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On the Asymptotic Determination of Invariant Manifolds for Autonomous Ordinary Differential Equations

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Abstract

A methodology to calculate the approximate invariant manifolds of dynamical systems defined through an m–dimensional autonomous vector field is presented. The technique is based on the calculation of formal symmetries and generalized normal forms associated to the vector field making use of Lie transformations for ordinary differential equations. Once a symmetry is determined up to a certain order, a reduction map allows us to pass from the equation in normal form to the orbit space, leading to the so–called reduced system of dimension $s < m$. Next, a non–degenerate p–dimensional invariant set of the reduced system is transformed, asymptotically, into a $(p+m-s)$–dimensional invariant set of the departure equation. We put three examples of normal forms computations and reduction process for Hamiltonian and dissipative systems. The procedure is illustrated by three applications: i) we characterize the set of all periodic orbits sufficiently close to the origin of the Hamiltonian vector field defined by the Hénon and Heiles family when the main frequencies do not satisfy a resonance condition; ii) we calculate the normally hyperbolic invariant manifold together with its stable and unstable manifold of an equilibrium point of type centre×centre×saddle for the three–degrees–of–freedom (3DOF) Hamilton function of the Rydberg atom, explaining the relevance of these invariant structures in the Transition State Theory; and iii) we apply our technique to the reduction process of the Lorenz equations, obtaining periodic orbits and some one–dimensional (1D) and 2D invariant sets.

Key words and expressions: Extended normal forms, Lie transformations, homology equation, invariant theory, mapping reductions, orbit spaces, reduced phase spaces, centre reduction, periodic orbits, nD invariant tori, normally hyperbolic invariant manifolds, Transition State Theory, averaging techniques, Hamiltonian functions, dissipative systems.

AMS (MOS) Subject Classification: 34C20, 34C14, 34C25, 34K19, 37J15, 37J40.

Resumen

En este trabajo se presenta una metodología para calcular variedades invariantes de un sistema dinámico definido mediante un sistema de m ecuaciones diferenciales autónomas. La técnica que empleamos se basa en el cálculo de simetrías asintóticas y formas normales generalizadas asociadas al campo vectorial que define la ecuación de origen, haciendo uso de transformaciones de Lie para ecuaciones diferenciales ordinarias. Una vez determinada la simetría hasta un cierto orden de aproximación un proceso de reducción permite formular la ecuación transformada en un espacio de dimensión s, estrictamente menor que m. El resultado central del trabajo establece que, bajo ciertas condiciones de regularidad, una variedad de dimensión p, invariante por el flujo del sistema dinámico correspondiente al sistema de ecuaciones reducido, se transforma mediante el cambio inverso al anterior, en otra variedad de dimensión $p + m - s$ que es aproximadamente invariante por el flujo del sistema dinámico correspondiente a la ecuación de partida. Además en el caso de que las variedades sean toros invariantes, la transformación asegura la existencia de toros invariantes de dimensión $p + m - s$ en el sistema original. La teoría desarrollada se ilustra a través de tres aplicaciones: i) caracterizamos el conjunto de todas las órbitas periódicas suficientemente cercanas al origen, de un problema de dinámica galáctica, en el que las frecuencias principales del sistema original no satisfacen una condición de resonancia; ii) calculamos la variedad invariante normalmente hiperbólica así como sus variedades estable e inestable de un punto crítico cuya estabilidad es de tipo centro×centro×silla correspondiente a un hamiltoniano de tres grados de libertad que modeliza la trayectoria de un átomo sujeto a la acción de un campo eléctrico y otro magnético dispuestos en direcciones perpendiculares, explicando la relevancia que tienen las estructuras geométricas invariantes en el lenguaje de la teoría del estado de transición en reacciones químicas; y iii) aplicamos la teoría al estudio del sistema disipativo de origen metereológico, llamada ecuación de Lorenz, obteniendo nuevas variedades invariantes de dimensón dos y órbitas periódicas, para ciertos valores de los parámetros del problema.

Palabras clave y expresiones: Formas normales extendidas, transformaciones de Lie, ecuación homológica, teoría de invariantes, aplicaciones de reducción, espacios orbitales, espacios fásicos reducidos, reducción a la variedad central, trayectorias periódicas, toros invariantes n–dimensionales, variedades invariantes normalmente hiperbólicas, teoría del estado de transición, técnicas de promedios, funciones hamiltonianas, sistemas disipativos.

1 Introduction and scope of the paper

The general setting of this paper is given through ordinary differential equations having the form

$$\frac{d\,\mathbf{x}(t)}{d\,t} \;=\; \mathbf{F}(\mathbf{x}(t);\varepsilon) = \sum_{i=0}^{L} \frac{\varepsilon^i}{i!}\mathbf{F}_i(\mathbf{x}(t)), \tag{1}$$

where t represents the independent variable, $\mathbf{x} \in \mathbf{R}^m$, ε stands for a dimensionless small parameter and for $0 \leq i \leq L$, $\mathbf{F}_i$ is a vector field with m components defined on an open set $\Omega \subseteq \mathbf{R}^m$. Note that L can be interpreted as the degree reached by the Taylor development of an analytic vector field, thus it can be infinity.

In particular, if $\mathbf{F}$ has a canonical character, there is a scalar field $\mathcal{H}$ such that Equation (1) is equivalent to

$$\mathcal{H}(\mathbf{q}(t),\mathbf{p}(t);\varepsilon) \;=\; \sum_{i=0}^{L} \frac{\varepsilon^i}{i!}\mathcal{H}_i(\mathbf{q}(t),\mathbf{p}(t)). \tag{2}$$

Many dynamical systems are modelled by a system of ordinary differential equations either of the type (1) or of the type (2). In both cases they are normally formed by the sum of a principal part ($\mathbf{F}_0$ or $\mathcal{H}_0$) plus the perturbation. These equations are very typical of Dynamical Systems Theory; for instance in stability and bifurcation analysis of equilibrium points, periodic orbits or singularity theories. Since (2) is a particular situation of (1) we shall present the results for the more general case, particularizing for (2) when dealing with Hamilton functions.

Analytical methods that deal with dynamical systems like (1) are based on the fact that the vector field $\sum_{i=1}^{L}(\varepsilon^i/i!)\,\mathbf{F}_i$ corresponds to a small perturbation of the principal part $\mathbf{F}_0$. In the context of Perturbation Theory [25, 33] our aim is to transform the initial problem to a simpler one by means of formal changes of variables.

Let us recall first some known concepts. A regular manifold is a p–dimensional set $M \subseteq \mathbf{R}^m$ $(0 \leq p \leq m)$ such that for each $\mathbf{x} \in M$ there is a neighbourhood $U_{\mathbf{X}}$ where one can find an invertible map, $\varphi : \mathbf{R}^m \to U_{\mathbf{X}}$, $\mathcal{C}^1$ at least. Given a differential equation like (1), defined in $\Omega \subseteq \mathbf{R}^m$, the manifold $M \subseteq \Omega$ is said to be invariant if the solution $\mathbf{x}(t;\varepsilon)$, with $\mathbf{x}(0) \in M$, is embedded in M for $-\infty < t < \infty$. As remarkable manifolds one has equilibrium points, periodic orbits, $(2 \leq p \leq m)$–dimensional tori or the stable, unstable and centre manifolds of critical points and the first integrals. More details can be looked up in Refs. [1, 4].

Within this framework, the purpose of the paper is to present a methodology for the computation of approximate, that is, asymptotic, invariant manifolds associated to a system

of the type (1). The central idea consists in constructing generalized (or extended) normal forms, i.e. different formal changes of variables which lead to different systems of differential equations (the normal forms) such that one extracts different invariant sets from each normal form. Thus, the initial equation gets transformed into different systems, each of them enjoying a different symmetry $\mathbf{T}$ up to a certain order of approximation. Hence, the calculation of a generalized normal form (or generalized normalized systems) accomplishes an effective reduction of the original system.

Making use of the Splitting Lemma (see [16] and references therein and see a different approach in [28]) it is readily proven that the transformed vector field can be split into two subsystems defined on two different invariant spaces. One of the subsystems, the so–called reduced system, contains the fundamental dynamics of the departure system. Actually, the reduction can be performed due to the fact that the vector field $\mathbf{T}$ is a continuous symmetry of the normal form system.

The invariant manifolds of the generalized normal forms are computed using standard methods, excepting for the case of the stable, unstable and centre manifolds associated to an equilibrium, as we shall see in Section 3. (Note that due to the reduction in the dimension of the equation, it is easier to find out the invariant manifolds in the reduced systems.) As the implementation of our method uses Lie transformations, once the invariant manifolds of the reduced system have been determined, one can use the inverse Lie transformation to approximate the invariant manifolds of the original differential equation.

More precisely, given the vector field $\mathbf{F}_0$, the first step consists in determining the set of independent vector fields $\mathbf{T}_i$ commuting with $\mathbf{F}_0$ (with the usual Lie brackets for vector fields), that is, the vector fields $\mathbf{T}_i$ belong to the centralizer of $\mathbf{F}_0$. Then, for each $\mathbf{T}_i$ one constructs a normal form so that this system is invariant under the action of the Lie group associated to $\mathbf{T}_i$, in other words, $\mathbf{T}_i$ is the formal symmetry of the normal form. The number of Lie transformations of the original system one can perform depends on the number of available independent vector fields $\mathbf{T}_i$.

The Lie transformation method for differential equations is based on previous work of Deprit for Hamiltonian systems [11] and was introduced by Kamel [25]. (see also the contribution by Henrard, Ref. [22].) Here we use the setting given by Meyer [33] through his General Perturbation Theorem. At this point we emphasize that our procedure is global in the sense that we do not use local expansions around equilibrium points. However, the convergence of the transformations is not discussed through the paper, though it is known that transformations based on normal form techniques diverge. Basically, a convergent transformation can be guaranteed if there is a nontrivial local one–parameter group of symmetries, see reference [58] and the recent book by Cicogna and Gaeta [6].

The connection of the General Perturbation Theorem with the reduction of a dynamical system through the introduction of symmetries has been given for polynomial vector fields in [46], see also a previous paper by Cicogna and Gaeta [5]. Here we enlarge those studies, considering analytic vector fields making use of a theorem by Schwarz [52]. The extension for non–polynomial vector fields is justified by the use of reduction techniques from the point of view of global analysis of dynamical systems. As examples of normal forms of non–polynomial vector fields we mention the case of perturbed Keplerian systems, see Ref. [9] and references therein.

The paper has eight sections. Section 2 recalls the General Perturbation Theorem and contains the required setting for generalizing the normal form approach. In Section 3 we describe the geometrical aspects of the reduction after the application of the generalized normal forms, dealing with the invariants of the Lie groups related to the symmetry introduced by the Lie transformations. We also show how the different reduced phase spaces are constructed and by means of Theorem 3.2 how the invariant manifolds of the normalized systems are related to the invariant manifolds of the original system. Section 4 is devoted to the construction of normal forsm and reduced phase spaces for the typical cases of problems in dynamical systems. In Section 5 we illustrate the technique with the Hénon and Heiles family of Hamilton functions for the special case in which the frequencies related to the principal part (quadratic terms) of the Hamiltonian are out of a resonant domain. Section 6 deals with the calculation of normally hyperbolic invariant manifolds for ($n \geq 2$)–dimensional Hamilton systems, concentrating on one case typical in atomic physics. Section 7 treats the problem of constructing invariant sets for the Lorenz equation by using various normal forms. Finally in Section 8 we outline the main remarks of the paper.

2 Formal symmetries through normal forms

2.1 Lie transformations for vector fields

Meyer's approach to the calculation of formal symmetries is based on Lie transformations. The paper of Meyer in this direction [33] is based on previous work by Kamel [25]. In [33] Meyer presents a Lie transformations treatment in the context of tensor fields. We start by recalling the Lie transformations method applied to analytic vector fields.

Let us consider the system

$$\frac{d\,\mathbf{x}(t)}{d\,t} \;=\; \mathbf{F}_0(\mathbf{x}(t)) + \sum_{i=1}^{\infty} \frac{\varepsilon^i}{i!}\mathbf{F}_i(\mathbf{x}(t)), \tag{3}$$

where t represents the time variable, $\mathbf{x} \in \mathbf{R}^m$, ε stands for a dimensionless small parameter and $\mathbf{F}_i$, $i \geq 0$ is a vector field with m components, which are analytic functions in $\mathbf{x}$. We

define by $[\,\cdot\,,\,\cdot\,]$ the Lie bracket of two vector fields $\mathbf{g}_1$ and $\mathbf{g}_2$ in $\mathbf{R}^m$, that is, $[\,\mathbf{g}_1\,,\,\mathbf{g}_2\,] = D\,\mathbf{g}_1(\mathbf{x})\,\mathbf{g}_2 - D\,\mathbf{g}_2(\mathbf{x})\,\mathbf{g}_1$.

Let us describe the typical algorithm of Lie transformations for ordinary differential equations. An analytic vector field (3) depending on a small parameter ε, is transformed into another vector field

$$\frac{d\,\mathbf{y}(t)}{d\,t} \;=\; \mathbf{G}_0(\mathbf{y}(t)) + \sum_{i=1}^{\infty} \frac{\varepsilon^i}{i!}\mathbf{G}_i(\mathbf{y}(t)), \tag{4}$$

where $\mathbf{G}_0(\mathbf{y}(t)) \equiv \mathbf{F}_0(\mathbf{x}(t))$, through a generating function

$$\mathbf{W}(\mathbf{x};\varepsilon) \;=\; \sum_{i=0}^{\infty} \frac{\varepsilon^i}{i!}\mathbf{W}_{i+1}(\mathbf{x}),$$

following the recursive formula

$$\mathbf{F}_i^{(j)} \;=\; \mathbf{F}_{i+1}^{(j-1)} + \sum_{k=0}^{i} \binom{i}{k} [\,\mathbf{F}_{i-k}^{(j-1)}\,,\,\mathbf{W}_{k+1}\,], \tag{5}$$

with $i \geq 0$, $j \geq 1$. Besides, $\mathbf{F}_i^{(0)} \equiv \mathbf{F}_i$ and $\mathbf{F}_0^{(i)} \equiv \mathbf{G}_i$ for all $i \geq 0$.

Note that $\mathbf{W}(\mathbf{x};\varepsilon)$ is conserved under the transformation and thus, it can also be expressed as $\mathbf{W}(\mathbf{y};\varepsilon)$, that is, $\mathbf{W}(\mathbf{x};\varepsilon) \equiv \mathbf{W}(\mathbf{y};\varepsilon)$.

Hence, Equation (5) yields the partial differential identity

$$\mathcal{L}_{\mathbf{F}_0}(\mathbf{W}_i) + \mathbf{G}_i \;=\; \widetilde{\mathbf{F}}_i, \tag{6}$$

where $\widetilde{\mathbf{F}}_i$ collects all the terms known from the previous orders plus $\mathbf{F}_i$. In this identity, called the homology equation, $\mathbf{W}_i$ and $\mathbf{G}_i$ must be determined according to the specific requirements of the Lie transform one performs. Besides, $\mathcal{L}_{\mathbf{F}_0}$ denotes the Lie operator associated to the Lie bracket of two vector functions, i.e. given two vector fields $\mathbf{g}_1$ and $\mathbf{g}_2$: $\mathcal{L}_{\mathbf{g}_1}(\mathbf{g}_2) = [\,\mathbf{g}_1\,,\,\mathbf{g}_2\,]$.

The transformation $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$ relates the "old" variables $\mathbf{x}$ with the "new" ones $\mathbf{y}$ and is a near–identity change of variables. The direct change is given by

$$\mathbf{x} \;\;=\;\; \mathbf{y} + \sum_{i=1}^{\infty} \frac{\varepsilon^i}{i!}\,\mathbf{y}_0^{(i)}. \tag{7}$$

Vectors $\mathbf{y}_0^{(i)}$, $i \geq 1$ are calculated recursively with the aid of

$$\mathbf{y}_i^{(j)} \;=\; \mathbf{y}_{i+1}^{(j-1)} + \sum_{k=0}^{i} \binom{i}{k} (\,\mathbf{y}_k^{(j-1)}\,,\,\mathbf{W}_{i+1-k}\,), \tag{8}$$

with $i \geq 0$, $j \geq 1$ and $\mathbf{y}_i^{(0)} \equiv \mathbf{0}$ for $i \geq 1$ and $\mathbf{y}_0^{(0)} \equiv \mathbf{y}$. Besides, given two vector fields $\mathbf{g}_1(\mathbf{y})$ and $\mathbf{g}_2(\mathbf{y})$, the operator $(\,\mathbf{g}_1\,,\,\mathbf{g}_2\,)$ is computed as $D\,\mathbf{g}_1(\mathbf{y})\,\mathbf{g}_2$. Consequently,

Equation (7) gives the set of co–ordinates $\mathbf{x}$ in terms of $\mathbf{y}$ with the use of the generating function $\mathbf{W}$.

Similar formulæcan be used to obtain the inverse transformation $\mathbf{y} = \mathbf{Y}(\mathbf{x};\varepsilon)$, which explicitly reads as

$$\mathbf{y} \;=\; \mathbf{x} + \sum_{i=1}^{\infty} \frac{\varepsilon^i}{i!}\, \mathbf{x}_i^{(0)}. \tag{9}$$

Now $\mathbf{x}_0^{(0)} \equiv \mathbf{x}$ and for $i \geq 1$ vectors $\mathbf{x}_i^{(0)}$ are calculated recursively by means of

$$\mathbf{x}_i^{(j)} \;=\; \mathbf{x}_{i-1}^{(j+1)} + \sum_{k=0}^{i-1} \binom{i-1}{k} \left(\mathbf{x}_{i-k-1}^{(j)} \,,\, \mathbf{W}_{k+1} \right), \tag{10}$$

with $i \geq 1$, $j \geq 0$. This time $\mathbf{x}_0^{(i)} \equiv \mathbf{0}$ for $i \geq 1$ and the Jacobians appearing in the operators of (10) are computed with respect to $\mathbf{x}$ and $\mathbf{W}_{k+1}$ is also written in $\mathbf{x}$.

Note that Equation (7) can be used to transform any function expressed in the old variables $\mathbf{x}$ as a function of the new variables $\mathbf{y}$. Similarly, Equation (9) is used to transform any function in $\mathbf{y}$ as a function of $\mathbf{x}$.

2.2 Generalized normal forms

The above method is formal in the sense that the convergence of the various series is not discussed. Moreover, the series diverge in many applications. However, the first orders of the transformed system can give interesting information and the process can be stopped at a certain order M. This means that these terms of the series are useful to construct both the transformed vector field and the generating function, since they are unaffected by the divergent character of the whole process. In these circumstances, the General Perturbation Theorem applies.

Theorem 2.1 *General Perturbation Theorem (Meyer). Let $M \geq 1$ be given, let $\{\mathcal{P}_i\}_{i=0}^{M}$, $\{\mathcal{Q}_i\}_{i=1}^{M}$ and $\{\mathcal{R}_i\}_{i=1}^{M}$ be sequences of vector spaces of analytic functions in $\mathbf{x} \in \mathbf{R}^m$ defined on a common domain Ω in $\mathbf{R}^m$ with the following properties:*

i) $\mathcal{Q}_i \subseteq \mathcal{P}_i$, $i = 1, \ldots, M$;

ii) $\mathbf{F}_i \in \mathcal{P}_i$, $i = 0, 1, \ldots, M$;

iii) $[\,\mathcal{P}_i\,,\,\mathcal{R}_j\,] \subseteq \mathcal{P}_{i+j}$, $i + j = 1, \ldots, M$;

iv) for any $\mathbf{D} \in \mathcal{P}_i$, $i = 1, \ldots, M$, one can find $\mathbf{E} \in \mathcal{Q}_i$ and $\mathbf{K} \in \mathcal{R}_i$ such that

$$\mathbf{E} = \mathbf{D} + [\,\mathbf{F}_0\,,\,\mathbf{K}\,].$$

Then, there is an analytic vector field $\mathbf{W}$*,*

$$\mathbf{W}(\mathbf{x};\varepsilon) = \sum_{i=0}^{M-1} \frac{\varepsilon^i}{i!}\, \mathbf{W}_{i+1}(\mathbf{x}),$$

with $\mathbf{W}_i \in \mathcal{R}_i$*,* $i = 1, \ldots, M$*, such that the change of variables* $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$ *is the general solution of the initial value problem*

$$\begin{aligned} \frac{d\,\mathbf{x}}{d\,\varepsilon} &= D\,\mathbf{W}(\mathbf{x};\varepsilon), \\ \mathbf{x}(0) &= \mathbf{y}, \end{aligned}$$

and transforms the convergent vector field

$$\mathbf{F}(\mathbf{x};\varepsilon) = \sum_{i=0}^{\infty} \frac{\varepsilon^i}{i!}\, \mathbf{F}_i(\mathbf{x}),$$

to the convergent vector field

$$\mathbf{G}(\mathbf{y};\varepsilon) = \sum_{i=0}^{M} \frac{\varepsilon^i}{i!}\, \mathbf{G}_i(\mathbf{y}) + \mathcal{O}(\varepsilon^{M+1}),$$

with $\mathbf{G}_i \in \mathcal{Q}_i$*,* $i = 1, \ldots, M$*.*

Proof See reference [33]. □

Now we are ready to extend Theorem 2.1 for the construction of formal symmetries for vector fields. For this we give a result in which we add an extra hypothesis.

Theorem 2.2 *Let* $M \geq 1$ *be given, let* $\{\mathcal{P}_i\}_{i=0}^{M}$*,* $\{\mathcal{Q}_i\}_{i=1}^{M}$ *and* $\{\mathcal{R}_i\}_{i=1}^{M}$ *be sequences of vector spaces of analytic functions in* $\mathbf{x} \in \mathbf{R}^m$ *defined on a common domain* Ω *in* $\mathbf{R}^m$ *and let* $\mathbf{T} \equiv \mathbf{T}(\mathbf{x})$ *be a vector field in some* $\{\mathcal{P}_i\}_{i=0}^{M}$ *with the following properties:*

i) $\mathcal{Q}_i \subseteq \mathcal{P}_i$*,* $i = 1, \ldots, M$*;*

ii) $\mathbf{F}_i \in \mathcal{P}_i$*,* $i = 0, 1, \ldots, M$*;*

iii) $[\,\mathcal{P}_i\,,\,\mathcal{R}_j\,] \subseteq \mathcal{P}_{i+j}$*,* $i + j = 1, \ldots, M$*;*

iv) for any $\mathbf{D} \in \mathcal{P}_i$*,* $i = 1, \ldots, M$*, one can find* $\mathbf{E} \in \mathcal{Q}_i$ *and* $\mathbf{K} \in \mathcal{R}_i$ *such that*

$$\mathbf{E} = \mathbf{D} + [\,\mathbf{F}_0\,,\,\mathbf{K}\,] \quad \textit{and} \quad [\,\mathbf{E}\,,\,\mathbf{T}\,] = \mathbf{0}.$$

Then, there is an analytic vector field $\mathbf{W}$*,*

$$\mathbf{W}(\mathbf{x};\varepsilon) = \sum_{i=0}^{M-1} \frac{\varepsilon^i}{i!}\, \mathbf{W}_{i+1}(\mathbf{x}),$$

with $\mathbf{W}_i \in \mathcal{R}_i$, $i = 1, \ldots, M$, *such that the change of variables* $\mathbf{x} = \mathbf{X}(\mathbf{y}; \varepsilon)$ *is the general solution of the initial value problem*

$$\begin{aligned} \frac{d\,\mathbf{x}}{d\,\varepsilon} &= D\,\mathbf{W}(\mathbf{x}; \varepsilon), \\ \mathbf{x}(0) &= \mathbf{y}, \end{aligned}$$

and transforms the convergent vector field

$$\mathbf{F}(\mathbf{x}; \varepsilon) = \sum_{i=0}^{\infty} \frac{\varepsilon^i}{i!}\, \mathbf{F}_i(\mathbf{x}),$$

to the convergent vector field

$$\mathbf{G}(\mathbf{y}; \varepsilon) = \sum_{i=0}^{M} \frac{\varepsilon^i}{i!}\, \mathbf{G}_i(\mathbf{y}) + \mathcal{O}(\varepsilon^{M+1}),$$

with $\mathbf{G}_i \in \mathcal{Q}_i$ *and* $[\,\mathbf{G}_i\,,\,\mathbf{T}\,] = \mathbf{0}$, $i = 1, \ldots, M$. *Besides, if* $[\,\mathbf{F}_0\,,\,\mathbf{T}\,] = \mathbf{0}$ *then* $\mathbf{T} \equiv \mathbf{T}(\mathbf{y})$ *is a formal symmetry of* $\mathbf{G}$.

