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INTEGRABLE APPROXIMATIONS OF DISCRETE DYNAMICAL SYSTEMS: CLASSICAL AND QUANTUM ASPECTS

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*Aos meus pais, $\frac{1}{2} [(Lúcia e Mauro) + (Mauro e Lúcia)]$,
pelos exemplos e contraexemplos.*

**Grau, teurer Freund, ist alle Theorie,
Und grün des Lebens goldner Baum.**

[Cinzenta, querido amigo, é toda teoria,
E verdejante a áurea árvore da vida.]

Johann W. von Goethe em *Fausto*, vol. 1.

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¹Estou falando de chimarrão!

Abstract

We have obtained Hamiltonians that approximate the orbits of a special class of discrete chaotic maps near all fixed points simultaneously, as long as these fixed points do not bifurcate. The Hamiltonians (or *integrable approximations*, as we will often call them) were obtained using two different procedures: a quantum one (based on the Baker-Hausdorff-Campbell expansion) and a classical one (based on center functions). Such integrable approximations were also shown to be the classical limit of a quantum Hamiltonian, where the commutator deformed into the Poisson bracket. The role of the integrable approximation as an element of the Lie algebras generated by operators and classical Hamiltonians is also discussed.

Resumo

Neste trabalho obtivemos hamiltonianos (aos quais nos referiremos muitas vezes como *aproximações integráveis*) que aproximam as órbitas de uma classe de mapas caóticos discretos em vizinhanças de todos os seus pontos fixos simultaneamente. Utilizamos para isso dois procedimentos distintos: um quântico (baseado na expansão de Baker-Hausdorff-Campbell) e um clássico (baseado nas funções de centro). Mostramos também que tais aproximações integráveis emergem como o limite clássico de hamiltonianos quânticos, com o comutador deformando-se no colchete de Poisson. É discutido também o papel das aproximações integráveis como um elemento da algebra de Lie gerada tanto por operadores quanto por hamiltonianos clássicos.

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Chapter 1

Introduction

This dissertation deals a lot with Classical Mechanics. Although we delve into Quantum Mechanics in the last chapter, many of the methods and objectives in it are stated and based on the formalism of Symplectic and Hamiltonian Geometry. We introduce here the essential language and notation that will be used in the following chapters and present