Proof It appears in reference [46] but we repeat it for sake of clarity in our exposition. Note that the difference between this result and Theorem 2.1 is that here we introduce the vector field $\mathbf{T}$. Condition *iv)* of Theorem 2.1 is slightly modified in the sense that we also require that functions $\mathbf{E} \in \mathcal{Q}_i$ satisfy $[\,\mathbf{E}\,,\,\mathbf{T}\,] = \mathbf{0}$. According to Theorem 2.1, $\mathbf{G}_i \in \mathcal{Q}_i$ and the additional thesis $[\,\mathbf{G}_i\,,\,\mathbf{T}\,] = \mathbf{0}$ is satisfied. □

The vector field $\mathbf{G}(\mathbf{y}; \varepsilon)$ is a generalized normal form of the original vector field (3). Note that the number of generalized normal forms depends on the different Lie transformations of $\mathbf{F}(\mathbf{x}; \varepsilon)$ one executes, or in other words, on the functionally independent symmetries $\mathbf{T}$ corresponding to $\mathbf{F}_0$. In this respect we can compute a formal symmetry of the original system by reversing the transformation. Specifically if the normal form calculations have been carried out to an order $M > 1$, then we determine $\mathbf{T}^*(\mathbf{x}; \varepsilon)$ as

$$\mathbf{T}^*(\mathbf{x}; \varepsilon) = \mathbf{T}(\mathbf{x}) + \sum_{i=1}^{M} \frac{\varepsilon^i}{i!}\, \mathbf{T}(\mathbf{x})_i^{(0)}, \tag{11}$$

where $\mathbf{T}(\mathbf{x})_i^{(0)}$ are calculated using

$$\mathbf{T}(\mathbf{x})_i^{(j)} = \mathbf{T}(\mathbf{x})_{i-1}^{(j+1)} + \sum_{k=0}^{i-1} \binom{i-1}{k} [\,\mathbf{T}(\mathbf{x})_{i-k-1}^{(j)}\,,\,\mathbf{W}_{k+1}\,], \tag{12}$$

with $i \geq 1$ and $j \geq 0$. Now $\mathbf{T}(\mathbf{x})_0^{(0)} \equiv \mathbf{T}(\mathbf{x})$ and for $i \geq 1$, $\mathbf{T}(\mathbf{x})_0^{(i)} \equiv 0$. Then $\mathbf{T}^*(\mathbf{x}; \varepsilon)$ is an asymptotic symmetry of $\mathbf{F}$, i.e. $[\,\mathbf{F}\,,\,\mathbf{T}^*\,] = \mathcal{O}(\varepsilon^{M+1})$. If we are in the symplectic context, this procedure extends classic results on the determination of formal integrals for Hamiltonian

systems, as thoise developed in Refs. [59, 60, 20, 17]. For ordinary differential equations, the construction generalized normal forms enlarges other criteria for the determinations of continuous asymptotic symmetries. Details can be found in references [44, 46, 47, 43].

We have to note that given a vector field $\mathbf{T}$ with $[\,\mathbf{F}_0\,,\,\mathbf{T}\,]=\mathbf{0}$ it is not always possible to solve the homology equation (6) due to the difficulties in finding out the pair $(\mathbf{G}_i,\mathbf{W}_i)$ satisfying it. Therefore, on some occasions we will stop the computation of a normal form at the order we had reached without difficulties.

3 Reduction to the orbit space

3.1 The Splitting Lemma

From a geometrical point of view, the consequence of introducing a symmetry by making use of Theorem 2.2 is that the dimension of the phase space where the transformed system is defined — the so–called reduced phase space — is reduced from m to s (s denoting the number of functionally–independent first integrals associated to $\mathbf{T}(\mathbf{y})$). Let us see how this is achieved with some detail.

Fixed $\varepsilon\in\mathbf{R}$, the system of differential equations (1) is defined over an open subset of $\mathbf{R}^m$. This is the phase space of the dynamical system determined by (1). Given an m–dimensional vector field $\mathbf{T}$ such that $[\,\mathbf{F}_0\,,\,\mathbf{T}\,]=0$, the application of Theorem 2.2, after truncating at order M, leads to the analytic vector field $\mathbf{H}(\mathbf{y};\varepsilon)$, e.g. the truncation of $\mathbf{G}$ at order M:

$$\frac{d\,\mathbf{y}}{d\,t}\;=\;\mathbf{H}(\mathbf{y};\varepsilon)\;=\;\sum_{i=0}^{M}\frac{\varepsilon^i}{i!}\mathbf{G}_i(\mathbf{y}),\tag{13}$$

where $\mathbf{H}_0\equiv\mathbf{F}_0$ and each $\mathbf{G}_i$ is constructed so that $[\,\mathbf{G}_i\,,\,\mathbf{T}\,]=\mathbf{0}$, for $1\leq i\leq M$.

Now we show how the transformation described in Section 2 is effective in the sense that we really simplify the departure system. We use for that a result obtained in reference [16], adapting it to our requirements. Associated to the one–parameter group of symmetries introduced through the Lie transformation there is an $(m-s)$–dimensional Lie group $G_{\mathbf{T}}$, such that $\mathbf{H}$ is $G_{\mathbf{T}}$–equivariant, that is, fixed $\varepsilon>0$, for any $\mathbf{y}\in\mathbf{R}^m$ and any $g\in G_{\mathbf{T}}$, $\mathbf{H}(\mathbf{y},\varepsilon)=\mathbf{H}(g\,\mathbf{y},\varepsilon)$.

Schwarz [52, 53] generalized a result given by Hilbert for polynomial first integrals for vector fields enjoying a continuous symmetry. Specifically, Schwarz showed that for any $G_{\mathbf{T}}$–equivariant vector field, there is a set of smooth functions defined on a domain $\Omega\subseteq\mathbf{R}^m$ (in other words, $\mathcal{C}^\infty(\Omega)$–functions) such that any $G_{\mathbf{T}}$–equivariant smooth function defined in Ω can be written as a $\mathcal{C}^\infty(\Omega)$–function of those functions. Besides, these functions, designated by $\varphi_i(\mathbf{y}), i=1,\ldots,r$ and $\mathbf{y}\in\Omega$, correspond to the r linearly–independent first integrals of the system $d\,\mathbf{y}(t)/d\,t=\mathbf{T}(\mathbf{y}(t))$, from which $1\leq s\leq r$ are functionally independent.

The set $\{\varphi_1, \ldots, \varphi_r\}$ receives the name of minimal integrity basis and it has the structure of a ring of scalar fields with the standard product and addition of $\mathcal{C}^\infty$–functions. Denote by $\mathcal{L}^*_{\mathbf{T}}(z(\mathbf{y}))$ the Lie derivative of a function $z : \Omega \to \mathbf{R}$ related to $\mathbf{T}$, e.g. $\mathcal{L}^*_{\mathbf{T}}(z(\mathbf{y})) = \langle\, D\, z(\mathbf{y})\,,\, \mathbf{T}\,\rangle$. So, $\mathcal{L}^*_{\mathbf{T}}(\varphi_i(\mathbf{y})) = 0$, $i \in \{1, \ldots, r\}$. Hence, the φ_i are the independent solutions of the linear partial differential equation $\mathcal{L}^*_{\mathbf{T}}(\varphi_i(\mathbf{y})) = 0$. Note that $s \leq m$ but r can be bigger than, equal to or smaller than m.

We build a smooth mapping $\varrho_{\mathbf{T}}$ over $\mathbf{R}^m$ as follows:

$$\begin{array}{rccc} \varrho_{\mathbf{T}}: & G_{\mathbf{T}} \times \mathbf{R}^m & \longrightarrow & \mathbf{R}^m \\ & (g\,,\,\mathbf{x}) & \mapsto & g\,\mathbf{x}. \end{array}$$

This mapping is a natural action of $G_{\mathbf{T}}$ on $\mathbf{R}^m$ because it satisfies the conditions: i) $\varrho_{\mathbf{T}}(g_1\, g_2, \mathbf{x}) = \varrho_{\mathbf{T}}(g_1, \varrho_{\mathbf{T}}(g_2, \mathbf{x}))$, $\forall g_1, g_2 \in G_{\mathbf{T}}$, $\forall \mathbf{x} \in \mathbf{R}^m$; and ii) $\varrho_{\mathbf{T}}(e, \mathbf{x}) = \mathbf{x}$ (e is the identity of the Lie group), $\forall \mathbf{x} \in \mathbf{R}^m$.

Let us define $\sim$ in such a way that $\mathbf{x} \sim \mathbf{x}'$ if and only if $\mathbf{x}$ and $\mathbf{x}'$ lie on the same $G_{\mathbf{T}}$–orbit of $\varrho_{\mathbf{T}}$. As $\sim$ is an equivalence relation on $\mathbf{R}^m$, it partitions $\mathbf{R}^m$ into $G_{\mathbf{T}}$–orbits, see reference [10]. Then we denote $\mathbf{p} = \{\varphi_1, \ldots, \varphi_r\}$ and $\bar{\mathbf{y}} = g\,\mathbf{y}$ the orbit of the action $\varrho_{\mathbf{T}}$ through the point $\mathbf{x} \in \mathbf{R}^m$. Thus, $\mathbf{p}(\mathbf{y}) \equiv g\,\mathbf{y}$ and we can define the orbit map (also called the reduction map) as the surjective map:

$$\begin{array}{rccc} \pi_{\mathbf{T}}: & \Omega \subseteq \mathbf{R}^m & \longrightarrow & \mathbf{R}^m/G_{\mathbf{T}} \\ & \mathbf{y} & \mapsto & \mathbf{p}. \end{array}$$

Now, related to the reduction map $\pi_{\mathbf{T}}$ and the vector field (13), there is a phase space defined as the s–dimensional quotient space $\mathbf{R}^m/G_{\mathbf{T}}$ (which is a semialgebraic manifold, the so–called orbit space, see details in [10]). Henceforth, the φ_i are also called the invariants of the reduction process. The reader can look up references [38, 57] for details about the theoretical aspects of the reduction under the introduction of a continuous symmetry. See also Ref. [8] for a computational treatment of the subject. However, the passage to the orbit space must be combined with an additional differential equation in the Lie group. Now we choose a set of co–ordinates on $G_{\mathbf{T}}$ to make the reduction explicit. Denoting $\mathbf{q} = \{\vartheta_1, \ldots, \vartheta_{m-s}\}$, the flow on $G_{\mathbf{T}}$ is indeed the time evolution of the variables $\vartheta_i \in G_{\mathbf{T}}$. We have the following result.

Theorem 3.1 *Splitting Lemma. Given the generalised normal form system (13) with* $\mathbf{H}$ *a smooth function of* ε *and* $\mathbf{y}$ *defined on* $\Omega \subseteq \mathbf{R}^m$*, it can be transformed into a triangular system as*

$$\begin{array}{rcl} \dfrac{d\,\mathbf{p}(t)}{d\,t} & = & \mathbf{a}(\mathbf{p}(t); \varepsilon) \,=\, \displaystyle\sum_{i=0}^{M} \frac{\varepsilon^i}{i!}\, \mathbf{a}_i(\mathbf{p}(t)), \\ \dfrac{d\,\mathbf{q}(t)}{d\,t} & = & \mathbf{b}(\mathbf{q}(t), \mathbf{p}(t); \varepsilon) \,=\, \mathbf{b}_0(\mathbf{p}(t)) + \displaystyle\sum_{i=1}^{M} \frac{\varepsilon^i}{i!}\, \mathbf{b}_i(\mathbf{q}(t), \mathbf{p}(t)), \end{array} \tag{14}$$

a *and* **b** *being smooth functions obtained constructively from* **H**, *and having dimensions* r *and* $m-s$, *respectively. Moreover, the vector fields* $\mathbf{b}_i$, $0 \leq i \leq M$, *are linear in* **q**.

Proof It is basically proven in Ref. [16] but here we propose a slight modification, see also [43]. The reason for appearance of **a** and **b** comes from the fact that they are constructed order by order in powers of ε. The first equation of (14) depends exclusively on the φ_i, it is named the reduced system and is defined over $\mathbf{R}^m/G_{\mathbf{T}}$, whereas the second equation of (14) is defined on the Lie group $G_{\mathbf{T}}$. The vector field **a** is constructed using the identity $d\,\mathbf{p}(t)/d\,t = (\partial\,\mathbf{p}/\partial\,\mathbf{y})\ \mathbf{H}(\mathbf{y};\varepsilon)$ and taking into account that the right–hand member of this equation can be expressed completely in terms of **p** (see Refs. [23, 16] for details and the seminal paper by Michel [35]). Thus, we make the identification

$$\mathbf{a}(\mathbf{p};\varepsilon)\ =\ D\,\mathbf{p}(\mathbf{y})\,\mathbf{H}(\mathbf{y};\varepsilon), \quad \text{that is,} \quad \mathbf{a}_i(\mathbf{p})\ =\ D\,\mathbf{p}(\mathbf{y})\ \mathbf{H}_i(\mathbf{y}).$$

For each i, the construction of the $\mathbf{b}_i$ is done with the aid of $\mathbf{a}_i$ and $\mathbf{H}_i$. It must be performed once the co–ordinates **q** have been calculated. Besides, $\mathbf{b}_0$ cannot depend on **q** since it is constructed from $\mathbf{F}_0$, and $\mathbf{F}_0$ is $G_{\mathbf{T}}$–equivariant, so it does not depend on **q**. The dimensions of **a** and **b** follow, respectively, from the dimensions of **p** and **q**. □

The first equation of (14) depends exclusively on the φ_i, it is named the reduced system and is defined on $\mathbf{R}^m/G_{\mathbf{T}}$, whereas the second equation of (14) is defined on the Lie group $G_{\mathbf{T}}$. The vector field **a** is constructed using the identity $d\,\mathbf{p}(t)/d\,t = D\,(\mathbf{p})\,\mathbf{H}(\mathbf{y};\varepsilon)$ and taking into account that the right–hand member of this equation can be expressed completely in terms of **p** (see Ref. [16] for details). Thus, we identify $\mathbf{a}(\mathbf{p};\varepsilon) = D\,(\mathbf{p})\,\mathbf{H}(\mathbf{y};\varepsilon)$. The construction of **b** is performed once the co–ordinates **q** have been calculated. Note that as there is not a unique set of co–ordinates, there is not a unique function **b**. Besides, $G_{\mathbf{T}}$ must be a connected compact group, otherwise the splitting does not hold in general. Theorem 3.1 is also called the Splitting Decomposition. A similar decomposition but of local character and based on geometric considerations is given in [28].

The relevant part of the normal form is given by the equation on the orbit space $\mathbf{R}^m/G_{\mathbf{T}}$. Moreover, if the solution of the equation involving the φ_i is known, then the solution of the remaining equation on $G_{\mathbf{T}}$ can be obtained. As there are $r-s$ functionally independent relations among the $\varphi_i(\mathbf{y})$, these relations are indeed the constraints determining the phase space where the normal form system in $\mathbf{R}^m/G_{\mathbf{T}}$ is defined. Besides, the basic properties of system (13) are also reflected in $\mathbf{R}^m/G_{\mathbf{T}}$. For instance, asymptotic expressions, at a certain order M, of the analytic integrals of the departure system must be found from the analysis of the normal form in the orbit space. The invariance of some subsets of $\mathbf{R}^m$ is formally preserved when passing to the orbit space, see a proof in Ref. [57]. This latter property will be essential in the computation of the invariant sets, as we shall see below.

For Hamiltonian systems we do not have to compute the co–ordinates $\mathbf{q}$, as the normal form Hamiltonian, by construction, is always a function depending exclusively on $\mathbf{p}$. Besides, the reduction is done by adding an extra step. First, Theorem 3.1 is applied and $\mathbf{p}$ and $\mathbf{a}$ are calculated. Then, as $\mathcal{T}$ is a constant of motion, one can fix a real value for it, i.e. $\mathcal{T} \equiv c \in I \subseteq \mathbf{R}$.

More concretely, if an initial Hamilton equation defines a dynamical system on a $(2\,n)$–dimensional phase space, that is, a system of n degrees of freedom, after a symplectic reduction, the transformed Hamiltonian lies on a phase space of dimension s, if s is even, or of dimension $s-1$ whether s is odd. Strictly speaking, there is an infinite number of reduced phase spaces, one for each value of $c \in I \subseteq \mathbf{R}$. Moreover, note that in the symplectic context, the Lie bracket of two vector fields is replaced by the Poisson bracket of two scalar fields $\mathcal{P}$ and $\mathcal{Q}$. That is, if $\mathcal{J}$ denotes the skew–symmetric matrix of order $2\,n$, the Poisson bracket is defined over an open domain of $\mathbf{R}^{2\,n}$ as the quantity

$$\{\,\mathcal{P}\,,\,\mathcal{Q}\,\}(\mathbf{x}) \,=\, \sum_{i=1}^{n} \left(\frac{\partial \mathcal{P}}{\partial x_i}\,\frac{\partial \mathcal{Q}}{\partial x_{i+n}} - \frac{\partial \mathcal{P}}{\partial x_{i+n}}\,\frac{\partial \mathcal{Q}}{\partial x_i} \right)$$

for $\mathbf{x} = (x_1, \ldots, x_{2n})$.

The relation of the procedure described through Theorem 3.1 and the method of averaging is rather clear, see for instance [51]. Indeed, it is easy to see that the passage from the original equation to the system defined on the orbit space can be interpreted as an average of the equation over all "angular" variables ϑ_i since the co–ordinates of the Lie group are absent in $\mathbf{R}^m/G_{\mathbf{T}}$. However, the way we have followed seems to be more transparent and general, as the reduction process does not depend on the variables we use, and the co–ordinates of $G_{\mathbf{T}}$ do not need to be actual angles, see some examples in Ref. [67].

Several reductions of a departure system can be performed successively. Indeed, if $\mathbf{T}_1, \ldots, \mathbf{T}_k$ correspond to k functionally independent vector fields commuting with the principal part of a dynamical system like (1), it is possible (at least theoretically) to apply up to k different reductions (conversions to normal forms followed by the passage to the corresponding invariants and the splitting decompositions). Thus, an originally m–dimensional system could be reduced to a system of dimension one. However, in practice it is quite unlikely to execute more than one transformation, due to the difficulty in solving the homology equation in the Lie transformation.

3.2 The reduced phase spaces

The co–ordinates of the orbit space (also called generators) are indeed the r linearly–independent first integrals related to $\mathbf{T}$. As pointed out before, the dimension of $\mathbf{R}^m/G_{\mathbf{T}}$ is s thus, there are s functionally independent invariants. However, the number r of linearly

independent invariants cannot be obtained in a systematic manner, and it depends on each reduction, that is, it is determined by the choice of the vector field $\mathbf{T}$, but $r \geq s$ is always satisfied. Notice that there must be at least $r - s$ relations involving the φ_i. These relations are used to define the reduced phase space.

This space can have singular points due to the existence of non–trivial isotropy subgroups. Specifically, given the Lie group $G_{\mathbf{T}}$ associated to $\mathbf{T}$ and its natural action $\varrho_{\mathbf{T}}$ on $\mathbf{R}^m$, the isotropy subgroup of a vector $\mathbf{x} \in \mathbf{R}^m$ is defined as $G_{\mathbf{T}}^{\mathbf{X}} = \{g \in G_{\mathbf{T}} \mid \varrho_{\mathbf{T}}(g, \mathbf{x}) = \mathbf{x}\}$. Now, if for all $\mathbf{x} \in \mathbf{R}^m$ the isotropy subgroup of $\mathbf{x}$ is trivial, the reduced phase space is a smooth manifold. This is the so–called regular reduction [31]. On the contrary, if there is an $\mathbf{x} \in \mathbf{R}^m$ such that its isotropy subgroup is non–trivial, the reduced phase space is a manifold with singularities. This reduction is called singular [2].

If the reduction is symplectic there is another possibility of introducing singularities in the reduced phase space. After determining the corresponding invariants and computing the reduced Hamiltonian up to the desired order, the value of $\mathcal{T}$ has to be fixed to a constant $c \in \mathbf{R}$. This constant appears as a parameter in the constraints which define the reduced phase spaces. In other words, one has a parametric family of reduced phase spaces with at least one parameter, the constant c. Thus, these reduced phase spaces have different number of singularities according to the values the parameter c takes. This situation cannot be detected by analyzing the corresponding isotropy subgroups. A straightforward way of calculating the singularities consists in parametrizing the reduced phase space and computing thereafter its gradient vector. The singularities are those points where the gradient vanishes.

3.3 Invariant manifolds of the original system

Now, it is time to formulate the main result of the paper, so that we can obtain the invariant sets of an initial system from the (reduced) invariant sets of their reduced systems.

Theorem 3.2 *Let the following differential equation*

$$\frac{d\,\mathbf{p}(t)}{d\,t} \;=\; \mathbf{a}(\mathbf{p}(t);\varepsilon) \;=\; \sum_{i=0}^{M} \frac{\varepsilon^i}{i!}\,\mathbf{a}_i(\mathbf{p}(t)) \tag{15}$$

be defined over a certain s–dimensional orbit space $\mathbf{R}^m/G_{\mathbf{T}}$. Let the vector field $\mathbf{a}$ be an r–dimensional smooth vector coming from a generalised normal form system (13), where $\mathbf{H}$ represents a smooth function defined over $\Omega \subseteq \mathbf{R}^m$ with $s \leq min\{r, m\}$. (There are $r - s$ essential constraint relations which are part of the definition of $\mathbf{R}^m/G_{\mathbf{T}}$.)

Suppose that $\mathbf{c}(\mathbf{t}, \mathbf{p}_0; \varepsilon)$ stands for an r–dimensional vector field defined over $\mathbf{R}^m/G_{\mathbf{T}}$, such that is obtained as a non–degenerate (isolated) p–dimensional invariant set of Equation (15)

with $p \leq s$, where we have chosen certain initial conditions $\mathbf{p}_0$ of $\mathbf{p}$ and p parameters defining $\mathbf{t} = (t_1, \ldots, t_p)$.

Then, there is a non–degenerate vector field $\mathbf{c}^*(\mathbf{u}, \mathbf{y}_0; \varepsilon)$ defined on $\mathbf{R}^m$ whose dimension is $p + m - s$ (so, $\mathbf{u} = (u_1, \ldots, u_{p+m-s})$ stands for the parameters of $\mathbf{c}^*$) and such that it represents an invariant set of $\mathbf{H}$, one of the truncated normal forms of a certain differential equation $\mathbf{F}$ in $\mathbf{R}^m$ (with notations for $\mathbf{F}$ and $\mathbf{H}$ given in Section 2 and 3). In particular, $\mathbf{H}$ stands for the normal form associated to the symmetry of the dominant part $\mathbf{F}_0$ that we have called $\mathbf{T}$. Moreover, $\mathbf{c}$ and $\mathbf{c}^*$ have the same type of stability.

Suppose that the equation $\mathbf{x} = \mathbf{X}(\mathbf{y}; \varepsilon)$ stands for the direct change of co–ordinates to order M, provided by the Lie transformation built to obtain $\mathbf{H}$ from $\mathbf{F}$ and $\mathbf{T}$. Suppose in addition that the set $\mathbf{c}^{\#}(\mathbf{v}, \mathbf{x}_0; \varepsilon)$ with the parameter–vector $\mathbf{v} = (v_1, \ldots, v_{p+m-s})$ and initial condition $\mathbf{x}_0 = \mathbf{X}(\mathbf{y}_0; \varepsilon)$, is constructed from $\mathbf{c}^*$ using the change $\mathbf{X}$. Then, $\mathbf{c}^{\#}$ represents an (approximate) invariant set of $\mathbf{F}$, up to an error $\mathcal{O}(\varepsilon^{M+1})$.

Furthermore, whenever the Lie transformation procedure converges in a domain $D \subseteq \Omega$ and $\mathbf{c}^*(\mathbf{u}, \mathbf{y}_0; \varepsilon) \in D$, the invariant structure $\mathbf{c}^{\#}$ converges to the exact invariant set of $\mathbf{F}$.

Finally, suppose that all variables on the Lie group ϑ_i $1 \leq i \leq m - s$, and the parameter–vector $\mathbf{t}$ represent actual angles. In addition suppose that the approximate invariant $\mathbf{c}^*$ depends smoothly on some external parameters $\mathbf{d} = (d_1, \ldots, d_\ell)$ such that we can write it as $\mathbf{c}^*(\mathbf{u}, \mathbf{y}_0; \mathbf{d}, \varepsilon)$. Then, whether the $(m \times m)$–matrix

$$\left(\frac{\partial\, \mathbf{c}^*(\mathbf{u}, \mathbf{y}; \mathbf{d}^*, \varepsilon)}{\partial \mathbf{y}} \right) (\mathbf{u}^T; \mathbf{y}_0; \mathbf{d}, \varepsilon)$$

(with $\mathbf{d}^* \to \mathbf{d}$ and $\mathbf{u}^T = (u_1^{T_1}, \ldots, u_{p+m-s}^{T_{p+m-s}})$ representing a fixed vector formed with the corresponding periods of the $p + m - s$ angle co–ordinates) has the eigenvalue 1 with multiplicity $p + m - s$, the invariant $(p + m - s)$–dimensional torus $\mathbf{c}^*$ can be continued into an invariant torus of the vector field $\mathbf{F}$, called $\mathbf{c}^{\#}$, with the same dimension and stability character.

Proof The demonstration is an application of Theorems 3.1 and 2.2 of this paper and an adequate use of the Implicit Mapping Theorem for the case of the invariant tori. See more details in [43]

In a first step one needs to calculate, when it will be possible, the invariant sets of the equation defined over $\mathbf{R}^m / G_{\mathbf{T}}$. Note that an invariant set (of dimension $0 \leq p \leq m$) associated to the system $d\,\mathbf{p}(t)/d\,t = \mathbf{a}(\mathbf{p}(t); \varepsilon)$ can be represented parametrically by the vector field $\mathbf{c}(\mathbf{t}, \mathbf{p}_0; \varepsilon)$ where $\mathbf{c}$ is r–dimensional, $\mathbf{t}$ designates a p–dimensional parameter–vector, and $\mathbf{p}_0$ stands for some initial conditions calculated in the process of the computation of the specific invariant manifold. Besides, ε remains fixed.

Once $\mathbf{c}$ is determined, we go back to the variable $\mathbf{y}$ by making use of the explicit expressions of the φ_i in terms of $\mathbf{y}$, by means of the reduction map $\pi_{\mathbf{T}}$. In other words, we

attach to each point of $\mathbf{R}^m/G_{\mathbf{T}}$, an $(m-s)$–dimensional set defined by the co–ordinates of $G_{\mathbf{T}}$. Thus, $\mathbf{c}$ is transformed into $\mathbf{c}^*(\mathbf{u},\mathbf{y}_0;\varepsilon)$ where $\mathbf{y}_0$ are derived from the initial condition $\mathbf{p}_0$ and $\mathbf{u}$ designates a parameter–vector with $p+m-s$ components, accounting for the p–free parameters of $\mathbf{c}$ plus $m-s$ co–ordinates related to ϑ_i, $1 \leq i \leq m-s$. In addition, $\mathbf{c}^*$ has dimension m. Due to the fact that the invariance of $\mathbf{c}$ with respect to the flow defined by (15) is preserved by $\pi_{\mathbf{T}}$, we have that $\mathbf{c}^*$ defines an isolated and exact $(p+m-s)$–invariant manifold of the ODE $d\,\mathbf{y}/d\,t = \mathbf{H}(\mathbf{y};\varepsilon)$ in $\mathbf{R}^m$, with the same stability as $\mathbf{c}$.

Next we recover the equation of the manifold in the original variable $\mathbf{x}$. This is achieved by using the change of variable $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$. Thus we pass from the m–dimensional vector $\mathbf{c}^*(\mathbf{u},\mathbf{y}_0;\varepsilon)$ to the m–dimensional vector $\mathbf{c}^*(\mathbf{u},\mathbf{y}_0;\varepsilon)$, with $\mathbf{x}_0 = \mathbf{X}(\mathbf{y}_0;\varepsilon)$ and $\mathbf{v}$ having the same meaning as $\mathbf{u}$. Again since the Lie transformation preserves the invariant character of the expressions, $\mathbf{c}^{\#}$ remains invariant in $\mathbf{R}^m$ with respect to the flow $d\,\mathbf{x}/d\,t = \mathbf{F}(\mathbf{x};\varepsilon)$, up to an approximation of order M. For a convergent Lie transformation, $\mathbf{c}^{\#}$ converges asymptotically to an exact invariant set of $\mathbf{F}$ provided that the invarint set lies entirely inside the domain D.

Finally, in the case of having $p+m-s$ angular co–ordinates (all the variables ϑ_i of $G_{\mathbf{T}}$ plus the p parameters of the invariant set $\mathbf{c}$), the reconstruction of $\mathbf{c}^{\#}$ is such that all components of the $(p+m-s)$–dimensional parameter–vector $\mathbf{u}$ represent angles. Thus, we need to construct a suitable Poincaré mapping and apply to it the Implicit Function Theorem, following to Meyer and Hall [34]. We define a cross section to the invariant tori $\mathbf{c}^*$ as the hyperplane Σ of codimension $p+m-s$ as follows

$$\begin{aligned}\Sigma \;=\; \{\mathbf{x}\in\mathbf{R}^m \mid \langle \mathbf{a}_i\,,\,\mathbf{y}-\mathbf{y}_0\rangle = 0 \quad \forall\,\mathbf{a}_i\in\mathbf{R}^m \quad \text{such that}\\ \langle \mathbf{a}_i\,,\,\mathbf{H}(\mathbf{y}_0;\varepsilon)\rangle \neq 0 \quad \text{for all} \quad 1\leq i\leq p+m-s\}.\end{aligned}$$

Since the $p+m-s$ parameters of $\mathbf{c}^*$ are angles, and $\mathbf{c}^*$ is an exact invariant set of $d\,\mathbf{y}/d\,t = \mathbf{H}(\mathbf{y};\varepsilon)$, we have by construction that $\mathbf{c}^*$ "starts" on Σ and after a "time" $\mathbf{u}^T = (u_1^{T_1},\ldots,u_{p+m-s}^{T_{p+m-s}})$ returns to the section. So, there is a vector $(u_{01}^{T_1},\ldots,u_{0\,p+m-s}^{T_{p+m-s}})$ such that if $\mathbf{y}$ is close to $\mathbf{y}_0$ on Σ, there is a "time" $\mathbf{Q}(\mathbf{y})$ close to $\mathbf{u}^T$ with $\mathbf{c}^*(\mathbf{Q}(\mathbf{y}),\mathbf{y};\varepsilon)$ is on Σ. Vector $\mathbf{Q}$ is called first return time and allows to define the Poincaré mapping $\mathbf{P}:\mathbf{y}\rightarrow\mathbf{c}^*(\mathbf{Q}(\mathbf{y}),\mathbf{y};\varepsilon)$. Clearly, $\mathbf{c}^*$ appears now as a fixed point of $\mathbf{P}$. Moreover, $\mathbf{P}$ is a smooth map and is used to build the function $\mathbf{E} = \mathbf{P}(\mathbf{y};\mathbf{d}^*,\varepsilon) - \mathbf{y}$, after adding the external parameters $\mathbf{d}^*$. Now, the Implicit Function Theorem is applied to the equation $\mathbf{E}=\mathbf{0}$. Note that $\mathbf{E}(\mathbf{y}_0;\mathbf{d},\varepsilon)$ vanishes and the matrix

$$\left(\frac{\partial\,\mathbf{c}^*(\mathbf{u},\mathbf{y};\mathbf{d}^*,\varepsilon)}{\partial\mathbf{y}}\right)(\mathbf{u}^T;\mathbf{y}_0;\mathbf{d},\varepsilon),$$

has the eigenvalue 1 with multiplicity $p+m-s$ (one eigenvalue 1 for each angle $\mathbf{u}_i$). Next, there is a smooth function $\tilde{\mathbf{y}}(\mathbf{d}^*,\varepsilon)$ such that $\mathbf{E}(\tilde{\mathbf{y}}(\mathbf{d}^*,\varepsilon);\mathbf{d}^*,\varepsilon)=\mathbf{0}$ for small ε and $\mathbf{d}^*\rightarrow\mathbf{d}$.

Thence, the torus $\mathbf{c}^*$ can be continued to a certain set $\mathbf{c}^\#$ for small ε and $\mathbf{d}^* \to \mathbf{d}$. Finally $\mathbf{c}^\#$ represents an $(p+m-s)$–dimensional torus of $\mathbf{F}$. □

In a first step one needs to calculate, when it will be possible, the invariant sets of the equation defined on $\mathbf{R}^m/G_{\mathbf{T}}$. Note that an invariant set (of dimension $0 \leq p \leq m$) associated to the system $d\,\mathbf{p}(t)/d\,t = \mathbf{a}(\mathbf{p}(t);\varepsilon)$ can be represented parametrically at least locally by the equation $\mathbf{p} = \mathbf{u}(\mathbf{c};\varepsilon)$, where $\mathbf{c}$ designates the p–parameter vector, that is, a vector with p constants, and $\mathbf{u}$ stands for a known r–dimensional vector field determined in the process of the computation of the specific invariant manifold. Besides, ε remains fixed.

Once $\mathbf{u}$ is obtained, we go back to the variable $\mathbf{y}$ by making use of the explicit expressions of the φ_i in terms of $\mathbf{y}$. Locally, we can express s components of the y_i in terms of ε, the c_i and $m-s$ components of the y_i. Without loss of generality we identify $\mathbf{d}_1 = \{y_1, \ldots, y_s\}$ and $\mathbf{d}_2 = \{y_{s+1}, \ldots, y_m\}$. Thus, $\mathbf{d}_1$ can be put in terms of ε, $\mathbf{c}$ and $\mathbf{d}_2$. Now, we can express the equation of the invariant manifold as $\mathbf{d}_1 = \mathbf{v}(\mathbf{c}, \mathbf{d}_2; \varepsilon)$ where $\mathbf{v}$ is a known vector field having dimension s. Due to the fact that the invariance of the equations is preserved by $\pi_{\mathbf{T}}$ we have that $\mathbf{v}$ defines an invariant manifold in $\mathbf{R}^m$.

The last step consists in recovering the equation of the manifold in the variable $\mathbf{x}$. For that we need to use the direct Lie transformation, that is, the change of variable $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$. Denoting by $\mathbf{e}_1$ the s components of $\mathbf{x}$ which can be written locally in terms of the other $m-s$ components of $\mathbf{x}$ (which are denoted by $\mathbf{e}_2$), we arrive at a formula of the type $\mathbf{e}_1 = \mathbf{w}(\mathbf{c}, \mathbf{e}_2; \varepsilon)$ where $\mathbf{w}$ is an s–dimensional vector field defining an invariant set of dimension $p+m-s$. Again $\mathbf{w}$ remains invariant in $\mathbf{R}^m$ up to an approximation of order M.

Estimates of the error committed by the application of Theorems 2.1 and 2.2 can be obtained from the theory developed for the method of averaging. In fact, taking into account that $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$, if we call $\mathbf{F}^*(\mathbf{y};\varepsilon) = \mathbf{F}(\mathbf{X}(\mathbf{y};\varepsilon);\varepsilon)$, then using Theorem 3.2 one can conclude that by choosing an adequate norm, $\|\mathbf{F}^*(\mathbf{y};\varepsilon) - \mathbf{G}(\mathbf{y};\varepsilon)\| = \mathcal{O}(\varepsilon^{M+1})$ on a time–scale $1/\varepsilon$, see references [51, 56] for details. This remark gives the key to know how accurate is the computation of the invariant manifolds.

At this point we must emphasize that the type of manifold of the original system determined through a certain normal form depends on the type of vector field $\mathbf{T}$ (on its invariants and its co–ordinates in $G_{\mathbf{T}}$). Take, for instance, a three–dimensional ordinary differential equation whose principal part $\mathbf{F}_0$ admits a symmetry $\mathbf{T}$, i.e. the Lie bracket $[\,\mathbf{F}_0\,,\,\mathbf{T}\,] = \mathbf{0}$. Suppose besides that the number of functionally independent invariants related to $\mathbf{T}$ is $s = 2$, that is, we have the scalar functions φ_1, φ_2, such that $\mathcal{L}^*(\varphi_i) = 0$, for $i = 1, 2$. Furthermore suppose that the co–ordinate in $G_{\mathbf{T}}$ is of angular type. We perform a normal form transformation so that we arrive at a two–dimensional system in $\dot{\varphi}_1, \dot{\varphi}_2$.

The equilibrium points of the normal form are zero–dimensional invariants in the two–dimensional space $\mathbf{R}^3/G_{\mathbf{T}}$, so $p = 0$ and these equilibria determine one–dimensional invariants in $\mathbf{R}^3$, since $p + m - s = 1$. In addition to that, as ϑ is an angle, the invariants of the original system computed through the equilibria of system $\dot{\varphi}_1 = \dot{\varphi}_2 = 0$, following the steps described in the last paragraphs, correspond to periodic orbits in $\mathbf{R}^3$, after applying Theorem 3.2 (see also examples in Refs.[51, 56]). Using a similar argument, the periodic orbits one can calculate in $\mathbf{R}^3/G_{\mathbf{T}}$ are in correspondence with two–dimensional invariant tori in $\mathbf{R}^3$ (in this case, $p = 1$ and $p + m - s = 2$). However, if ϑ is not an angle, the corresponding one–dimensional and two–dimensional manifolds of the original system are not periodic orbits nor invariant tori.

An important application of the reduction techniques concerns with the analysis of the stability of equilibrium points. On some occasions the reduction of the vector field to the centre manifold helps in establishing the stability character of the critical point under study, see for instance the examples of [19, 61]. The reduction to the centre manifold for Hamiltonian vector fields can be looked up in Refs. [36, 24]. In this sense, the computation up to high order of the centre manifolds of equilibrium points can be done in the framework of normal forms theory, see the approach followed in [13]. Moreover, using the generalized normal form point of view we can get the reduction to the centre, stable and unstable manifolds. (Notice that the reduction to the stable manifold is useful from the point of view of calculating approximations of the solution of the original ODE in the neighbourhood of an equilibrium, because of the stability character of the stable manifold of an equilibrium point, see [42].)

Without loss of generality we suppose that the equilibrium in study is the origin of $\mathbf{R}^m$. Under these circumstances, the principal vector field $\mathbf{F}_0(\mathbf{x})$ becomes a linear system $A\,\mathbf{x}$ with A a constant matrix of dimension $m \times m$. Thus, the search of vector fields $\mathbf{T}$ commuting with $A\,\mathbf{x}$ simplifies to look for matrices T such that $A\,T = T\,A$. Now, adequate choices of T provide the determination of the centre, stable and unstable manifolds, together with the reduction of some specific equilibria to those manifolds, as exposed in the following.

First of all it is advisable to write A in Jordan canonical form. Suppose then that A has n_s eigenvalues with negative real part, n_u eigenvalues with positive real part and n_c eigenvalues with null real part, then $n_s + n_u + n_c = m$. Moreover we arrange A in such a way that we put all the eigenvalues with null real part at the beginning, then the eigenvalues with negative real part and finally the eigenvalues with positive real part. In order to compute the centre manifold associated to the origin (the equilibrium) we choose a diagonal matrix T whose n_c first components are zero, whereas the rest of entries, $n_s + n_u$, are non–zero real numbers such that they do not satisfy any resonance condition among them. Then,

clearly $A\,T = T\,A$ and we could perform the normal form computation and $T\,\mathbf{y}$ becomes a symmetry of the truncated normal form.

Now, from $d\,\mathbf{y}/d\,t = T\,\mathbf{y}$ we have that $s = n_c$ and $\varphi_1 = y_1, \ldots, \varphi_s = y_s$ and $\vartheta_1 = y_{s+1}, \ldots, \vartheta_{m-s} = y_m$. So we can pass from the normal form to the reduced system which has dimension s, and corresponds to the differential equation associated to the centre manifold. To compute the co–ordinates of the centre manifold we construct the change of variable putting the original variables in terms of the transformed ones (direct change) by following the technique based on Lie transformations, Refs. [25, 45], obtaining $\mathbf{x} = \mathbf{X}(\mathbf{y}; \varepsilon)$. Finally, we substitute $y_{s+1} = y_{s+2} = \ldots = y_m \equiv 0$, arriving at the equations defining the s–dimensional centre manifold of the origin corresponding to the departure system. In a similar manner we would compute the stable and unstable manifolds of the origin, defining a diagonal matrix T having either n_s or n_u zeroes in their corresponding places, whereas the rest of terms are non-zero real numbers that do not satisfy any resonance condition.

The calculation of invariant manifolds of a Hamiltonian vector field $\mathcal{H} = \mathcal{H}_0 + \varepsilon\,\mathcal{H}_1 + \ldots$ is a particular situation of the theory exposed above. However, one has to choose the integrals $\mathcal{T}$ (Hamilton functions) of the principal part $\mathcal{H}_0$ and perform the Lie transformations in the symplectic frame, see Refs. [44, 45, 50]. Moreover, as the reduction is now symplectic, and $\mathcal{T}$ takes a fixed value $c \in \mathbf{R}$, once we calculate a certain invariant set in the reduced phase space, we can determine a family (parametrized by c) of invariant sets of the original Hamiltonian. Thus, we will talk about families of periodic orbits, or families of p–dimensional invariant tori, etc.

4 Examples of normal forms, reduction techniques and invariant theory

4.1 A case of a semisimple Hamiltonian in $\mathbf{R}^4$

According to Ref. [45] the number of polynomial Hamilton functions in $\mathbf{R}^4$ with real parameters and whose dominant part is a quadratic polynomial is fourteen. One of the cases corresponds to a Hamiltonian whose dominant term is $\mathcal{H}_0 = a\,x\,X + b\,y\,Y$ (a and b are real nonzero constants, x and y refer to positions and X and Y to their velocities. An application of this case is a particle under the influence of a double–well potential, see Ref. [10].

Given a Hamiltonian $\mathcal{H} = \mathcal{H}_2 + \mathcal{H}_3 + \cdots$ where each $\mathcal{H}_i$, $i \geq 1$ is a homogeneous polynomial in x, y, X and Y of degree $i + 2$ with real parameters, the task is to seek a formal change of co–ordinates $(x', y', X', Y') \to (x, y, X, Y)$ so that it is used to transform $\mathcal{H}$ into another Hamiltonian $\mathcal{K} = \mathcal{K}_0 + \mathcal{K}_1 + \cdots$ where $\mathcal{K}_0 \equiv \mathcal{H}_0$ and each $\mathcal{K}_i$, with $i \geq 1$ is a homogeneous polynomial in x', y', X' and Y' of degree $i + 2$ but such that the Poisson brackets $\{\mathcal{K}_i\,, \mathcal{T}\} = 0$, for $i \geq 0$ and a certain polynomial $\mathcal{T}$. Now, two possibilities are

in order: either the quotient a/b is not a rational number, thus $\mathcal{H}_0$ defines a non–resonant system and the normal form theory for polynomial Hamiltonians [55, 34] yields a system of dimension zero with trivial phase space; either a/b is a negative or positive integer and the normal form approach yields a one–dimensional phase space if we choose $\mathcal{T} = \mathcal{H}_0$.

If there are resonances, a and b can be taken integers and relatively primes without loss of generality. Moreover, we can always suppose that $|b| \geq |a|$.

The invariants of the normalization are taken as:

$$\varphi_1 = x\,X, \quad \varphi_2 = y\,Y, \quad \varphi_3 = x^{|b|}\,Y^{|a|}, \quad \varphi_4 = X^{|b|}\,y^{|a|}.$$

Note that φ_3 and φ_4 are polynomials of degree $|a| + |b|$. There are four linearly independent invariants, and are different according to the signs of a and b.

The identity which connects them is:

$$\varphi_1^{|b|}\,\varphi_2^{|a|} \;=\; \varphi_3\,\varphi_4. \tag{16}$$

We add the condition $\mathcal{T} = c \in \mathbf{R}$. Putting φ_2 in terms of φ_1, formula (16) is now:

$$\varphi_1^{|b|}\,(c - a\,\varphi_1)^{|a|} \;=\; b^{|a|}\,\varphi_3\,\varphi_4. \tag{17}$$

The reduced Hamiltonian $\mathcal{K}$ is computed straightforwardly using the approach of [34], after truncation defines a system of one degree of freedom in φ_1, φ_2, φ_3 and φ_4, that is in the orbit space defined through (16).

The singularities can be determined by parametrizing Equation (16) in the frame defined by φ_1, φ_2, φ_3 and φ_4. The gradient vector is

$$\left(|b|\,\varphi_1^{|b|-1}\,\varphi_2^{|a|}\,,\; |a|\,\varphi_1^{|b|}\,\varphi_2^{|a|-1}\,,\; -\varphi_4\,,\; -\varphi_3\right).$$

Now, three possibilities are in order: i) if $|b| > |a| > 1$ the gradient vanishes at $(0, \varphi_2, 0, 0)$ and $(\varphi_1, 0, 0, 0)$; ii) if $|b| > |a| = 1$ then the gradient vanishes at $(0, \varphi_2, 0, 0)$ and iii) if $|b| = |a| = 1$ the gradient is null at $(0, 0, 0, 0)$. Now we take into account the condition $a\,\varphi_1 + b\,\varphi_2 = c$ and pass to the three–dimensional space determined by φ_1, φ_3 and φ_4. Then, the singular points are $(0, 0, 0)$ and $(c/a, 0, 0)$ in subcase i); $(0, 0, 0)$ in subcase ii) and $(0, 0, 0)$ in subcase iii) if and only if $c = 0$. That is, one has zero singular points if $|b| = |a| = 1$ and $c \neq 0$, two singular points if $|b| > |a| > 1$ and $c \neq 0$ and one singular point in the rest of the cases.

Then, the reduction is regular only if $|b| = |a| = 1$ and $c \neq 0$. Otherwise it is singular. Several phase spaces are depicted in Figures 1 and 2.

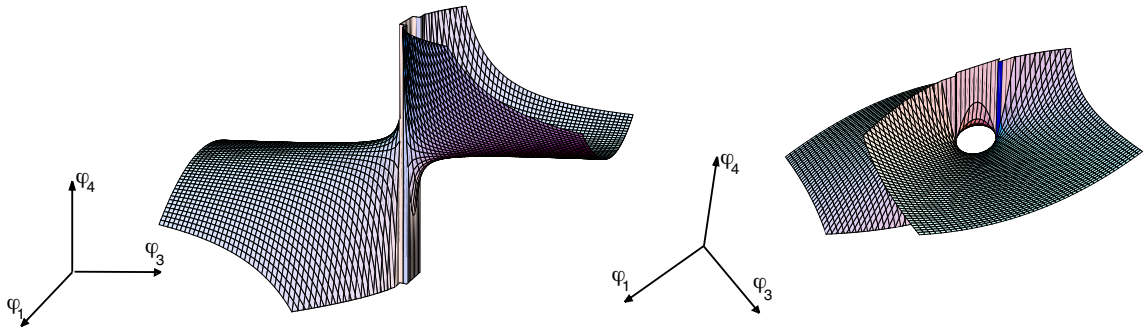

Figure 1: Two views of the reduced phase space for $\mathcal{T} = a\,x\,X + b\,y\,Y$, $|a| = |b|$ and $c \neq 0$. The surface is regular.

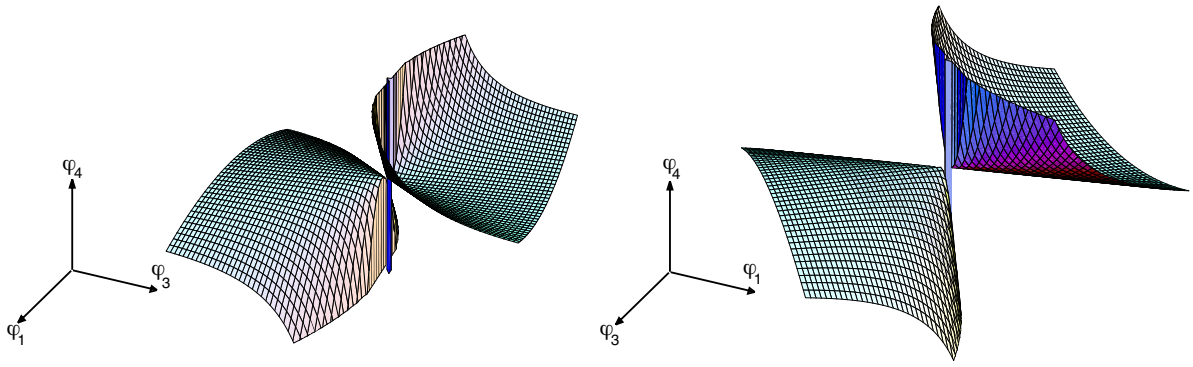

Figure 2: Two views of the reduced phase space for $\mathcal{T} = a\,x\,X + b\,y\,Y$, $|a| = |b|$ and $c = 0$. The origin is the only singular point of the surface.

4.2 A perturbed Keplerian system

Here we briefly analyze the reduction procedure for artificial satellites orbiting the Earth at low altitudes. W do not plan give a full theory of artificial satellites, but to present the guidelines for the construction of a normal form for some artificial satellites, see also [39, 40, 41]. The gravity potential written in spherical co–ordinates (r, λ, β) in a reference frame fixed to the Earth, admits the representation independent of the time:

$$\mathcal{V} = -\frac{\mu}{r} \sum_{n \geq 2} \left(\frac{\alpha}{r}\right)^n \sum_{0 \leq m \leq n} (C_{n\,m} \cos m\,\lambda + S_{n\,m} \sin m\,\lambda)\ P_{n\,m}(\sin \beta), \tag{18}$$

where μ denotes the gravitational constant, α is the mean equatorial radius of the Earth, $C_{n\,m}$ and $S_{n\,m}$ stand for the tesseral coefficients and $P_{n\,m}$ is the associated Legendre function of degree n and order m, see the details in [12]. Thus the energy of the system is given by the sum of the unperturbed Hamiltonian — composed by the two–body part and Coriolis part — and the potential $\mathcal{V}$ is the sum $\mathcal{H} = \mathcal{H}_K + \mathcal{H}_C + \mathcal{V}$ where, in mixed Delaunay

variables (ℓ, g, ν, L, G, N) and polar–nodal variables $(r, \vartheta, \nu, R, G, N)$ (see the definitions of these co–ordinates in [41]), one has

$$\mathcal{H}_K \,=\, -\frac{\mu^2}{2\,L^2} \quad \text{and} \quad \mathcal{H}_C \,=\, -\Omega\, N,$$

where $L^2 = \mu\, a$ and a stands for the semi–major axis and N refers to the third component of the angular momentum vector.

In the context of an artificial satellite theory, one needs to order the terms of $\mathcal{H}$ according to an asymptotic expansion in order to build a perturbation theory. In general, the full unperturbed part of the Hamiltonian is placed at zeroth order while the perturbation is distributed at first and second orders. However, as we restrict ourselves to the case of low altitude satellites, where the angular velocity of the Earth (i.e. Ω) is much smaller than the initial mean motion of the satellite, n_0, we propose a different scheme to distribute $\mathcal{H}$. This scaling is possible as $|\mathcal{H}_K|$ is much bigger than $\Omega\,|N|$. Now, if one chooses the small parameter ε equal to Ω/n_0, then the Keplerian terms remains at zeroth order while the term $-\Omega\, N$ is placed at first order. Then, as the influence of the terms containing the harmonic coefficients is smaller than the one produced by $-\Omega\, N$, the terms factorized by $C_{n\,m}$ and $S_{n\,m}$ are relegated to higher orders.

In the case of the French SPOT satellite the initial conditions for the semi–major axis, the eccentricity and the orbital inclination are respectively, $a = 7200.141\,\text{km}$, $e = 0.01$ and $I = 98^o$. The perturbing potential is distributed as follows: the term factorized by $C_{2\,0}$ is placed at order two and the rest of the potential, $\mathcal{V}$, goes to order seven. Now, we have that the small parameter is $\varepsilon = \Omega/n_0 \approx 1/14$. The Hamiltonian of the problem in Whittaker variables reads as a power series of ε:

$$\mathcal{H} \,=\, \mathcal{H}_0 + \varepsilon\,\mathcal{H}_1 + \frac{\varepsilon^2}{2!}\,\mathcal{H}_2 + \frac{\varepsilon^7}{7!}\,\mathcal{H}_7, \tag{19}$$

where

$$\mathcal{H}_0 \,=\, \tfrac{1}{2}\left(R^2 + \frac{\Theta^2}{r^2}\right) - \frac{\mu}{r}, \qquad \mathcal{H}_1 \,=\, -n_0 N, \qquad \mathcal{H}_2 \,=\, -\frac{\mu}{r}\left(\frac{\alpha}{r}\right)^2 \bar{C}_{2\,0}\, P_2(s\,\sin\,\vartheta),$$

$$\begin{aligned}\mathcal{H}_7 \,=\, & -\frac{\mu}{r}\sum_{n\geq 3}\left(\frac{\alpha}{r}\right)^n \bar{C}_{n\,0}\, P_n(s\,\sin\,\vartheta) \\ & -\frac{\mu}{r}\sum_{n\geq 2}\left(\frac{\alpha}{r}\right)^n \sum_{1\leq m\leq n} (\bar{C}_{n\,m}\,\cos\,m\,\lambda + \bar{S}_{n\,m}\sin m\,\lambda)\, P_{n\,m}\,(s\,\sin\,\vartheta),\end{aligned}$$

with $s = \sin\, I = (1 - (N/G)^2)^{1/2}$. We still maintain the spherical longitude λ for simplicity in the notation, assuming that it must be expressed in polar–nodal variables. Besides the "bar" harmonic coefficients satisfy the relations

$$C_{2\,0} \,=\, \frac{\varepsilon^2}{2!}\,\bar{C}_{2\,0},\; C_{n\,m} \,=\, \frac{\varepsilon^7}{7!}\,\bar{C}_{n\,m} \text{ and } S_{n\,m} \,=\, \frac{\varepsilon^7}{7!}\,\bar{S}_{n\,m}, \text{ for } n \geq 3,\, m \geq 0 \text{ or } n = 2,\, m \geq 1.$$

Once the Hamiltonian is written adequately, we apply a symplectic transformation with the aim of doing L a formal integral and eliminating ℓ from the normal form $\mathcal{K}$.

As a first step we have to put $\mathcal{H}_2$ and $\mathcal{H}_7$ in terms of non–negative powers of R and integer powers of r. Then we have to take $\mathcal{K}_i$ as the averages:

$$\mathcal{K}_i \,=\, \frac{1}{2\,\pi}\,\int_0^{2\,\pi}\,\widetilde{\mathcal{H}}_i\,d\,\ell \qquad \text{for} \qquad i \geq 2,$$

where $\widetilde{\mathcal{H}}_i$ is calculated following the instructions provided by the Lie transformation.

We have pushed the computations of the normal form to order nine, that is, the global error of our computations is of the size $\varepsilon^{10} \approx 3.45\,10^{-12}$. Up to order seven, the procedure is carried out in a standard manner, resulting equivalent results to those obtained by Coffey and Deprit for the zonal problem (e.g. considering only the first sum in $\mathcal{H}_7$, see [7] for details). Nevertheless, in the calculation of $\mathcal{K}_8$, we have to deal with terms of the type $P_i\,\varphi\,\cos\,i\,h$ and $Q_i\,\varphi\,\sin\,i\,h$ (where $h \equiv \nu$ is the argument of the node, $\varphi = f - \ell$ is the difference between the true and mean anomaly and is called the equation of the centre, P_i and Q_i are functions of the moments). The appearance of these terms is due to the fact that in the Lie process one needs to compute $\{\,-n_0\,H\,,\,\mathcal{W}_7\,\}$, where $H \equiv N$ and $\mathcal{W}_7$ stands for the generator of normalization at order seven. Therefore, the calculation of the quadrature of φ over ℓ must be done so that to obtain the expression of the generator of order eight in closed form. While these terms do not contribute to the transformed Hamiltonian of order eight (i.e. their average with respect to the mean anomaly is zero), one needs to calculate their primitives with respect to ℓ in order to complete the generating function $\mathcal{W}_8$.

Now the intermediate Hamiltonian $\widetilde{\mathcal{H}}_8$ is computed in closed form. Now one expresses everything in terms of $z_E = \exp(\imath\,E)$ (E designates the eccentric anomaly) and the integral $\int \widetilde{\mathcal{H}}_8^{\#}(z_E)\,d\,z_E$ must be calculated. At this step, all the terms in $\widetilde{\mathcal{H}}_8^{\#}$ are of the form

$$z_E^q, \quad z_E^q\,\mathrm{Li}_2[(1+\eta)^{-1}\,e\,z_E], \quad z_E^q\,\mathrm{Li}_2[(1+\eta)^{-1}\,e\,{z_E}^{-1}]$$

and $\mathcal{W}_9$ is computed in closed form, yielding the polylogarithmic function of third order. (The variable e denotes the eccentricity of the orbit, that is, $e = (1-(G/L)^2)^{1/2}$ and η is defined such that $\eta^2 + e^2 = 1$.) See Figure 3 for the representation of the polylogarithmic function of complex argument. The process can be continued to higher orders in closed form. At order ten one obtains the polylogarithm of fourth order and so on. Note that Hamiltonian $\mathcal{K} = \mathcal{K}_0 + \varepsilon\,\mathcal{K}_1 + (\varepsilon^2/2)\,\mathcal{K}_3 + \ldots + (\varepsilon^9/9!)\,\mathcal{K}_9$ defines a dynamical system with two degrees of freedom in the variables g and h.

Once $\mathcal{K}$ is determined we should perform the reduction process. Since $\mathcal{K}$ depends only on two angles, it defines a 2DOF system, which is diffeomorphic to $S^2 \times S^2$. The details on the reduction can be seen in Ref. [9]. Notice that the equilibria of the Hamiltonian defined

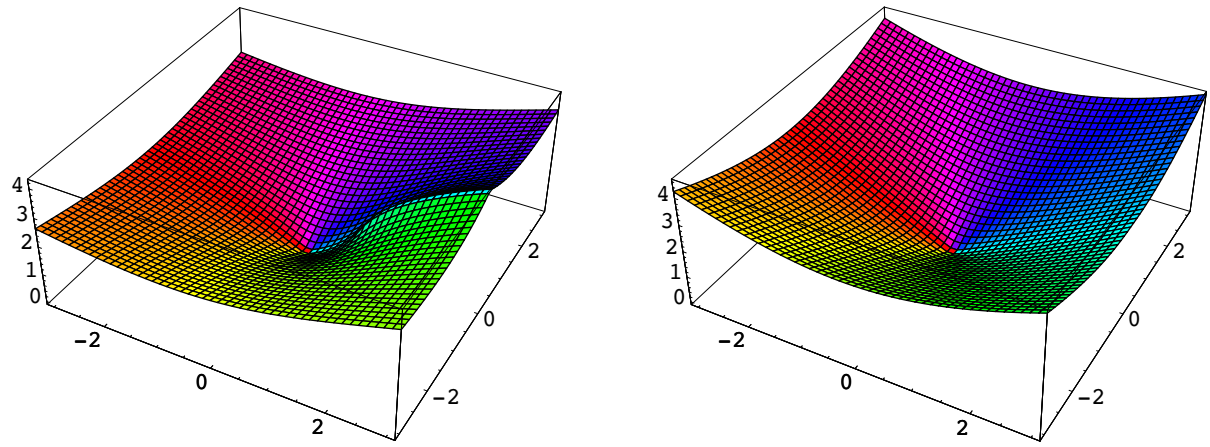

Figure 3: On the left, the polylogarithm of second order with complex argument. On the right, the polylogarithm of order 6 with complex argument.

on $S^2 \times S^2$ correspond to periodic orbits of the original Hamiltonian in the real system. See also details and more examples in Refs. [40, 41].

4.3 A non–Hamiltonian EDO

One of the applications of the theory developed before concerns the cases of polynomial dynamical systems whose linear parts have nilpotent real matrices. In these situations the application of the Normal Form Theorem [32, 13, 4] does not produce a new formal symmetry. The full classification for two–and-three–dimensional cases has been treated in [67]. Here we deal with 3×3–matrices with real entries. See also more details in Ref. [46].

Consider the system

$$\frac{d\,\mathbf{x}}{d\,t} = A\,\mathbf{x} + \mathbf{f}(\mathbf{x}), \tag{20}$$

where $\mathbf{x} = (x_1, x_2, x_3)^t \in \mathbf{R}^3$ and A is either

$$A_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Let us suppose that the vector field $\mathbf{f}(\mathbf{x})$ has three components $f_1(\mathbf{x})$, $f_2(\mathbf{x})$ and $f_3(\mathbf{x})$ corresponding to arbitrary Taylor series in $\mathbf{x}$ starting at degree two. Clearly A_1, A_2 and A_3 are nilpotent since $A_1^2 = A_3^2 = 0$ and $A_2^3 = 0$. Systems (20) are studied from the Stability Theory point of view with the aim of analyzing if the origin can be stable. Besides, scalar equations of the form $d^3x/dt^3 + f(x, dx/dt, d^2x/dt^2)$, where f has a Taylor expansion starting at degree two, can be written in the form (20) with $A = A_2$. Because of symmetric

considerations we study (20) with $A = A_1$ and A_2, as the case A_3 can be readily inferred from the analysis for A_1.

Note that due to the form taken by the function $\mathbf{f}$ we have the freedom of calculating the normal forms and the generating functions in a compact manner, which allows to simplify the notations and calculations. Besides, the Lie transformations are executed easily to any order and in one step. In a real application we should cut the Taylor expansions at an order M but the rest of the formulae apply straightforwardly. In addition to this, we should scale the system defined by (20), say $\mathbf{x} \to \varepsilon\,\mathbf{x}'$, so as to introduce a dimensionless small parameter $\varepsilon > 0$. In this manner the equation would appear in the appropriate setting to apply a perturbation theory. However we can avoid this step as we do the Lie transformation in one step. Thus from now on we can fix the value of ε, that is, without loss of generality we make $\varepsilon = 1$.

First of all we apply the Normal Form Theorem. Since $A = A_N$ and $A_S = 0$ (for both A_1 and A_2), no symmetry is going to appear as a consequence of this transformation and therefore the Splitting Lemma does not apply. Note that they are the only matrices (and their Jordan–equivalent) in three dimensions whose semisimple part is zero. More concretely, Equations (20) are converted into:

$$\frac{d\,\mathbf{y}}{d\,t} = A\,\mathbf{y} + \mathbf{g}(\mathbf{y}), \tag{21}$$

with $\mathbf{y} = (y_1, y_2, y_3)^t$, $\mathbf{g} = (g_1, g_2, g_3)^t$ and

$$g_1(\mathbf{y}) \,=\, \alpha(y_1, y_2), \quad g_2(\mathbf{y}) \,=\, y_2\,\beta(y_1, y_2), \quad g_3(\mathbf{y}) \,=\, y_3\,\beta(y_1, y_2) + \gamma(y_1, y_2),$$

for $A = A_1$ whereas for $A = A_2$

$$g_1(\mathbf{y}) = \alpha(y_1), \quad g_2(\mathbf{y}) \,=\, \frac{y_2}{y_1}\,\alpha(y_1) + \beta(y_1),$$
$$g_3(\mathbf{y}) = \frac{y_2^2}{2\,y_1^2}\,\alpha(y_1) + \frac{y_2}{y_1}\,\beta(y_1) + \gamma(y_1, 2\,y_1\,y_3 - y_2^2).$$

For the choice $A = A_1$ the Taylor series of $\alpha(y_1, y_2)$ and $\gamma(y_1, y_2)$ start at degree two and the Taylor series of $\beta(y_1, y_2)$ starts at degree one. For $A = A_2$ the Taylor series $\alpha(y_1)$, $\beta(y_1)$, $\gamma(y_1, 2\,y_1\,y_3 - y_2^2)$ start at degree two. So, in all the cases the vector field $\mathbf{g}$ has polynomial components in $\mathbf{y}$ starting at degree two. The corresponding generating functions are also polynomial as we have made use of the Normal Form Theorem. Because systems (21) have been constructed through the application of the Normal Form Theorem, then $[\,A^t\,\mathbf{y}\,,\,\mathbf{g}(\mathbf{y})\,] = \mathbf{0}$. As the two systems (20) and (21) are defined over $\mathbf{R}^3$, their reduced phase spaces coincide although the transformed systems are simpler than the original ones.

As a second choice we take $T = A_1$ and $T = A_2$, respectively. Note that there are other matrices commuting with A_1 and A_2 but here we only focus on the determination of formal

symmetries with $T = A$. Now, we have to solve $\mathcal{L}_A(\mathbf{w}) + \mathbf{g} = \mathbf{f}$, where $\mathbf{g} \in \ker(\mathcal{L}_T)$ and $\mathbf{w}$ is a solution of $\mathcal{L}_A(\mathbf{w}) = \mathbf{f} - \mathbf{g}$. The application of Theorem 2.2 yields the reduced system

$$\frac{d\,\mathbf{y}}{d\,t} = A\,\mathbf{y} + \mathbf{g}(\mathbf{y}), \tag{22}$$

where for $A = A_1$

$$g_1(\mathbf{y}) \;=\; \alpha(y_1, y_3), \quad g_2(\mathbf{y}) \;=\; y_2\,\beta(y_1, y_3) + \gamma(y_1, y_3), \quad g_3(\mathbf{y}) \;=\; y_3\,\beta(y_1, y_3), \tag{23}$$

and for $A = A_2$

$$\begin{aligned} g_1(\mathbf{y}) &= \frac{y_1}{y_3}\,\alpha(y_3) + \frac{y_2}{y_3}\,\beta(y_3) + \gamma(2\,y_1\,y_3 - y_2^2, y_3), \\ g_2(\mathbf{y}) &= \frac{y_2}{y_3}\,\alpha(y_3) + \beta(y_3), \quad g_3(\mathbf{y}) \;=\; \alpha(y_3). \end{aligned} \tag{24}$$

When $A = A_1$ the Taylor series of $\alpha(y_1, y_2)$ and $\gamma(y_1, y_3)$ start at degree two and the Taylor series of $\beta(y_1, y_3)$ at degree one. When $A = A_2$ the Taylor series $\alpha(y_3)$, $\beta(y_3)$, $\gamma(2\,y_1\,y_3 - y_2^2, y_3)$ start at degree two. Again, in all the cases the vector field $\mathbf{g}$ has homogeneous polynomial components in $\mathbf{y}$ starting at degree two.

For $A = A_1$

$$\begin{aligned} w_1(\mathbf{y}) \;&=\; -\frac{y_2}{y_3}\,\alpha(y_1, y_3) + \frac{1}{y_3}\int f_1(\mathbf{y})\,d\,y_2, \\ w_2(\mathbf{y}) \;&=\; -\frac{y_2^2}{y_3}\,\beta(y_1, y_3) - \frac{y_2}{y_3}\,\gamma(y_1, y_3) + \frac{1}{y_3}\int f_2(\mathbf{y})\,d\,y_2 \\ &\quad + \frac{1}{y_3^2}\int\left(\int f_3(\mathbf{y})\,d\,y_2\right)\,d\,y_2, \\ w_3(\mathbf{y}) \;&=\; -y_2\,\beta(y_1, y_3) + \frac{1}{y_3}\int f_3(\mathbf{y})\,d\,y_2. \end{aligned}$$

For $A = A_2$, the expression for $\mathbf{w}(\mathbf{y})$ is more involved. Indeed, it is not possible to give an explicit formula in terms of a general vector field $\mathbf{f}$. Hence, one needs to substitute $\mathbf{f}$ in terms of polynomials starting at degree two. We have done it with Mathematica but for an arbitrary polynomial vector field $\mathbf{f}$ of degree two and with three components; the resulting expression for $\mathbf{w}$ is quite big. For the two choices of A, $\mathbf{w}$ is a rational function having y_3 in the denominators. Thus the reductions are not defined if $y_3 = 0$. From this point of view, the open domain (subset of $\mathbf{R}^3$) which has to be chosen to define the transformation must exclude the line $y_3 = 0$. This makes the normal forms useless for analyzing the origin. However, it is also possible to use (22) in other points of the corresponding reduced phase space.

Note that $[\,T\,\mathbf{y}\,,\,A\,\mathbf{y} + \mathbf{g}(\mathbf{y})\,] = \mathbf{0}$ for both normal forms. Therefore $T\,\mathbf{y}$ is a symmetry of the transformed systems, up to a certain order, and we can apply Theorem 3.1. We obtain two functionally–independent first integrals in both cases. For $A = A_1$ one has $\varphi_1(\mathbf{y}) = y_1$

and $\varphi_2(\mathbf{y}) = y_3$ whereas for $A = A_2$, $\varphi_1(\mathbf{y}) = 2\,y_1\,y_3 - y_2^2$ and $\varphi_2(\mathbf{y}) = y_3$. In both cases we have $r = s = 2$ and then $m - s = 1$.

For $A = A_1$ an adequate choice of ϑ (the co–ordinate associated to the Lie group G_T) consists in identifying it with y_2. The reason is that φ_1 and φ_2 are precisely y_1 and y_3. Thus, equation (23) becomes the polynomial system:

$$\frac{d\,\varphi_1}{d\,t} \;=\; \alpha(\varphi_1, \varphi_2), \quad \frac{d\,\varphi_2}{d\,t} \;=\; \varphi_2\,\beta(\varphi_1, \varphi_2). \tag{25}$$

The remaining one–dimensional system is defined by the polynomial system:

$$\frac{d\,\vartheta}{d\,t} \;=\; \varphi_2 + \gamma(\varphi_1, \varphi_2) + \beta(\varphi_1, \varphi_2)\,\vartheta.$$

Note that the second equation is linear in ϑ. Besides, the dynamics (existence of equilibria, periodic trajectories and asymptotic expressions of the analytic first integrals) of the initial system (20) can be analyzed in Equation (25), excepting in the axis $y_3 = 0$.

For $A = A_2$ we can make $\vartheta = y_2$ (we also could have chosen $\vartheta = y_1$). Thus, the splitting is as follows:

$$\frac{d\,\varphi_1}{d\,t} \;=\; \frac{2\,\varphi_1}{\varphi_2}\,\alpha(\varphi_2) + 2\,\varphi_2\,\gamma(\varphi_1, \varphi_2), \quad \frac{d\,\varphi_2}{d\,t} \;= \alpha(\varphi_2), \tag{26}$$

whereas the one–dimensional equation reads as:

$$\frac{d\,\vartheta}{d\,t} \;=\; \varphi_2 + \beta(\varphi_2) + \frac{\alpha(\varphi_2)}{\varphi_2}\,\vartheta.$$

Note that the second equation is linear in ϑ and both systems are polynomial in φ_1, φ_2. On this occasion, except for the axis $y_3 = 0$, we can analyze system (26) to infer qualitative properties of the departure system (20).

The Lie group associated to each T is the one–dimensional set $G_T = \{\exp(T\,t) \in GL(\mathbf{R}^3) \mid t \in \mathbf{R}\}$, where for $T = A_1$ and $T = A_2$ we have respectively:

$$\exp(T\,t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & t \\ 0 & 0 & 1 \end{pmatrix}, \quad \exp(T\,t) = \begin{pmatrix} 1 & t & t^2/2 \\ 0 & 1 & t \\ 0 & 0 & 1 \end{pmatrix}.$$

We define the natural action

$$\begin{array}{rccc} \varrho_T : & G_T \times (\mathbf{R}^3 \setminus \{y_3 = 0\}) & \longrightarrow & \mathbf{R}^3 \setminus \{y_3 = 0\} \\ & (\exp(T\,t)\,,\,\mathbf{y}) & \mapsto & \exp(T\,t)\,\mathbf{y}. \end{array}$$

These mappings are natural actions of G_T on $\mathbf{R}^3 \setminus \{y_3 = 0\}$. Thus, systems (25) and (26) are defined over $(\mathbf{R}^3 \setminus \{y_3 = 0\})/G_T$, which are the reduced phase spaces. As for the two choices of T, the corresponding φ_1 runs over $\mathbf{R}$ whereas φ_2 runs over $\mathbf{R} \setminus \{0\}$, then both reduced

phase spaces can be identified with $\mathbf{R}\times(\mathbf{R}\setminus\{0\})$, that is, $(\mathbf{R}^3\setminus\{y_3=0\})/G_T \cong \mathbf{R}\times(\mathbf{R}\setminus\{0\})$. This time, the transformation has permitted to reduce the dimension of the phase space by one.

Notice that if one is interested in studying the initial system (20) in a vicinity of $y_3 = 0$ by means of normal form calculations, the only way is to resort to the analysis of system (21) in $\mathbf{R}^3$.

Finally, the isotropy subgroups are trivial for all $\mathbf{y} \in \mathbf{R}^3 \setminus \{y_3 = 0\}$. This implies that both reductions are regular in this subset of $\mathbf{R}^3$.

5 New periodic orbits and 2D–tori in the planar Hénon and Heiles family

In the following we plan to analyze the behaviour of the Hénon and Heiles family — see references [21, 18] — given by the Hamilton function $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ where

$$\begin{aligned} \mathcal{H}_0(x,y,X,Y) &= \tfrac{1}{2}\,(X^2+Y^2) + \tfrac{1}{2}\,(\omega_1^2\,x^2 + \omega_2^2\,y^2), \\ \mathcal{H}_1(x,y) &= \alpha\,x^3 + \beta\,x\,y^2. \end{aligned} \tag{27}$$

The unknown $\mathbf{x}' = (x, y, X, Y)$ is formed by the positions x, y and their corresponding velocities X, Y. Therefore, the physical dimensions of x and y are length whereas X and Y are length/time. Besides, ω_1 and ω_2 are strictly positive constants with dimensions 1/time. Finally, α and β are real constants with dimensions $1/(\text{length}\,\text{time}^2)$. This problem has been dealt with in Ref. [43], here

First, a dimensionless small parameter $\varepsilon > 0$ is introduced by means of the symplectic change $\mathbf{x}' \longrightarrow \varepsilon\,\mathbf{x}$. Dividing then the new Hamiltonian by ε^2 and using the same notation for $\mathcal{H}$ and for the variables, e.g. $\mathbf{x} = (x, y, X, Y)$, we arrive at the new system defined by $\mathcal{H} = \mathcal{H}_0 + \varepsilon\,\mathcal{H}_1$, with the same expressions for $\mathcal{H}_0$ and $\mathcal{H}_1$ as in (27). Now, $\mathcal{H}$ is associated with the four–dimensional differential system $d\,\mathbf{x}(t)/d\,t = \mathbf{F}(\mathbf{x}(t))$ with $\mathbf{F}(\mathbf{x}) = \mathbf{F}_0(\mathbf{x}) + \varepsilon\,\mathbf{F}_1(\mathbf{x})$. Besides, $\mathbf{F}_0(\mathbf{x}) = A\,\mathbf{x}$, $\mathbf{F}_1(\mathbf{x}) = (0, 0, -3\,\alpha\,x^2 - \beta\,y^2, -2\,\beta\,x\,y)^t$ and

$$A = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\omega_1^2 & 0 & 0 & 0 \\ 0 & -\omega_2^2 & 0 & 0 \end{pmatrix}.$$

Notice that as the eigenvalues of A are $\pm\,\imath\,\omega_1$ and $\pm\,\imath\,\omega_2$ (where $\imath$ designates the imaginary unit), the original system is already in the centre manifold and no reductions to the stable or unstable manifolds are possible.

Whenever ω_1/ω_2 is rational, the "standard" normal form transformation for Hamilton functions, see for instance [10], can be applied to system $\mathcal{H}$ producing a new Hamiltonian

$\mathcal{K}$, such that, truncating this latter at any order, it enjoys the function $\mathcal{K}_0 \equiv \mathcal{H}_0$ as a new integral. Therefore, by applying singular reduction in the symplectic context, the truncated Hamilton function $\mathcal{K}$ is written as a system of one degree of freedom. Now, depending on the value of ω_1/ω_2, that is, on the type of resonance, we will have a different reduced phase space, and consequently a different dynamics. For instance, in the case 1/1, the reduced phase space is a two–sphere, but for $\omega_1/1$ with $\omega_1 > 1$ it is a balloon, and for ω_1/ω_2 with $\omega_1 > \omega_2 > 1$, it has the shape of an onion, see also [45].

However, if ω_1/ω_2 is not a rational number things go rather different. In this situation it is still possible to apply the normalization procedure in such a way that $\mathcal{K}_0$ becomes a new integral up to a certain order. Nevertheless, as there is no pair of integers (i, j) satisfying $i\,\omega_1 + j\,\omega_2 = 0$, e.g. the resonant condition, no term is kept in the new Hamiltonian, in other words, $\mathcal{K}_i \equiv 0$ for $i \geq 1$. Therefore, truncating at any order $\mathcal{K}$ defines a system of zero degrees of freedom with a trivial dynamics. Hence, the calculation of the normal form (the usual one) does not work for our requirements of analyzing the dynamics of system $\mathcal{H}$ by means of normal forms.

Alternatively, we can use the theory developed in the previous sections computing various normal forms and various invariant manifolds. In fact, we restrict ourselves to the case in which ω_1/ω_2 is not rational and such that $i\,\omega_1 + j\,\omega_2 \not\approx 0$ with $i, j \in \{-5, \ldots, 5\}$. Indeed, in case that $i\,\omega_1 + j\,\omega_2 \approx 0$ with $i, j \in \{-5, \ldots, 5\}$, we would use a detuning "trick", see some examples of this technique in Ref. [51, 56].

Then, we need linear vector fields commuting with the Hamiltonian — using the Lie bracket operator — with $\mathbf{F}_0(\mathbf{x}) = A\,\mathbf{x}$, i.e. we look for matrices T commuting with A. Thus, we shall require T to be of the form $T = \mathcal{J}\,\bar{T}$ where $\bar{T}$ is a symmetric matrix. So, the matrix $\bar{T}$ must be the following: $\bar{T} = \operatorname{diag}\{\omega_1^2\,t_1, \omega_2^2\,t_2, t_1, t_2\}$ with t_1 and t_2 arbitrary constants. Hence, the corresponding integrals associated to T are of the form $\mathcal{T}_a(\mathbf{x}) = \frac{1}{2}\,(X^2 + \omega_1^2\,x^2)$ (related with $T_a = \mathcal{J}\operatorname{diag}\{\omega_1^2, 0, 1, 0\}$ and $\mathbf{T}_a(\mathbf{x}) = T_a\,\mathbf{x}$) and $\mathcal{T}_b(\mathbf{x}) = \frac{1}{2}\,(Y^2 + \omega_2^2\,y^2)$ (related with $T_b = \mathcal{J}\operatorname{diag}\{0, \omega_2^2, 0, 1\}$ and $\mathbf{T}_b(\mathbf{x}) = T_b\,\mathbf{x}$) and any linear combination $r_1\,\mathcal{T}_a + r_2\,\mathcal{T}_b$. It means that we have two functionally–independent integrals to perform normal forms computations. Observe now that if we take $\mathcal{T} = \mathcal{T}_a + \mathcal{T}_b$ we shall arrive at the Hamiltonian $\mathcal{K}$ described before. Thus, we discard this option and maintain two candidates: $\mathcal{T}_a$ and $\mathcal{T}_b$. So, we shall make two normalizations.

5.1.1 Making $\mathcal{T}_a$ the new integral

We want to construct a Hamilton function $\mathcal{K}_a = \mathcal{K}_{a0} + \varepsilon\,\mathcal{K}_{a1} + \ldots + (\varepsilon^M/M!)\,\mathcal{K}_{aM} + \mathcal{O}(\varepsilon^{M+1})$ such that $\{\,\mathcal{K}_a\,,\,\mathcal{T}_a\,\} = \mathcal{O}(\varepsilon^{M+1})$. Thus, starting at order 1 we determine, step by step, a pair $(\mathcal{K}_{ai}, \mathcal{W}_{ai})$ verifying $\{\,\mathcal{K}_{ai}\,,\,\mathcal{T}_a\,\} = 0$ and $\mathcal{L}_{\mathbf{F}_0}(\mathcal{W}_{ai}) + \mathcal{K}_{ai} = \widetilde{\mathcal{H}_{ai}}$, where $\widetilde{\mathcal{H}_{ai}}$ collects the terms known from the previous orders plus $\mathcal{H}_i$. Implicitly, we pass from the co–ordinates $\mathbf{x}$ to the new co–ordinates $\mathbf{y} = (x', y', X', Y')$ and the direct and inverse changes of variables can be constructed, formally, with the help of the generator $\mathcal{W}_a$.

We use complex–symplectic variables (u, v, U, V):

$$u = \tfrac{1}{\sqrt{2}}\,\left(x - \tfrac{\imath}{\omega_1}\,X\right), \qquad U = \tfrac{1}{\sqrt{2}}\,\left(X - \imath\,\omega_1\,x\right),$$
$$v = \tfrac{1}{\sqrt{2}}\,\left(y - \tfrac{\imath}{\omega_2}\,Y\right), \qquad V = \tfrac{1}{\sqrt{2}}\,\left(Y - \imath\,\omega_2\,y\right),$$

to perform the computation in an easier manner. Now, we have that $\mathcal{H}_0 = \imath\,(\omega_1\,u\,U + \omega_2\,v\,V)$ and the perturbation $\mathcal{H}_1$ is a homogeneous polynomial in u, v, U, V of degree three. Besides, the terms of the perturbation $\mathcal{H}_i$ are homogeneous polynomials of degree $i+2$ in the complex–symplectic variables. The Lie operator associated to the principal part of $\mathcal{H}$ reads as

$$\mathcal{L}_{\mathbf{F}_0} \;=\; \imath\,\left[\omega_1\,\left(u\,\tfrac{\partial}{\partial u} - U\,\tfrac{\partial}{\partial U}\right) + \omega_2\,\left(v\,\tfrac{\partial}{\partial v} - V\,\tfrac{\partial}{\partial V}\right)\right]. \tag{28}$$

Thus, the monomial $z = u^j\,v^k\,U^\ell\,V^m$, for positive integers j, k, ℓ and m, belongs to $\ker\,(\mathcal{L}_{\mathcal{T}_a})$, e.g. satisfies $\{\,z\,,\,\mathcal{T}_a\,\} = 0$, if and only if $j = \ell$. Moreover, if z is not in this kernel we take the monomial $w = \imath\,z/(\omega_1\,(j-\ell) + \omega_2\,(k-m))$ and then the identity $\mathcal{L}_{\mathbf{F}_0}(w) = z$ holds. This completes the way the normal form transformation can be carried out at any order $i \geq 1$. We should stress that if $j \neq \ell$ the expression $\omega_1\,(j-\ell) + \omega_2\,(k-m)$ never vanishes, due to the non–resonant condition satisfied by ω_1 and ω_2.

Using the symbolic processor Mathematica, Version 4.1 [65], we have pushed the computation to calculate the new Hamiltonian and the corresponding generating function up to third order (fifth–degree terms) yielding that $\mathcal{K}_{a1} = \mathcal{K}_{a3} \equiv 0$, but we do not write down the results in Cartesians as they involve quite long expressions.

Now we can determine a formal integral of Hamiltonian $\mathcal{H}$, by means of $\mathcal{T}_a$ and $\mathcal{W}_a$. Simply, we have to use Equations (11) and (12) up to $M = 3$, obtaining a polynomial $\mathcal{T}_a^*$ in x, y, X and Y of degree 3, functionally independent of $\mathcal{H}$ and such that $\{\mathcal{H}\,,\,\mathcal{T}_a^*\} = 0$. The lowest degree terms of $\mathcal{T}_a^*$ are $\frac{1}{2}\,(X^2 + \omega_1^2\,x^2)$.

Next we calculate the first integrals — the invariant polynomials — associated to the system $d\,\mathbf{y}(t)/d\,t = T_a\,\mathbf{y}(t)$, i.e. the equation related to the constant of motion $\mathcal{T}_a$. They are readily determined using the procedure described in Subsection 3.1. We obtain three linearly

and functionally–independent polynomials: $\varphi_1 = y'$, $\varphi_2 = Y'$ and $\varphi_3 = \frac{1}{2}\,(X'^2 + \omega_1^2\, x'^2)$, see also [45]. Thus, $s \equiv r = 3$ and we transform the original system $\mathcal{H}$ into the system $\mathcal{K}_a$ which, after being truncated, can be entirely written in terms of φ_1, φ_2 and φ_3. Now, we fix a value for $\varphi_3 \equiv c \geq 0$ arriving at a Hamiltonian $\bar{\mathcal{K}_a}(\varphi_1, \varphi_2; \varepsilon, c)$ which defines a system (family of Hamiltonians) of one degree of freedom in the reduced phase space whose generators are $\varphi_1 \in \mathbf{R}$ and $\varphi_2 \in \mathbf{R}$. The constants $\alpha, \beta, \varepsilon, \omega_1$ and ω_2 are the external parameters of the system, whereas c is the internal one. This parametrization yields the plane $O\,\varphi_1\,\varphi_2$, and corresponds to the surface where $\bar{\mathcal{K}_a}$ is defined and therefore, the reduction is regular. Specifically, after dropping some constant terms, we have

$$\begin{aligned}
&\bar{\mathcal{K}_a}(\varphi_1, \varphi_2; \varepsilon, c) = \tfrac{1}{2}\,(\varphi_2^2 + \omega_2^2\,\varphi_1^2) \\
&+ \frac{\varepsilon^2\,\beta}{2\,\omega_1^4\,(\omega_1^2 - 4\,\omega_2^2)}\,\{\beta\,\omega_1^2\,\varphi_1^2\,\left[-2\,c + (\omega_1^2 - 2\,\omega_2^2)\,\varphi_1^2 - 2\,\varphi_2^2\right] \\
&+ 3\,\alpha\,c\,\left[(\omega_1^2 - 3\,\omega_2^2)\,\varphi_1^2 - \varphi_2^2\right]\}\,.
\end{aligned} \tag{29}$$

Notice that, as the transformation is symplectic, we have no need of computing explicitly the splitting (i.e. the co–ordinate of the orbit space, which has dimension one) though we can infer that it is an angle. Indeed, using action–angle variables $(\psi_1, I_1, \psi_2, I_2)$ with $I_1 = \frac{1}{2}\,(X'^2 + \omega_1^2\, x'^2)$, $I_2 = \frac{1}{2}\,(Y'^2 + \omega_2^2\, y'^2)$, the angle ψ_1 defined such that $\cos(\psi_1) = X'/(\omega_1^2\, x'^2 + X'^2)^{1/2}$, $\sin(\psi_1) = \omega_1\, x'/(\omega_1^2\, x'^2 + X'^2)^{1/2}$ and the angle ψ_2 defined through $\cos(\psi_2) = Y'/(\omega_2^2\, y'^2 + Y'^2)^{1/2}$, $\sin(\psi_2) = \omega_2\, y'/(\omega_2^2\, y'^2 + Y'^2)^{1/2}$, we have that the fact of calculating $\bar{\mathcal{K}_a}$ is completely equivalent to the "elimination" of the associated angle ψ_1. That is, the co–ordinate $\vartheta \in G_{T_a}$ should be chosen as the angle ψ_1.

Now, we are ready to construct the differential system in φ_1 and φ_2, either using the explanation given immediately after Theorem 3.1 or equivalently, taking into account that $\dot{\varphi_i} = \{\,\varphi_i\,,\,\bar{\mathcal{K}_a}\,\}$ for $i = 1, 2$. The result is:

$$\begin{aligned}
\frac{d\,\varphi_1}{d\,t} &= \varphi_2 + \frac{\varepsilon^2\,\beta}{\omega_1^4\,(\omega_1^2 - 4\,\omega_2^2)}\,\varphi_2\,(3\,\alpha\,c + 2\,\beta\,\omega_1^2\,\varphi_1^2), \\
\frac{d\,\varphi_2}{d\,t} &= -\omega_2^2\,\varphi_1 + \frac{\varepsilon^2\,\beta}{\omega_1^4\,(\omega_1^2 - 4\,\omega_2^2)}\,\varphi_1\,\{3\,\alpha\,c\,(\omega_1^2 - 3\,\omega_2^2) \\
&\qquad -2\,\beta\,\omega_1^2\,\left[c - (\omega_1^2 - 2\,\omega_2^2)\,\varphi_1^2 + \varphi_2^2\right]\},
\end{aligned} \tag{30}$$

which corresponds to the first equation of (14).

Observe that the equilibria of the equation (30) are those points of the form

$$(\varphi_1(\alpha, \beta, \omega_1, \omega_2, \varepsilon, c), \varphi_2(\alpha, \beta, \omega_1, \omega_2, \varepsilon, c))$$

for which $\dot{\varphi_1} \equiv \dot{\varphi_2} = 0$. These points are in correspondence with families, parametrized by $c \geq 0$, of periodic orbits of the system defined by $\mathcal{H}$, as the variable eliminated ψ_1 is an

angle. We shall compute them next. Moreover, the periodic orbits of (30) will represent families of two–dimensional "deformed" tori of the departure Hamiltonian with parameter c. Ways to obtain periodic orbits of differential systems are standard, see reference [51], but the process to obtain them can be quite cumbersome due to the number of parameters we have. Therefore, we shall not search them in the present work.

As well, it is possible to construct the (non–symplectic) three–dimensional differential system, adding the equation for $\dot{\varphi_3}$. The equilibria of such a system in $\mathbf{R}^3$ would give rise to periodic orbits of the fourth–dimensional system, the periodic orbits of the reduced system would refer to two–dimensional deformed invariant tori whereas the two–dimensional invariant tori would be in correspondence with three–dimensional tori of the original Hamiltonian. Following this alternative we would get a richer understanding of the original system, but we would loose the Hamiltonian character of the process and, for example, we could not apply KAM theory.

5.1.2 Making $\mathcal{T}_b$ the new integral

This time we build a Hamiltonian $\mathcal{K}_b = \mathcal{K}_{b0} + \varepsilon\,\mathcal{K}_{b1} + \ldots + (\varepsilon^M/M!)\,\mathcal{K}_{bM} + \mathcal{O}(\varepsilon^{M+1})$ such that $\{\,\mathcal{K}_b\,,\,\mathcal{T}_b\,\} = \mathcal{O}(\varepsilon^{M+1})$. As in the latter section, we have to proceed step by step, calculating first $\mathcal{K}_{b1}$, then $\mathcal{W}_{b1}$, after that $\mathcal{K}_{b2}$, then $\mathcal{W}_{b2}$ and so on. The passage from $\mathcal{H}$ to $\mathcal{K}_b$ is performed through the change of variable $\mathbf{x} \to \mathbf{y} = (x', y', X', Y')$ which can be determined —up to order M — by means of $\mathcal{W}_b$. Notice that $\mathbf{y}$ has nothing to do with the variable $\mathbf{y}$ introduced in Section 5.1.1.

Similarly to the previous case, for positive integers j, k, ℓ and m, the monomial $z = u^j\,v^k\,U^\ell\,V^m$ belongs to $\ker(\mathcal{L}_{\mathcal{T}_b})$, e.g. $\{\,z\,,\,\mathcal{T}_b\,\}$ is identically null, if and only if $k = m$. Besides, if z is not in this kernel we take $w = \imath\,z/(\omega_1\,(j-\ell) + \omega_2\,(k-m))$ and the identity $\mathcal{L}_{\mathbf{F}_0}(w) = z$ is readily satisfied. Therefore, the transformation can be executed up to any order $i \geq 1$. Now, we remark that if $k \neq m$ then $\omega_1\,(j-\ell) + \omega_2\,(k-m)$ is not null. The calculations have been carried out to order three.

The determination of a formal integral of Hamiltonian $\mathcal{H}$ is carried out by means of $\mathcal{T}_b$ and $\mathcal{W}_b$. The application of Equations (11) and (12) up to $M = 3$, yields a polynomial $\mathcal{T}_b^*$ in x, y, X and Y of degree 3, functionally independent of $\mathcal{H}$ and such that $\{\mathcal{H}\,,\,\mathcal{T}_b^*\} = 0$. This time, the quadratic part of $\mathcal{T}_b^*$ is $\frac{1}{2}\,(Y^2 + \omega_2^2\,y^2)$.

On this occasion the invariants associated to $d\,\mathbf{y}(t)/d\,t = T_b\,\mathbf{y}(t)$ (i.e. with the constant of motion $\mathcal{T}_b$) are: $\varphi_1 = x'$, $\varphi_2 = X'$ and $\varphi_3 = \frac{1}{2}\,(Y'^2 + \omega_2^2\,y'^2)$. Again $s \equiv r = 3$ and the original Hamiltonian $\mathcal{H}$ is converted into $\mathcal{K}_b$ which, after truncation is expressed as a function of φ_1, φ_2 and φ_3. Fixing a value for $\varphi_3 \equiv c \geq 0$ we arrive at the Hamiltonian $\bar{\mathcal{K}_b}(\varphi_1, \varphi_2; \varepsilon, c)$ which defines a system of one degree of freedom lying on a plane parametrized by φ_1 and φ_2. The

reduction is again regular. As in the latter section, c is the internal parameter, whereas the rest of constants stand for the external ones. After dropping some constant terms we obtain:

$$\begin{aligned}
&\bar{\mathcal{K}_b}(\varphi_1,\varphi_2;\varepsilon,c) = \tfrac{1}{2}\,(\varphi_2^2+\omega_1^2\,\varphi_1^2) + \frac{\varepsilon}{2\,\omega_2^2}\,\varphi_1\,(\beta\,c+2\,\alpha\,\omega_2^2\,\varphi_1)\\
&+\frac{\varepsilon^2\,\beta^2\,c}{\omega_2^2\,(\omega_1^2-4\,\omega_2^2)}\,\varphi_1^2+\ \frac{\varepsilon^3\,\beta^2\,c}{24\,\omega_2^6\,(\omega_1^2-\omega_2^2)\,(\omega_1^2-4\,\omega_2^2)^2}\,\varphi_1\times\\
&\times\ \{3\,\alpha\,\omega_2^2\ [-3\,c\,\omega_2^2+4\ (\omega_1^4-4\,\omega_1^2\,\omega_2^2+6\,\omega_2^4)\ \varphi_1^2+4\ (\omega_1^2-4\,\omega_2^2)\ \varphi_2^2]\\
&+2\,\beta\ [3\,c\ (\omega_1^4-4\,\omega_1^2\,\omega_2^2+6\,\omega_2^4)+\ 4\,\omega_2^2\ ((-\omega_1^4+4\,\omega_1^2\,\omega_2^2-12\,\omega_2^4)\ \varphi_1^2\\
&-(4\,\omega_1^2-13\,\omega_2^2)\ \varphi_2^2)]\}\,.
\end{aligned}\tag{31}$$

We do not calculate the co–ordinate of the orbit space but with the same argument we used for $\mathcal{T}_a$ we know that indeed, the angle removed through the transformation is the angle ψ_2, as it is the conjugate of the action $I_2=\frac{1}{2}\,(Y'^2+\omega_2^2\,y'^2)$.

Proceeding as in the latter section, we compute the differential system of equations, yielding:

$$\begin{aligned}
\frac{d\,\varphi_1}{d\,t} &= \varphi_2-\frac{\varepsilon^3\,\beta^2\,c}{3\,\omega_2^4\,(\omega_1^2-\omega_2^2)\,(\omega_1^2-4\,\omega_2^2)^2}\,\varphi_1\,\varphi_2\times\\
&\quad\times(-3\,\alpha\,\omega_1^2+8\,\beta\,\omega_1^2+12\,\alpha\,\omega_2^2-26\,\beta\,\omega_2^2),\\
\frac{d\,\varphi_2}{d\,t} &= -\omega_1^2\,\varphi_1-\frac{\varepsilon}{2\,\omega_2^2}\,(\beta\,c+6\,\alpha\,\omega_2^2\,\varphi_1^2)-\frac{2\,\varepsilon^2\,\beta^2\,c\,\varphi_1}{\omega_2^2\,(\omega_1^2-4\,\omega_2^2)}\\
&\quad+\frac{\varepsilon^3\,\beta^2\,c}{24\,\omega_2^6\,(\omega_1^2-\omega_2^2)\,(\omega_1^2-4\,\omega_2^2)^2}\times\\
&\quad\times\{-3\,c\ [-3\,\alpha\,\omega_2^4+2\,\beta\ (\omega_1^4-4\,\omega_1^2\,\omega_2^2+6\,\omega_2^4)]\\
&\quad+12\,\omega_2^2\ [-3\,\alpha\ (\omega_1^4-4\,\omega_1^2\,\omega_2^2+6\,\omega_2^4)\\
&\quad+2\,\beta\ (\omega_1^4-4\,\omega_1^2\,\omega_2^2+12\,\omega_2^4)]\ \varphi_1^2\\
&\quad+4\,\omega_2^2\ [-3\,\alpha\,\omega_1^2+8\,\beta\,\omega_1^2+12\,\alpha\,\omega_2^2-26\,\beta\,\omega_2^2]\ \varphi_2^2\}\,.
\end{aligned}\tag{32}$$

As before, the critical points of (32) are the roots of $\dot{\varphi_1}\equiv\dot{\varphi_2}=0$. These points are related with families of periodic orbits of $\mathcal{H}$, as the variable eliminated ψ_2 is angular. It will be the subject of next section. Again the periodic orbits of (32) will represent families of two–dimensional tori of $\mathcal{H}$. It could be possible to work with the differential system formed by $\dot{\varphi_1}$, $\dot{\varphi_2}$ and $\dot{\varphi_3}$ with the same considerations mentioned in Section 5.1.1.

5.2.1 Analysis of $\bar{\mathcal{K}}_a$

Solving system (30) with Mathematica produces the following critical points (φ_1, φ_2) in the plane $O\,\varphi_1\,\varphi_2$, up to order three, e.g. committing a global error of size ε^4:

$$(1)\ (0\,,\,0),$$

$$(2)\ \left(\pm\frac{\sqrt{\varepsilon^2\ (3\,\alpha-2\,\beta)\ \beta\,c\,\omega_1^2-(9\,\varepsilon^2\,\alpha\,\beta\,c+\omega_1^6)\ \omega_2^2+4\,\omega_1^4\,\omega_2^4}}{\varepsilon\,\beta\,\omega_1\,\sqrt{-2\,\omega_1^2+4\,\omega_2^2}}\,,\,0\right),$$

$$(3)\ \left(\pm\frac{\sqrt{-3\,\varepsilon^2\,\alpha\,\beta\,c\ -\omega_1^6+4\,\omega_1^4\,\omega_2^2}}{\sqrt{2}\,\varepsilon\,\beta\,\omega_1},\right.$$
$$\left.\pm\frac{\sqrt{-(2\,\varepsilon^2\,\beta^2\,c+\omega_1^6)\,\omega_1^2+(-3\,\varepsilon^2\,\alpha\,\beta\,c+5\,\omega_1^6)\,\omega_2^2-4\,\omega_1^4\,\omega_2^4}}{\sqrt{2}\,\varepsilon\,|\beta|\,\omega_1}\right).$$

Of course, the latter points are equilibria whether they represent real expressions, $\omega_1 \neq \sqrt{2}\,\omega_2$ and $\varepsilon\,\beta \neq 0$. If $\omega_1 = \sqrt{2}\,\omega_2$, the critical points are:

$$(1')\ (0\,,\,0),$$

$$(2')\ \left(\pm\frac{\sqrt{-3\,\varepsilon^2\,\alpha\,\beta\,c+8\,\omega_2^6}}{2\,\varepsilon\,\beta\,\omega_2}\,,\,\pm\frac{\sqrt{-\varepsilon^2\,\beta\,c\,(3\,\alpha+4\,\beta)+8\,\omega_2^6}}{2\,\varepsilon\,|\beta|}\right),$$

when it has sense. These points can also be obtained from (3) by replacing ω_1 by $\sqrt{2}\,\omega_2$. For $\varepsilon = 0$ or $\beta = 0$ the only equilibrium is the origin. Thus, the number of critical points can be one, three, five or seven, depending on the values the parameters take.

Let us denote the expressions under the three square roots of points (2) and (3) by:

$$\begin{aligned} c_1 &= \varepsilon^2\ (3\,\alpha-2\,\beta)\ \beta\,c\,\omega_1^2-(9\,\varepsilon^2\,\alpha\,\beta\,c+\omega_1^6)\ \omega_2^2+4\,\omega_1^4\,\omega_2^4,\\ c_2 &= -3\,\varepsilon^2\,\alpha\,\beta\,c\ -\omega_1^6+4\,\omega_1^4\,\omega_2^2,\\ c_3 &= -(2\,\varepsilon^2\,\beta^2\,c+\omega_1^6)\,\omega_1^2+(-3\,\varepsilon^2\,\alpha\,\beta\,c+5\,\omega_1^6)\,\omega_2^2-4\,\omega_1^4\,\omega_2^4. \end{aligned}$$

So, the existence of points (2) is assured whether $c_1 \geq 0$, whereas the points (3) are real when $c_2 \geq 0$ and $c_3 \geq 0$. Now, it is easy to see that the points (2) coalesce in the origin if and only if $c_1 = 0$. In addition to that, the four points (3) get reduced to two points in the axis $O\,\varphi_2$ for $c_2 = 0$ and to the two points (2) if $c_3 = 0$. Thus, the changes in the signs of c_1, c_2 and c_3 must be considered as the bifurcating conditions. Moreover, if $c_1 \equiv c_2 = 0$ or $c_1 \equiv c_3 = 0$ or $c_2 \equiv c_3 = 0$ then $\beta = 3\,\alpha\,(\omega_1^2 - 2\,\omega_2^2)/(2\,\omega_1^2)$ and the only critical point is $(0, 0)$.

The stability of the equilibria is analyzed by applying Morse Lemma — we refer to Ref. [1] for a proof and various applications — to Hamiltonian $\bar{\mathcal{K}}_a$ in the neighbourhoods of the

critical points. Thus, we conclude that the origin (1) is a centre if and only if $c_1\,c_2 > 0$ and a saddle whenever $c_1\,c_2 < 0$, whereas it is degenerate either if $c_1 = 0$ or $c_2 = 0$. Similarly, points (2) are centres if and only if $c_1\,c_3/(\omega_1^2 - 2\,\omega_2^2) > 0$ and saddles when $c_1\,c_3/(\omega_1^2 - 2\,\omega_2^2) < 0$. These equilibria become degenerate when $c_1 = 0$ or $c_3 = 0$. For the points (3), we deduce that they always correspond to saddles and become degenerate when $c_2 = 0$ or $c_3 = 0$. In the situations of degeneration it is not so clear what to decide about the stability of the equilibria, but this analysis is out of the scope of this paper.

For the case $\omega_1 = \sqrt{2}\,\omega_2$ and $\varepsilon\,\beta \neq 0$ we call

$$c_1' \;=\; -3\,\varepsilon^2\,\alpha\,\beta\,c + 8\,\omega_2^6, \qquad c_2' \;=\; -\varepsilon^2\,\beta\,c\,(3\,\alpha + 4\,\beta) + 8\,\omega_2^6,$$

and, obviously the existence of equilibria (2') is guaranteed provided that $c_1' \geq 0$ and $c_2' \geq 0$. When $c_1' = 0$ the four equilibria (2) coalesce in two points lying in the axis $O\,\varphi_2$ whereas in the case $c_2' = 0$ the two resulting points are placed in the axis $O\,\varphi_1$. Finally, the four equilibrium points get reduced to the origin for $c_1' \equiv c_2' = 0$. The application of Morse Lemma to the critical points reveals that the four points (2'), when they exist, are saddles and become degenerate for $c_1' = 0$ or $c_2' = 0$. Moreover, on this occasion, the origin is a centre when $c_1'\,c_2' > 0$, a saddle if $c_1'\,c_2' < 0$ and a degenerate point if and only if $c_1' = 0$ or $c_2' = 0$. Again we do not discuss the degeneration limits.

In the remaining cases, that is, when $\varepsilon\,\beta = 0$, as the only equilibrium is the origin, the application of Morse Lemma is rather simple. Indeed, when either $\varepsilon = 0$ or $\beta = 0$ the origin is always a centre and the dynamics of the resulting systems is trivial.

5.2.2 Analysis of $\bar{\mathcal{K}}_b$

Solving on this occasion system (32) with Mathematica produces the following equilibria (we have considered approximations up to order two):

$$\left(\frac{-2\,\varepsilon^2\,\beta^2\,c - q\,\omega_1^2\,\omega_2^2 \pm \sqrt{d}}{6\,\varepsilon\,\alpha\,q\,\omega_2^2}\,,\,0\right) \tag{33}$$

with

$$d \;=\; 4\,\varepsilon^4\,\beta^4\,c^2 - q\,\omega_2^2\,\left(6\,\varepsilon^2\,\alpha\,\beta\,c\,q - 4\,\varepsilon^2\,\beta^2\,c\,\omega_1^2 - q\,\omega_1^4\,\omega_2^2\right),$$

$q = \omega_1^2 - 4\,\omega_2^2$ does not vanishes, $\varepsilon\,\alpha \neq 0$ and the parameters are combined so that they yield a real expression, e.g they must verify $d \geq 0$. For $\alpha = 0$ the two critical points get reduced to

$$\left(-\frac{\varepsilon\,\beta\,c\,q}{2\,(2\,\varepsilon^2\,\beta^2\,c + q\,\omega_1^2\,\omega_2^2)}\,,\,0\right), \tag{34}$$

which is a valid point if $f = 2\,\varepsilon^2\,\beta^2\,c + q\,\omega_1^2\,\omega_2^2 \neq 0$. When $f = 0$ it is not hard to see that there is no equilibria. Finally, in the case $\varepsilon = 0$ the only critical point is $(0, 0)$.

In order to determine the stability of the equilibrium points we apply Morse Lemma to Hamiltonian $\bar{\mathcal{K}}_b$, using a Taylor expansion centered at the corresponding critical points. We conclude that, provided that $d \geq 0$, the point defined in (33) with positive sign in front of the square root is a centre for $q > 0$ and a saddle for $q < 0$, whereas the point with negative sign in front of the square root is a saddle when $q > 0$ and becomes a centre for $q < 0$. Besides, when $d = 0$ the two equilibria coalesce in one, which is a degenerate equilibrium, and when $d < 0$ the two equilibria disappear. This is the scenario for a saddle–centre bifurcation (depending smoothly on the variation of d). The application of Morse Lemma to the equilibrium (34) reveals that this point is a centre if and only if $f > 0$ and $q > 0$ or $f < 0$ and $q < 0$, whereas it becomes a saddle when $f < 0$ and $q > 0$ or $f > 0$ and $q < 0$. (Recall that $s \neq 0$ is the condition for the existence of the equilibrium and $q \neq 0$ is always true.) Finally, in the limit case $\varepsilon = 0$ the origin remains a centre. In Figure 4 we show the occurrence of a Hamiltonian saddle–centre bifurcation. See the details in Ref. [66]. It is noticeable to say that the saddle–centre bifurcation is typical of the Hénon and Heiles Hamiltonian in two and 3DOF, see Refs. [66, 15, 29].

All the critical points determined in the last paragraphs are in correspondence with periodic orbits of the initial system $\mathcal{H}$ and these orbits can be calculated up to order ε^4 when related to $\bar{\mathcal{K}}_a$ and to order ε^3 for those points obtained from $\bar{\mathcal{K}}_b$. The same holds for the families of two–dimensional deformed tori, constructed from the periodic orbits obtained from the systems $\bar{\mathcal{K}}_a$ and $\bar{\mathcal{K}}_b$.

As an example, let us specify how to get a family of periodic orbits from a particular equilibrium point $(\varphi_1^0, \varphi_2^0)$ obtained from $\bar{\mathcal{K}}_a$, following the steps detailed in Subsection 3.3. First, observe that φ_1^0 and φ_2^0 are written in terms of α, β, ω_1, ω_2, ε and c. Thus, taking into account that $\varphi_1 = y'$ and $\varphi_2 = Y'$, we write a point $\mathbf{y}^0 = (x', \varphi_1^0, X', \varphi_2^0)$ and then using that $c = \frac{1}{2}\,(X'^2 + \omega_1^2\, x'^2)$ and that $\cos(\psi_1) = X'/(\omega_1^2\, x'^2 + X'^2)^{1/2}$ and $\sin(\psi_1) = \omega_1\, x'/(\omega_1^2\, x'^2 + X'^2)^{1/2}$ we rewrite $\mathbf{y}^0$ as the expression $\mathbf{y}^0 = (\sqrt{2\,c}\,\sin(\psi_1)/\omega_1, \varphi_1^0, \sqrt{2\,c}\,\cos(\psi_1), \varphi_2^0)$. Now, making use of $\mathcal{W}_a$ we construct the direct change $\mathbf{x} = \mathbf{X}(\mathbf{y}; \varepsilon)$, through formula (7). Replacing now $\mathbf{y}$ by $\mathbf{y}^0$ we obtain explicitly an expression of the type $\mathbf{x}^0 = \mathbf{X}(\mathbf{y}^0; \varepsilon)$, which, for fixed α, β, ε, ω_1 and ω_2 gives the equation of the periodic orbits in $\mathbf{R}^4$ parametrized by $\psi_1 \in [0, 2\,\pi)$.

Note that the periodic orbits appear in families, as we still have the parameter $c \geq 0$. In analogous manner we can obtain the periodic orbits from the critical points obtained from $\bar{\mathcal{K}}_b$, parametrized this time by $\psi_2 \in [0, 2\,\pi)$. Moreover, the stability of the non–degenerate critical points coincides with the stability of the periodic orbits in the departure phase space.

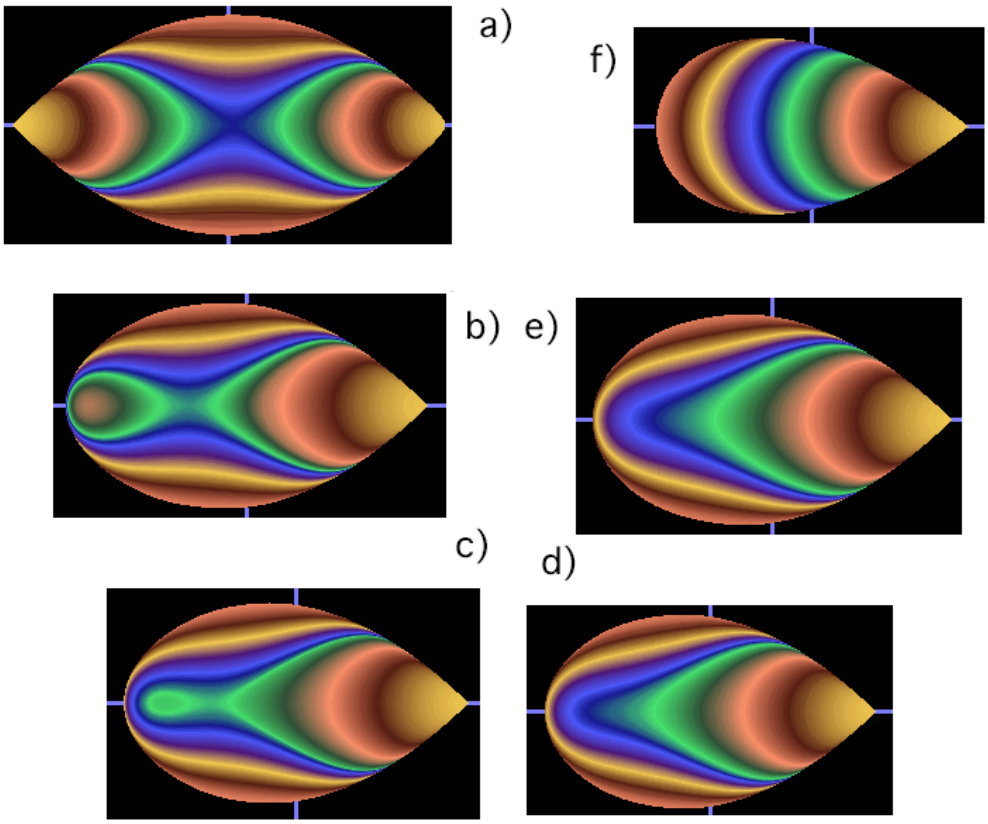

Figure 4: A Hamiltonian saddle–centre bifurcation scenario in six pictures, borrowed from reference [66].

5.3 Two–dimensional invariant tori of $\mathcal{H}$

Another way to obtain two–dimensional tori of $\mathcal{H}$ consists in applying a new normalization to either $\bar{\mathcal{K}}_a$ or $\bar{\mathcal{K}}_b$, with the aim of making $\mathcal{T}_b$ (in the first case) or $\mathcal{T}_a$ (in the second case) the new integral. This would be exactly equivalent to the application of a normal form to $\mathcal{H}$ choosing as the new integral $\mathcal{T}_a + \mathcal{T}_b$. Thus, the new reduced system, called $\mathcal{S}$, could be written in terms of I_1 and I_2 and would have zero degrees of freedom and therefore a trivial dynamics. However, one could still compute $\dot{\psi}_i = \partial \mathcal{S}/\partial I_i$ and the equilibrium points obtained from this latter system would correspond to families of two–tori in the Euclidean space $\mathbf{R}^4$ with angles $\psi_1, \psi_2 \in [0, 2\,\pi)$ parametrized by the constants $c_1 = I_1 \geq 0$ and $c_2 = I_2 \geq 0$.

By proceeding as the previous paragrapsh we have computed families of 2D–dimensional tori. Pushing the normal form transformations to order two, we arrive at a unique point (c_1, c_2) where:

$$\begin{aligned} c_1 &= -\frac{4\,{\omega_1}^4\,(\omega_1^2 - 4\,\omega_2^2)\,(3\,\beta\,{\omega_1}^4 - 2\,(3\,\alpha + 2\,\beta)\,{\omega_1}^2\,{\omega_2}^2 + 24\,\alpha\,{\omega_2}^4)}{\beta\,\varepsilon^2\,[(-9\,\alpha^2 - 48\,\alpha\,\beta + 16\,\beta^2)\,{\omega_1}^4 + 12\,\alpha\,(\alpha + 16\,\beta)\,{\omega_1}^2\,{\omega_2}^2 + 96\,\alpha^2\,{\omega_2}^4]}, \\ c_2 &= \frac{4\,{\omega_1}^2\,{\omega_2}^2\,(\omega_1^2 - 4\,\omega_2^2)\,[2\,(3\,\alpha - 2\,\beta)\,\beta\,{\omega_1}^4 - 3\,\alpha\,(5\,\alpha + 8\,\beta)\,{\omega_1}^2\ {\omega_2}^2 + 60\,\alpha^2\,{\omega_2}^4)]}{\beta^2\,\varepsilon^2\,[(-9\,\alpha^2 - 48\,\alpha\,\beta + 16\,\beta^2)\,{\omega_1}^4 + 12\,\alpha\,(\alpha + 16\,\beta)\,{\omega_1}^2\ {\omega_2}^2 + 96\,\alpha^2\,{\omega_2}^4]}, \end{aligned}$$

provided that $\omega_1^2 \neq 4\,\omega_2^2$, and whenever $\omega_1 \neq 2\,[(2 \times 11^{1/2} - 5)/3]^{1/2}\,\omega_2$ then $\alpha = 2\,(7 \times 11^{1/2} - 27)/15\,\beta$. Besides, we exclude also those values, of α, β that make null the denominators of c_1 and c_2.

For $\omega_1 = \pm\,2\,\omega_2$ we obtain, using the second–order normal form:

$$c_1 = \frac{512\,(3\,\alpha - 4\,\beta)\,{\omega_2}^6}{\beta\,(9\,\alpha^2 + 48\,\alpha\,\beta + 4\,\beta^2)\,\varepsilon^2}, \qquad c_2 = \frac{64\,(-15\,\alpha^2 + 24\,\alpha\,\beta + 4\,\beta^2)\,{\omega_2}^6}{\beta^2\,(9\,\alpha^2 + 48\,\alpha\,\beta + 4\,\beta^2)\,\varepsilon^2},$$

for $9\,\alpha^2 + 48\,\alpha\,\beta + 4\,\beta^2 \neq 0$.

Finally, the second–order normal form for the case $\omega_1 \neq 2\,[(2 \times 11^{1/2} - 5)/3]^{1/2}\,\omega_2$ and $\alpha = 2\,(7 \times 11^{1/2} - 27)/15\,\beta$ produces an infinite set of equilibria in the reduced phase space, concretely, the plane

$$c_1 + c_2 = \frac{32\,(7 \times 11^{1/2} - 8)\,\omega_2^6}{35\,\beta^2\,\varepsilon^2},$$

if c_1, c_2 vary along $\mathbf{R}^+$. In this latter case the computations should be carried out to order four, in order to avoid the degeneracy. We leave this case.

Finally, the 2D–tori are reconstructed inverting the Lie transformation to second order in ε, obtainig therefore explicit expressions of the tori associated to $\mathcal{H}$ up to terms in ε^3.

6 Invariant manifolds in Transition State Theory

6.1 The normally hyperbolic invariant manifold and the transition state

The geometrical structures which regulate transformations in dynamical systems with three or more degrees of freedom play an important role in the qualitative understanding on some differential equations. The treatment initiated in Ref [63] is based on the analysis of the $(2\,n-3)$–dimensional normally hyperbolic invariant manifold (NHIM) in n-degree-of-freedom systems associated with a centre$\times\cdots\times$centre$\times$saddle in the phase space flow in the $(2\,n-1)$–dimensional energy surface. The theory of NHIMs was commenced by Fenichel [14] and generalized by Wiggins [62] for nonlinear systems. The NHIM bounds a $(2\,n-2)$–dimensional surface, called a "transition state" in chemical reaction dynamics, which partitions the energy surface into volumes characterized as "before" and "after" the transformation. This surface is the long–sought momentum–dependent transition state beyond two degrees of freedom. The $(2\,n-2)$–dimensional stable and unstable manifolds associated with the $(2\,n-3)$–dimensional NHIM are impenetrable barriers with the topology of multidimensional spherical cylinders. The phase flow interior to these spherical cylinders passes through the transition state as the system undergoes its transformation. The phase flow exterior to these spherical cylinders is directed away from the transition state and, consequently, will never undergo the transition. The explicit forms of these phase space barriers can be evaluated using normal form theory. We follow Wiggins *et al.* [63] in our exposition.

Consider a Hamilton function of the type:

$$\begin{aligned} H &= \sum_{i=1}^{n-1} \frac{\omega_i}{2}\left(p_i^2+q_i^2\right) + \lambda q_n p_n \\ &\quad + f_1(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1},\mathcal{I}) + f_2(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1}), \end{aligned} \tag{35}$$

up to arbitrarily high order where $(q_1,\ldots,q_n,p_1,\ldots,p_n)$ denote $(2\,n)$-dimensional canonical co–ordinates, $\mathcal{I}\equiv p_n q_n$ and f_1, f_2 are at least third order, i.e., they are responsible for the nonlinear terms in the Hamiltonian vector field, and $f_1(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1},0)=0$. The NHIM associated to a Hamilton vector field like H is:

$$\begin{aligned} \mathcal{M}_h^{2\,n-3}(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1}) &= \sum_{i=1}^{n-1} \frac{\omega_i}{2}\left(p_i^2+q_i^2\right) \\ &\quad + f_2(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1}) = h = constant > 0. \end{aligned} \tag{36}$$

The NHIM acts as a multidimensional saddle "point". The dynamics occurs in the $(2\,n-1)$–dimensional energy surface given by setting H in the initial Hamiltonian to be a positive

constant h. If we set $q_n = p_n = 0$ in the vector field associated to H, then $\dot{q}_n = \dot{p}_n = 0$. Therefore $q_n = p_n = 0$ is a $(2\,n-2)$–dimensional invariant manifold. Its intersection with the $(2\,n-1)$–dimensional energy surface, is the NHIM, given by (36).

Another advantage of computing the normal form is that the stable and unstable manifolds of $\mathcal{M}_h^{2\,n-3}$ are known explicitly. They are $(2\,n-2)$–dimensional objects, acting as multidimensional separatrices. They are given by:

$$\begin{aligned} W^s\left(\mathcal{M}_h^{2\,n-3}\right) = \Bigg\{ & (q_1,\ldots,q_n,p_1,\ldots,p_n) \,|\, \sum_{i=1}^{n-1} \frac{\omega_i}{2}\left(p_i^2+q_i^2\right) \\ & + f_2(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1}) = h = constant > 0,\, q_n = 0 \Big\}\,, \\ W^u\left(\mathcal{M}_h^{2\,n-3}\right) = \Bigg\{ & (q_1,\ldots,q_n,p_1,\ldots,p_n) \,|\, \sum_{i=1}^{n-1} \frac{\omega_i}{2}\left(p_i^2+q_i^2\right) \\ & + f_2(q_1,\ldots,q_{n-1},p_1,\ldots,p_{n-1}) = h = constant > 0,\, p_n = 0 \Big\}\,. \end{aligned} \tag{37}$$

The Hamiltonian vector field (35) has an equilibrium point at the origin which has a $(2\,n-2)$–dimensional centre manifold given by $p_n = q_n = 0$, a one–dimensional stable manifold given by $q_i = p_i = 0$, $i = 1,\ldots,n-1$, $p_n = -\lambda q_n$, and a one–dimensional unstable manifold given by $q_i = p_i = 0$, $i = 1,\ldots,n-1$, $p_n = \lambda q_n$. It is easy to check that the stable and unstable manifolds of the origin have the same energy as the origin, i.e., $h = 0$. We say that they are isoenergetic. However, the centre manifold of the origin is not isoenergetic. The intersection of the centre manifold of the origin with the energy surface is given by:

$$\tfrac{1}{2}\sum_{i=1}^{n-1} p_i^2 + \tfrac{1}{2}\sum_{i=1}^{n-1} \omega_i^2 q_i^2 = h = constant.$$

This is the normally hyperbolic invariant $(2\,n-3)$–dimensional sphere we described earlier. Hence we see that the centre manifold of the origin is foliated by a one–parameter (normally the energy) family of normally hyperbolic invariant $(2\,n-3)$–dimensional spheres.

Now we construct the transition state. It has the following properties:

- It will be of dimension $2\,n-2$ in the $(2\,n-1)$–dimensional energy surface.
- Trajectories that cross the transition state correspond to reactive trajectories.
- The $(2\,n-3)$–dimensional saddle sphere will play an important role in the construction of the transition state.
- The transition state is a true "surface of no return" for this linear Hamiltonian system.

The transition state for this system is obtained by setting $q_n = 0$. Now we look at this in the full $(2\,n)$–dimensional phase space. Setting $q_n = 0$ on the energy surface gives the equation:

$$\tfrac{1}{2}\sum_{i=1}^{n} p_i^2 + \tfrac{1}{2}\sum_{i=1}^{n-1} \omega_i^2 q_i^2 = h = constant. \tag{38}$$

This is the transition state. It is a $(2\,n-2)$–dimensional sphere. The sphere has two "halves": $p_n > 0$ and $p_n < 0$. The sphere is divided into these two halves by $p_n = 0$, which corresponds to the saddle sphere $S_h^{2\,n-3}$. All reacting trajectories must pass through this transition state. The forward reactive trajectories pass through the sphere with $p_n > 0$ and the backward reactive trajectories pass through the sphere with $p_n < 0$.

6.2 Application to the Rydberg atom

The treatment of [63] and [54] has the advantage of supplying a practical algorithm, demonstrating its use on a strongly coupled nonlinear Hamiltonian, the hydrogen atom in crossed electric and magnetic fields. We take the example from reference [54].

The Hamiltonian in atomic units ($e = \hbar = m_e = 1$) for the hydrogen atom in crossed electric and magnetic fields in Cartesian co–ordinates is given by:

$$H \;=\; \tfrac{1}{2}\,(P_1^2 + P_2^2 + P_3^2) - \frac{1}{R} + \left[\frac{\omega_c}{2}\,(x_1\,P_2 - x_2\,P_1) + \frac{\omega_c^2}{8}(x_1^2 + x_2^2) - \sigma x_1\right], \tag{39}$$

where $R = (x_1^2 + x_2^2 + x_3^2)^{1/2}$, ω_c is the cyclotron frequency in atomic units of 2.35×10^5 Tesla and σ is the electric field in atomic units of 5.14×10^{11} V/m. Co–ordinates x_1, x_2 and x_3 are the Cartesian components of the electron's position vector with respect to a reference frame centered at the nucleus of the atom. The moments P_1, P_2 and P_3 refer to the velocities associated to x_1, x_2 and x_3, respectively.

Scaling the co–ordinates by ω_c, that is, $x_i' = \omega_c^{2/3}\,x_i$ and $P_i' = \omega_c^{-1/3}\,P_i$, for $i = 1, 2, 3$, and dropping the primes in order not to complicate the notation, the Hamiltonian becomes:

$$\mathcal{H} = \tfrac{1}{2}\,(P_1^2 + P_2^2 + P_3^2) - \frac{1}{R} + \left[\frac{1}{2}\,(x_1\,P_2 - x_2\,P_1) + \tfrac{1}{8}\,(x_1^2 + x_2^2) - \sigma\,x_1\right],$$

where $\mathcal{H} = \omega_c^{-2/3} H$ is the scaled energy and $\sigma = \omega_c^{-4/3}\,\sigma$ is the scaled electric field. We adopt the experimentally interesting value of $\sigma = 0.58$ in our calculations.

The equilibrium point of interest for the Hamilton vector field must satisfy that the linearization of $\mathcal{H}$ around it is of the type saddle×centre×centre. Thus we select:

$$\mathbf{X}_0 = (x_1, x_2, x_3, P_1, P_2, P_3) = (\sigma^{-1/2}, 0, 0, 0, -\tfrac{1}{2}\sigma^{-1/2}, 0). \tag{40}$$

We translate the fixed point to the origin via the following co–ordinate shift:

$$\hat{x}_1 = x_1 - \sigma^{-1/2}, \quad \hat{x}_2 = x_2, \quad \hat{x}_3 = x_3, \quad \hat{P}_1 = P_1, \quad \hat{P}_2 = P_2 + \tfrac{1}{2}\,\sigma^{-1/2}, \quad \hat{P}_3 = P_3.$$

The new Hamiltonian (that we call again H) is then given by:

$$H \;=\; \tfrac{1}{2}\,(\hat{P}_1^2 + \hat{P}_2^2 + \hat{P}_3^2) - \frac{1}{\mathcal{R}} + \tfrac{1}{2}\,(\hat{x}_1\hat{P}_2 - \hat{x}_2\hat{P}_1) + \tfrac{1}{8}\,(\hat{x}_1^2 + \hat{x}_2^2) - \sigma\,\hat{x}_1 - \sigma^{1/2},$$

where $\mathcal{R} = ((\hat{x}_1 - x_s)^2 + \hat{x}_2^2 + \hat{x}_3^2)^{1/2}$ and $x_s = -\sigma^{-1/2}$. From this point on we drop the hats from the variables with the understanding that our equilibrium point has been translated to the origin.

In order to compute the normal form up to a finite order N we will need the Taylor expansion of the Hamiltonian about the origin up through this order:

$$H' = H + 2\sigma^{\frac{1}{2}} = \sum_{n=2}^{N} H_n, \tag{41}$$

where H_n denotes a homogeneous polynomial in six variables of degree n. We begin by making a Taylor expansion of the term $1/\mathcal{R}$ in the three position variables around the origin up to eighth degree, because the normalization procedure will be pushed up to sixth order, which involves polynomial terms of eighth degree. The terms of the development of $1/\mathcal{R}$ which contribute to the main part of the Hamiltonian are the ones up to second order:

$$\frac{1}{\mathcal{R}} = \sqrt{\sigma} - \sigma\,x_1 + \sigma^{3/2}\,x_1^2 - \tfrac{1}{2}\,\sigma^{3/2}\,(x_2^2 + x_3^2) + \mathcal{O}((x_1^2 + x_2^2 + x_3^2)^{3/2}). \tag{42}$$

Since the origin is an equilibrium point the first order terms of the expansion of the Hamiltonian vanish. The constant term is irrelevant to the dynamics. The first relevant terms are the second order terms, which are:

$$\begin{aligned} H_2 \;=\; & \tfrac{1}{2}\,(P_1^2 + P_2^2 + P_3^2) + \tfrac{1}{2}\,(x_1P_2 - x_2P_1) + \left(\tfrac{1}{8} - \sigma^{3/2}\right)\,x_1^2 + \left(\tfrac{1}{8} + \tfrac{1}{2}\,\sigma^{3/2}\right)\,x_2^2 \\ & + \tfrac{1}{2}\,\sigma^{3/2}\,x_3^2. \end{aligned} \tag{43}$$

6.3 Transformation of the linear part of Hamilton's equations

We now construct a change of variables to reduce the Hamiltonian (43) to its real normal form:

$$H_2 = 2\,\eta\,\tilde{x}_1\,\tilde{P}_1 + \nu_1\,(\tilde{x}_2^2 + \tilde{P}_2^2) + \nu_2\,(\tilde{x}_3^2 + \tilde{P}_3^2), \tag{44}$$

where η, ν_1 and ν_2 are positive constants and due to the choice of parameter we have made, they do not satisfy a resonance condition. We omit the details about we constructed the linear and symplectic transformation are they are quite long. The details are in [54].

Next, in order to obtain the complex normal form associated to (43) we apply the complexifying change:

$$\tilde{x}_1 = q_3,\ \tilde{x}_2 = \frac{q_2 + \imath\, p_2}{\sqrt{2}},\ \tilde{x}_3 = \frac{q_1 + \imath\, p_1}{\sqrt{2}},\ \tilde{P}_1 = p_3,\ \tilde{P}_2 = \frac{\imath\, q_2 + p_2}{\sqrt{2}},\ \tilde{P}_3 = \frac{\imath\, q_1 + p_1}{\sqrt{2}} \tag{45}$$

which leads to the new Hamiltonian:

$$H_2 = \imath\, \omega_1\, q_1\, p_1 + \imath\, \omega_2\, q_2\, p_2 + \mu\, q_3\, p_3, \tag{46}$$

after making the identification $\mu = 2\,\eta$, $\omega_1 = 2\,\nu_2$ and $\omega_2 = 2\,\nu_1$ (note that the reaction co–ordinate is "3" now). Hence, the nonlinear terms included in H_i, $i > 2$ must be transformed adequately following the same steps used to calculate (46).

The next step is the calculation of the normal form. We plan to reach sixth order in the normalization procedure, which means that the normal form will be an eighth–degree polynomial in $\mathbf{q} = (q_1, q_2, q_3)$ and $\mathbf{p} = (p_1, p_2, p_3)$. Therefore we have to calculate terms in the Taylor development of $1/\mathcal{R}$ up to degree eight before normalizing. We start by describing the process we shall perform.

6.4 Transformation to normal form up to order 6

We apply the Lie method to the complexified Hamiltonian $H' = \sum_{i=2}^{8} H_i$ where H_2 is given by (46) and each H_i, $i > 2$ is a homogeneous polynomial of degree i in the complex co–ordinates q and p obtained after expanding $1/\mathcal{R}$ in power series of q_i and p_i. Thus, our plan consists in carrying out the calculations up to polynomials of degree eight, e.g. up to sixth order in the normal form. In this way, we construct a change of co–ordinates from the old ones: $\mathbf{q} = (q_1, q_2, q_3)$ and $\mathbf{p} = (p_1, p_2, p_3)$ to the new ones: $\mathbf{q}' = (q_1', q_2', q_3')$ and $\mathbf{p}' = (p_1', p_2', p_3')$. We drop the primes to avoid tedious notation.

We identify H_2 with $\mathcal{H}_0$ and each H_{i+2} with $\mathcal{H}_i/i!$, $i \leq 6$. Then, we must recall that terms belonging to $\widetilde{\mathcal{H}_i}$ are monomials in p and q of degree $i+2$ with real or complex coefficients c. So, a monomial of degree $i+2$: $m_i = c\, q_1^{j_1}\, q_2^{j_2}\, q_3^{j_3}\, p_1^{k_1}\, p_2^{k_2}\, p_3^{k_3}$ such that $\sum_{l=1}^{3}(j_l + k_l) = i + 2$, belongs to the kernel of $\mathcal{L}_{H_2}$ (and therefore must be incorporated to the new Hamiltonian) if and only if $j_1 = k_1$, $j_2 = k_2$ and $j_3 = k_3$; otherwise its contribution to the new Hamiltonian is zero and the part corresponding to the generating function $\mathcal{W}_i$ becomes $m_i/(\mu\,(k_3 - j_3) +$

$\imath\left(\omega_1\left(k_1-j_1\right)+\omega_2\left(k_2-j_2\right)\right)\big)$. This is the key point in solving the homology equation (6) at each order i.

We rescale the co–ordinates, say $(\mathbf{q}^*,\mathbf{p}^*)\rightarrow\varepsilon\left(\mathbf{q},\mathbf{p}\right)$, to introduce the small parameter ε and adopt then the formulæof Section 2. Afterwards we set $\varepsilon=1$ and drop the stars to simplify our notation further. We call the normal form $K=\sum_{i=2}^{8}K_i$, and in diagonal complex co–ordinates (the transformed ones $\mathbf{q}'$ and $\mathbf{p}'$, that we have renamed $\mathbf{q}$ and $\mathbf{p}$) reads as follows:

$$K(\mathbf{p},\mathbf{q})=\sum_{j,k,l}^{4}a(j,k,l)(p_1q_1)^j(p_2q_2)^k(p_3q_3)^l, \tag{47}$$

with coefficients given by:

$a(1,0,0)$	$1.3292326209360146\,\imath$
$a(0,1,0)$	$1.9630114596221002\,\imath$
$a(0,0,1)$	1.2728995840709765
$a(2,0,0)$	$1.084118969828125 \times 10^{-1}$
$a(0,2,0)$	$6.432737304520157 \times 10^{-2}$
$a(0,0,2)$	$-2.412298516241746 \times 10^{-1}$
$a(1,1,0)$	$3.8502889530602764 \times 10^{-3}$
$a(1,0,1)$	$-5.709272495222898\,\imath \times 10^{-1}$
$a(0,1,1)$	$-4.029118438454696\,\imath \times 10^{-1}$
$a(3,0,0)$	$5.563568366758172\,\imath \times 10^{-3}$
$a(0,3,0)$	$-1.140865632382711\,\imath \times 10^{-3}$
$a(0,0,3)$	$-3.4607990223896906 \times 10^{-2}$
$a(2,1,0)$	$1.84708258092598\,\imath \times 10^{-2}$
$a(2,0,1)$	$-9.804116149675277 \times 10^{-2}$
$a(1,2,0)$	$-5.26869060648934\,\imath \times 10^{-2}$
$a(0,2,1)$	$-2.3139914837113457 \times 10^{-1}$
$a(1,0,2)$	$4.004377334411079\,\imath \times 10^{-2}$
$a(0,1,2)$	$2.76105499066869\,\imath \times 10^{-1}$
$a(1,1,1)$	$-9.949641599540471 \times 10^{-2}$
$a(4,0,0)$	$9.18992415784192 \times 10^{-3}$
$a(0,4,0)$	$3.921799630947499 \times 10^{-3}$
$a(0,0,4)$	$4.005710239128329 \times 10^{-2}$
$a(3,1,0)$	$1.2123807670174411 \times 10^{-2}$
$a(2,2,0)$	$1.1847669375067585 \times 10^{-2}$
$a(1,3,0)$	$2.5741638128707816 \times 10^{-2}$
$a(3,0,1)$	$-1.0660011034295587\,\imath \times 10^{-1}$
$a(2,0,2)$	$-3.307549676029244 \times 10^{-1}$
$a(1,0,3)$	$2.2562472925332147\,\imath \times 10^{-1}$
$a(0,3,1)$	$-6.01563793667196\,\imath \times 10^{-2}$
$a(0,2,2)$	$-1.7149257534732887 \times 10^{-1}$
$a(0,1,3)$	$3.281124863222212\,\imath \times 10^{-1}$
$a(2,1,1)$	$-2.4216727696341944\,\imath \times 10^{-1}$
$a(1,2,1)$	$2.2830888537513132\,\imath \times 10^{-2}$
$a(1,1,2)$	$-4.781394388287208 \times 10^{-1}$

(48)

Each H_i for $2 \leq i \leq 8$ in the last normal form Hamiltonian is a homogeneous polynomial of degree i. The generating function is also a polynomial in $\mathbf{q}$ and $\mathbf{p}$ of degree eight but it is too long to publish. Specifically, $\mathcal{W} = \sum_{i=1}^{6} \mathcal{W}_i/i!$ is written as $W = \sum_{i=3}^{8} W_i$ where each W_i is a homogeneous polynomial in $(\mathbf{q}, \mathbf{p})$ of degree i. Then, W_3 consists of 32 monomials, W_4 consists of 64 monomials, W_5 consists of 136 monomials, W_6 consists of 216 monomials, W_7 consists of 416 monomials and, finally, W_8 consists of 656 monomials.

Once W has been determined, we can calculate the new co–ordinates (or any function of them) as functions of the old ones and vice versa. This will be used later on.

Taking into account the considerations of Section 3.3, we have estimated the global error of the transformation, taking $\|(\hat{\mathbf{x}}, \hat{\mathbf{P}})\| \leq 10^{-2}$ — which is enough for our computation concerning transition state theory — and $\sigma = 0.58$. In the table below we show the error when the transformation is truncated at different orders i with $1 \leq i \leq 6$:

order 1	$7.51681572767062 \times 10^{-7}$
order 2	$7.440374042482777 \times 10^{-9}$
order 3	$1.3601828348825097 \times 10^{-10}$
order 4	$2.2895973941086116 \times 10^{-12}$
order 5	$3.813254946932333 \times 10^{-14}$
order 6	$5.676373185504885 \times 10^{-16}$

Thence, the transformation carried out at order 6 are such that the computations involved reach double precision. Let us note in addition that for the 6th order, each term of the composed series has around 13000 monomials, this is the reason why we omit the expressions here.

6.5 Exact solutions for the trajectories near the transition state

We write the integrals in terms of the real normal form co–ordinates following (45) as follows:

$$J_1 = \tilde{x}_1 \tilde{P}_1 = q_3 p_3, \quad J_2 = \tfrac{1}{2}\left(\tilde{P}_2^2 + \tilde{x}_2^2\right) = \imath q_2 p_2, \quad J_3 = \tfrac{1}{2}\left(\tilde{P}_3^2 + \tilde{x}_3^2\right) = \imath q_1 p_1. \tag{49}$$

Note that the truncated normal form Hamiltonian can be expressed entirely in terms of these integrals, that is, $K = K(J_1, J_2, J_3)$.

Using (49) and the chain rule, Hamilton's equations can be written as follows:

$$\begin{aligned}
\dot{\tilde{x}}_1 &= \frac{\partial K}{\partial \tilde{P}_1} = \frac{\partial K}{\partial J_1}\frac{\partial J_1}{\partial \tilde{P}_1} = \frac{\partial K}{\partial J_1}\tilde{x}_1, \\
\dot{\tilde{P}}_1 &= -\frac{\partial K}{\partial \tilde{x}_1} = -\frac{\partial K}{\partial J_1}\frac{\partial J_1}{\partial \tilde{x}_1} = -\frac{\partial K}{\partial J_1}\tilde{P}_1, \\
\dot{\tilde{x}}_2 &= \frac{\partial K}{\partial \tilde{P}_2} = \frac{\partial K}{\partial J_2}\frac{\partial J_2}{\partial \tilde{P}_2} = \frac{\partial K}{\partial J_2}\tilde{P}_2, \\
\dot{\tilde{P}}_2 &= -\frac{\partial K}{\partial \tilde{x}_2} = -\frac{\partial K}{\partial J_2}\frac{\partial J_2}{\partial \tilde{x}_2} = -\frac{\partial K}{\partial J_2}\tilde{x}_2, \\
\dot{\tilde{x}}_3 &= \frac{\partial K}{\partial \tilde{P}_3} = \frac{\partial K}{\partial J_3}\frac{\partial J_3}{\partial \tilde{P}_3} = \frac{\partial K}{\partial J_3}\tilde{P}_3, \\
\dot{\tilde{P}}_3 &= -\frac{\partial K}{\partial \tilde{x}_3} = -\frac{\partial K}{\partial J_3}\frac{\partial J_3}{\partial \tilde{x}_3} = -\frac{\partial K}{\partial J_3}\tilde{x}_3.
\end{aligned} \tag{50}$$

It is important to note that $\partial K/\partial J_i$, $i = 1, 2, 3$, are constants on trajectories. Hence, once the initial condition of a trajectory is chosen, evolution of the trajectory is given by a linear system whose coefficients are constant, but depend on the trajectory.

This simple form of Hamilton's equations in the normal form co–ordinates near the transition state enables us to construct trajectories having any possible behaviour near the transition state. These trajectories can then be visualized in the original co–ordinates using the transformation constructed in Section 6.6.

6.6 Transformation back to the original co–ordinates

In order to construct the change of co–ordinates back to the original co–ordinates i.e.,

$$(\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{P}_1, \hat{P}_2, \hat{P}_3),$$

we make use of the generating function W. Indeed we simply have to evaluate Poisson brackets but without solving any partial differential equations. Therefore the computational effort is much smaller than the one corresponding to the calculation of the normal form Hamiltonian and the generating function.

With the inverse of the linear change given in (45) the complex formal integrals are transformed into real expressions as functions of $(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \tilde{P}_1, \tilde{P}_2, \tilde{P}_3)$. As a final step we need to perform a new linear change of variables, inverting the matrix C and expressing consequently the three integrals in terms of $(\hat{x}_1, \hat{x}_2, \hat{x}_3, \hat{P}_1, \hat{P}_2, \hat{P}_3)$. We do not display the formulæof these integrals as they are quite long.

Next we build the direct change of co–ordinates $\mathbf{x} = \mathbf{X}(\mathbf{y}; \varepsilon)$ given through formula (7). Notice that in this particular case $\mathbf{x}$ represents $(\mathbf{q}, \mathbf{p})$ and $\mathbf{y}$ stands for $(\mathbf{q}', \mathbf{p}')$ (since we are explicitly discussing the transformation from the final step of the normalization back to the original co–ordinates we have returned the primes to the notation). Alternatively we can compute the change in real co–ordinates. For achieving this we first write W in real variables $(\tilde{\mathbf{x}}', \tilde{\mathbf{P}}') = (\tilde{x}_1', \tilde{x}_2', \tilde{x}_3', \tilde{P}_1', \tilde{P}_2', \tilde{P}_3')$ using the inverse of (45). Thence we calculate $(\tilde{\mathbf{x}}, \tilde{\mathbf{P}}) = (\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \tilde{P}_1, \tilde{P}_2, \tilde{P}_3)$ by means of (7). Note that on this occasion $\mathbf{x}$ in the formula $\mathbf{x} = \mathbf{X}(\mathbf{y}; \varepsilon)$ means $(\tilde{\mathbf{x}}, \tilde{\mathbf{P}})$ whereas $\mathbf{y}$ represents $(\tilde{\mathbf{x}}', \tilde{\mathbf{P}}')$. With this second route $\tilde{x}_1$ is expressed as a function of 913 monomials in $(\tilde{\mathbf{x}}', \tilde{\mathbf{P}}')$, whereas $\tilde{x}_2$ consists of 777 monomials and $\tilde{x}_3$ consists of 679 monomials. The momentum $\tilde{P}_1$ appears as a function of 913 terms in $(\tilde{\mathbf{x}}', \tilde{\mathbf{P}}')$, $\tilde{P}_2$ consists of 796 monomials and finally the formula for $\tilde{P}_3$ consists of 679 monomials in $(\tilde{\mathbf{x}}', \tilde{\mathbf{P}}')$.

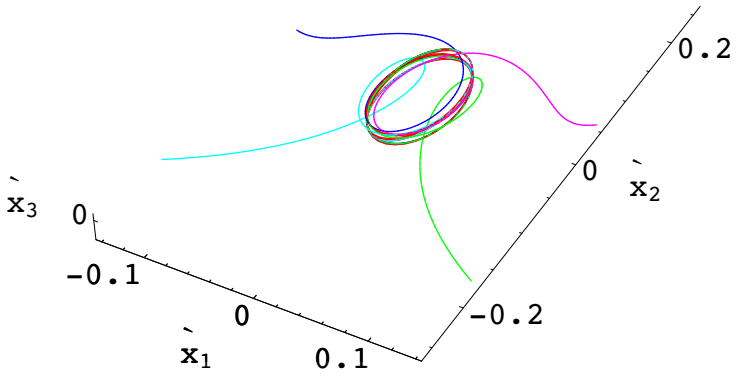

Figure 5: Different projections for trajectories in the NHIM.

6.7 Trajectories near the NHIM for the hydrogen atom in crossed electric and magnetic fields

We now want to show trajectories near the NHIM. We start by computing explicitly the co–ordinates of the NHIM, anmd its manifolds in the original co–ordinates. Notice that, once h is fixed, J_2 and J_3 are given a value, the asymptotic expressions of $\mathcal{M}_h^3$, $W^s\left(\mathcal{M}_h^3\right)$ and $W^u\left(\mathcal{M}_h^3\right)$ as well as the transition state can be now easily obtained, up to $M = 6$, with the direct real change of co–ordinates. Indeed, the NHIM is parametrized in terms of two parameters whereas $W^s\left(\mathcal{M}_h^3\right)$ and $W^u\left(\mathcal{M}_h^3\right)$ need three independent parameters to be properly defined. We remark that we do not use numerical approximations to this high–dimensional structures as Koon *et al.* do [27], more the contrary we have "at hand" the (literal) polynomial expressions of all these objects, up to degree 6.

In the normal form co–ordinates we have that $J_1 = 0$ on the NHIM and on its stable and unstable manifolds. Using (50) we can compute trajectories on the NHIM and on any branch of the stable and unstable manifold that we desire. Then these trajectories can be transformed back into the original co–ordinates. This is shown in Figures 5 and 6. In each figure we take $J_3 = (\tilde{P}_3^2 + \tilde{x}_3^2)/2 = 0.001$ and $J_2 = (\tilde{P}_2^2 + \tilde{x}_2^2)/2 = 0.000953096$. In all of the figures the yellow trajectory is on the NHIM: $\tilde{P}_1 = \tilde{x}_1 = 0$.

The light green is the trajectory on the forward unstable manifold of the NHIM with $\tilde{P}_1 = 0$, $\tilde{x}_1 = 0.00001 \exp\left(1.2728t\right)$. The blue trajectory is on the backward unstable manifold of the NHIM with $\tilde{P}_1 = 0$, $\tilde{x}_1 = -0.00001 \exp\left(1.2728t\right)$.

The dark green trajectory is on the forward stable manifold of the NHIM with $\tilde{P}_1 = 2 \exp\left(-1.2728t\right)$, $\tilde{x}_1 = 0$. The pink trajectory is on the backward stable manifold of the

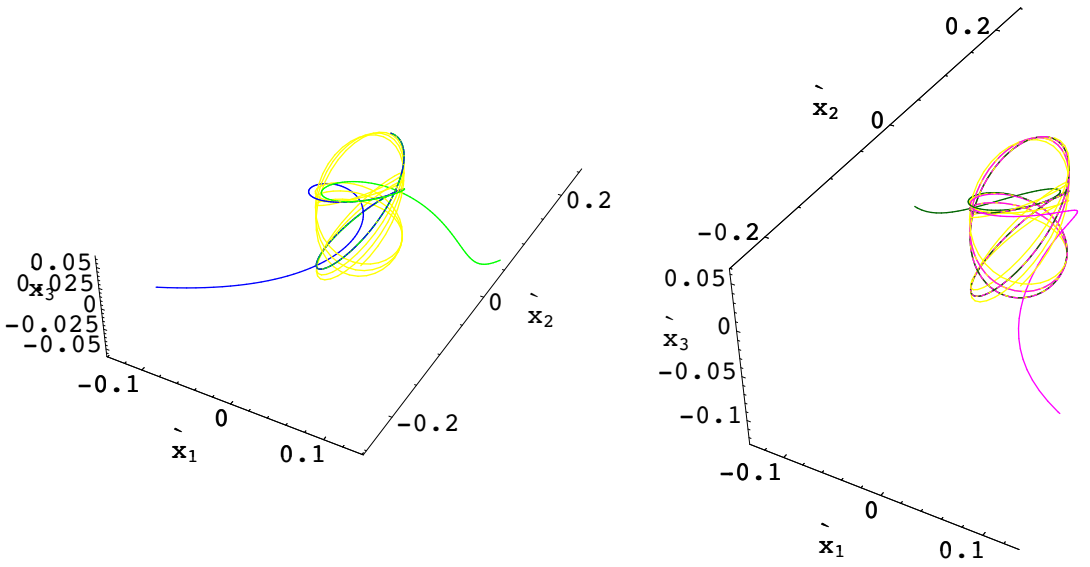

Figure 6: Different projections for trajectories in the NHIM and in the unstable manifold of the NHIM on left and trajectories in the NHIM and in the stable manifold of the NHIM on right.

NHIM with $\tilde{P}_1' = -2\exp(-1.2728t)$, $\tilde{x}_1 = 0$.

We can compute trajectories in either the forward or backward stable and unstable manifolds. These trajectories are simply chosen and computed for the normal form vector field (50). The normal form transformation then allows us to visualize them in the original co–ordinates. In other words, we have complete control and knowledge of the exact dynamical trajectories near the transition state in a 3DOF system. This is the first time this has been demonstrated for a 3DOF chemical or atomic system.

Thus, the solution provided through normal forms, leads naturally to the multidimensional generalization of a saddle "point" and its associated separatrices. Indeed, the approach given in Ref. [54] and here, makes explicit the long–sought classical structures that act as transition states in phase space beyond 2DOF. Indeed, the theory for 2DOF is a classic matter, see for instance [64]. We show that the rigorous way to describe the notion of a "barrier" in phase space is through invariant manifolds.

7 Analysis of the Lorenz system

We apply the theory o the Lorenz system [30] given by:

$$\frac{dx}{dt} = \sigma(y-x), \quad \frac{dy}{dt} = rx - y - xz, \quad \frac{dz}{dt} = xy - bz \tag{51}$$

where σ, b and r are positive parameters and t represents the time variable. Our aim now is to apply the method described in Section 2 to system (51) with the goal of analyzing the Lorenz equations in a vicinity of the origin. Calculations have been done with Mathematica.

7.1 Some invariant sets for $\sigma = 10$, $b = 8/3$ and $r > 1$

We start with the standard values for the parameters given by Lorenz, that is, we fix $\sigma = 10, b = 8/3$ and $r > 1$ (the case $0 < r \leq 1$ must be treated separately). The classical Lorenz system has been widely analyzed (see, for instance the book by Verhulst [56] and references therein) mainly in regards to its chaotic behaviour and the existence of an strange attractor. However, up to our knowledge, no systematic analysis concerning the possible appearance of periodic orbits and other invariant structures has been performed.

Expanding (51) around the origin (which is obviously an equilibrium point) we have that the linear part is given by $A\,\mathbf{x}$ where $\mathbf{x} = (x, y, z)$ and

$$A = \begin{pmatrix} -10 & 10 & 0 \\ r & -1 & 0 \\ 0 & 0 & -8/3 \end{pmatrix},$$

having eigenvalues: $\lambda_{1,2} = \frac{1}{2}\left(-11 \pm \sqrt{81 + 40\,r}\right)$ and $\lambda_3 = -8/3$. Now we make the corresponding (linear) change of variables $\mathbf{x} \to \mathbf{x}'$, so that A becomes diagonal, say A_J, with the eigenvalues in its diagonal. Besides we scale the system, say $\mathbf{x}' \to \varepsilon\,\mathbf{x}''$, so as to introduce a dimensionless small parameter $\varepsilon > 0$.

Clearly, as A_J is a semisimple the application of Theorem 2.1 produces a change of variable $\mathbf{x}'' \to \mathbf{y}$ and a vector field $\mathbf{g}$ for which $A_J\,\mathbf{y}$ is a symmetry up to a certain order $M \geq 1$. Now, some resonant relations among the eigenvalues of A_J must hold in order not to reduce $\mathbf{g}$ to $A_J\,\mathbf{y}$. Letting then $\lambda_{1,2}/\lambda_3 = n \in \mathbf{N}$, r must be equal to $(4\,n - 15)(8\,n - 3)/45$. Hence, it is not hard to prove that the first integrals associated to $A_J\,\mathbf{y}$ are $\varphi_1 = y_1^{-n}\,y_3$ and $\varphi_2 = y_1^{-33/8+n}\,y_2$ from where we deduce that $s = 1$, e.g. we would transform a three–dimensional vector field into a one–dimensional one. We have applied the Normal Form Theorem for polynomial vector fields (see Refs. [32, 13]), e.g. the "standard" polynomial transformation order by order starting at order one. We have reached order 3, i.e. the computations have been carried out up to fourth–degree polynomials in $\mathbf{y}$, obtaining $\mathbf{g}_1 = \mathbf{g}_2 = \mathbf{g}_3 \equiv \mathbf{0}$. It only means that $\mathbf{g}(\mathbf{y};\varepsilon) = A_J\,\mathbf{y} + \mathcal{O}(\varepsilon^4)$ but we have not pushed the computations further.

Alternatively we apply Theorem 2.2 with adequate matrix T such that $A_J\,T = T\,A_J$. Since $r > 1$ the eigenvalues are all different, thence we deduce that T must be diagonal, i.e. $T = \mathrm{diag}\,\{t_1, t_2, t_3\}$ with $t_i \in \mathbf{R}$ arbitrary. It immediately implies that there are no periodic

orbits of the Lorenz equation for the specific values of σ and b given above, at least periodic orbits close to the origin. However, different choices of t_i lead to different generalized normal forms and consequently, to different invariant sets.

For example, taking $t_3 \equiv t_2 \equiv t_1/2$ and $t_1 \in \mathbf{R}$ we have that the computation of the normal form carries out the change of variables: $\mathbf{x}'' \equiv (x, y, z) \rightarrow \mathbf{y} \equiv (x', y', z')$. The expression for the transformed system can be see in Refs. [48, 49]. Now, the reduction goes as follows. The first integrals are $\varphi_1 = y'/\sqrt{x'}$, $\varphi_2 = z'/\sqrt{x'}$ whereas the co–ordinate in G_T is $\vartheta = x'$. Now, the reduced system is defined on $\mathbf{R}^2$ as:

$$\begin{aligned}
\dot{\varphi_1} &= (12\,r)^{-1}\,\left(54\,\varphi_1\,\varphi_2 + 3\,\left(9+\sqrt{81+40\,r}\right)\,{\varphi_1}^2 - 3\,\left(-9+\sqrt{81+40\,r}\right)\,{\varphi_2}^2\right.\\
&\qquad \left. -2\,r\,\left(25+3\,\sqrt{81+40\,r}\right)\right)\,\varphi_1,\\
\dot{\varphi_2} &= (12\,r)^{-1}\,\left(54\,\varphi_1\,\varphi_2 + 3\,\left(9+\sqrt{81+40\,r}\right)\,{\varphi_1}^2 - 3\,\left(-9+\sqrt{81+40\,r}\right)\,{\varphi_2}^2\right.\\
&\qquad \left. +2\,r\,\left(-25+3\,\sqrt{81+40\,r}\right)\right)\,\varphi_2.
\end{aligned}$$

The corresponding equilibria are:

$$(0,0),\ \left(\pm\frac{\sqrt{9+60\,r-\sqrt{81+40\,r}}}{\sqrt{30}},0\right),\ \left(0,\pm\frac{\sqrt{9+60\,r+\sqrt{81+40\,r}}}{\sqrt{30}}\right).$$

By means of the direct Lie transformation we calculate the invariant manifold and the result is depicted in Figure 7. Next we are going to calculate the stable manifold associated to $\mathbf{0}$. As A (or A_J) has two negative eigenvalues and one positive, the dimension of the stable manifold is two. We then take $T = \mathrm{diag}\,\{0, 0, 1\}$ and apply the generalized normal form transformation to the Lorenz system. The normal form has been calculated to third order, see also [48].

This time the reduction achieves the computation of the differential system in the stable manifold. According to the choice of T we have $\varphi_1 = y_1$, $\varphi_2 = y_2$ and $\vartheta = y_3$. The reduced system is defined on $\mathbf{R}^2$, and is given by:

$$\begin{aligned}
\dot{\varphi_1} &= -\frac{8}{3}\,\varphi_1 - \frac{9+\sqrt{81+40\,r}}{2\,r}\,{\varphi_2}^2\\
&\qquad -\frac{27\,\left(3\,\left(81+40\,r\right)\,\left(57+58\,r\right)+\sqrt{81+40\,r}\,\left(1539+2\,r\,\left(973+360\,r\right)\right)\right)}{50\,r^2\,\left(81+40\,r\right)\,\left(133+72\,r\right)}\,\varphi_1\,{\varphi_2}^2,\\
\dot{\varphi_2} &= -\tfrac{1}{2}\,\left(81+40\,r\right)^{-1/2}\,\left(133+72\,r\right)^{-1}\,\left(\left(10773-2660\,\varphi_1-360\,{\varphi_1}^2+11152\,r\right.\right.\\
&\qquad \left.\left. -1440\,\varphi_1\,r+2880\,r^2+\left(1463+792\,r\right)\,\sqrt{81+40\,r}\right)\right)\,\varphi_2.
\end{aligned}$$

By means of the direct Lie transformation we calculate the two–dimensional stable manifold of the origin, as it appears in Figures 8 and 9 for different values of r.

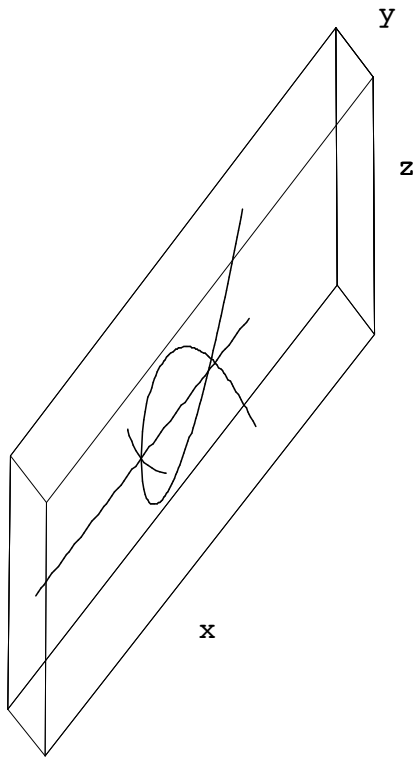

Figure 7: Invariant sets of the origin in the Lorenz system related to $T = \mathrm{diag}\,\{t_1, t_1/2, t_1/2\}$.

In Ref. [42] we proposed a transformation with the aim of integrating analytically the reduced equations, inverting back the transformation and resolving an initial value problem for equation (51), with $r = 28$, i.e. its classic value and adequate initial conditions. For achieving this we take $T = \mathrm{diag}\,\{1, \sqrt{2}, 0\}$, thus $A_J\,T = T\,A_J$. Besides $s = r = 1$ and the invariant $\varphi = y_3$ and $\vartheta_1 = y_1$ and $\vartheta_2 = y_2$. Note that the key point to obtain only one invariant (and consequently transforming the initial system to a simpler one) is the non–resonant conditions among the entries of T. After computing the normal form up order three, we pass to the reduced equations, yielding that:

$$\dot{\varphi} \;=\; \tfrac{1}{2}\,(-11 + \sqrt{1201})\,\varphi + \frac{15\,(1201 - 1689\,\sqrt{1201})}{134512\,(25 + 3\,\sqrt{1201})}\,\varphi^3, \tag{52}$$

and

$$\begin{aligned} \dot{\vartheta}_1 \;&=\; \frac{\left(-9 + \sqrt{1201}\right)}{56}\,\varphi^2 - \frac{\left(238268911748107 + 3427671328157\,\sqrt{1201}\right)}{3389702400\,\left(32622739 + 543621\,\sqrt{1201}\right)}\,\varphi^4 - \tfrac{8}{3}\,\vartheta_1, \\ \dot{\vartheta}_2 \;&=\; \frac{3\,\left(1893759619 - 24165531\,\sqrt{1201}\right)}{10117320080\,\left(25 + 3\,\sqrt{1201}\right)}\,\varphi^3 - \frac{\left(11 + \sqrt{1201}\right)}{2}\,\vartheta_2. \end{aligned} \tag{53}$$

The solutions of (52) and (53) can be obtained straightforwardly as φ is firstly written explicitly as a function of time. Then, this expression of φ is inserted in the linear (and

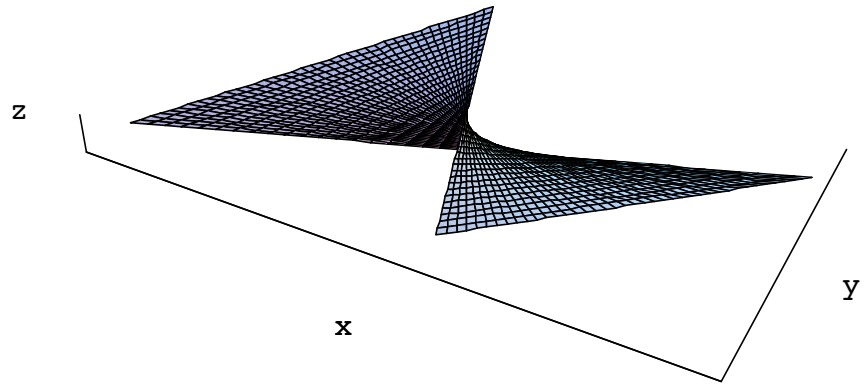

Figure 8: Local stable manifold of the origin for $r = 1.32$.

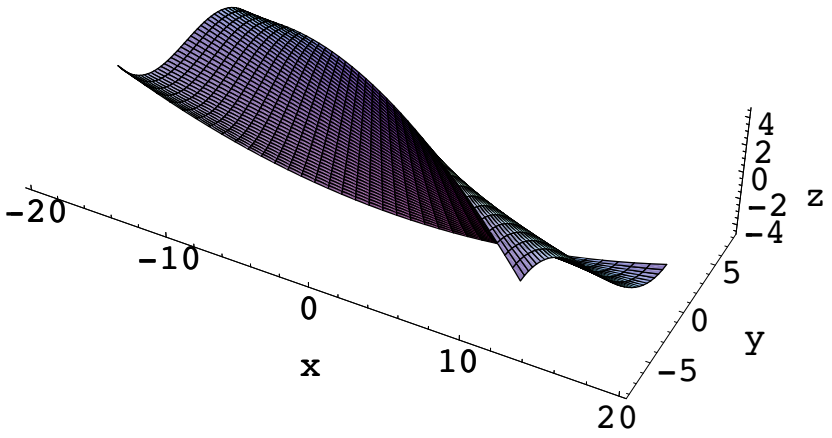

Figure 9: Local stable manifold of the origin for $r = 3.205189$.

separate) equations (53) getting expressions of ϑ_1 and ϑ_2 in terms of t. The process ends going back to the original variables by means of the inverse Lie transformation, obtaining therefore analytic expressions of $x(t)$, $y(t)$ and $z(t)$. See the entire calculations in [42].

7.2 Some periodic orbits for other values of σ, b and r

As we have not found out periodic orbits for $\sigma = 10$ and $b = 8/3$, we are going to treat σ, b and r as positive constants and look for possible relations among the three parameters so as to get some closed trajectories. Furthermore we also assume that $b > 1$ and $r > 1$. The canonical Jordan form of A is

$$A_J = \operatorname{diag}\left\{-b\,,\,\tfrac{1}{2}\left(-1-\sigma-\sqrt{(1-\sigma)^2+4\,r\,\sigma}\right)\,,\,\tfrac{1}{2}\left(-1-\sigma+\sqrt{(1-\sigma)^2+4\,r\,\sigma}\right)\right\}.$$

The first step is to determine whether T_1, T_2 and T_3 can be candidates to perform normal forms. We then have to discard T_2, but T_1 and T_3 commute with A_J if and only if $\sigma(b) =$

$b(b-1)/(b+r-1)$.

Now, in order not to have a trivial first order normal form and therefore, in order to search for periodic orbits, we make the identification $r(b) = (1+\sqrt{2})\,(b-1)^2/(1+\sqrt{2}+b)$. Replacing now this value of r in the condition for σ of the latter paragraph we obtain that $\sigma(b) = (1+\sqrt{2}+b)/(2+\sqrt{2})$. Note that both $\sigma(b)$ and $r(b)$ are positive if $b > 1$. Moreover, $r(b) > 1$ if and only if $b > 1+\sqrt{2}$. We have pushed the computations up to second order (homogeneous polynomial vector fields of degree three) finding out that $\mathbf{g}_2$ vanishes. We do not write the explicit expressions of the normal form and the reduced system in $\varphi_1 = y_1^2+y_2^2$, $\varphi_2 = y_3$, however we present the three equilibria of the reduced system:

$$(0,0), \quad \left(0, \pm\frac{\sqrt{b-1}\,\sqrt{b}\,\sqrt{34+2\,b\,(5\,b-19)+\sqrt{2}\,(24+b\,(7\,b-27))}}{1+\sqrt{2}+b}\right). \tag{54}$$

Now the periodic orbits of the initial Lorenz system are calculated passing from the invariants to the variable $\mathbf{y}$. Note that, apart from the origin, the two other equilibria have co–ordinate $\varphi_1 = 0$, or, in other words, they are closed trajectories with a small radius $\mathcal{O}(\varepsilon^3)$. Next, using the direct Lie transformation, we express everything in terms of $\mathbf{x}''$ and, finally, the original variable $\mathbf{x}$ are recovered with the (inverse) linear change used to introduce the canonical Jordan form of A. According to (54), it is not difficult to deduce that when $b > 1+\sqrt{2}$ there are always three equilibria (three quasi–periodic orbits of the initial system), two of them being stable and one unstable. This situation is maintained for all $b > 1+\sqrt{2}$. Similar results are obtained from the normal form constructed with the aid of T_3.

Finally, concerning the estimation of the global error of the computations carried out in this section, since the asymptotic change of variables has been performed up to order three, if we choose $\varepsilon = 10^{-2}$ and $\|\mathbf{x}\| \leq 0.1$, then the global error is $E(\mathbf{x}) \leq 1.33969 \times 10^{-7}$, which is valid on a time–scale $t \approx 100$. More details about the treatment of the error appear in [42].

8 Concluding remarks

The present paper establishes a methodology to analyze an autonomous ODE from a qualitative point of view. More specifically we have given some techniques to calculate different invariant sets for dynamical systems of Hamiltonian and dissipative character.

In fact, our technique carries out a reduction in the dimension of the departure system by means of the introduction of a symmetry through the change of variable. Then, we take advantage of this reducibility with the goal of extracting from the simpler systems qualitative information (about stability and possible bifurcations, existence of periodic orbits or chaotic regions in phase space, calculation of formal integrals of Hamilton functions, analysis of

possible chemical reactions, construction of seminumerical schemes to integrate some ODEs, etc.) valuable for the original equation.

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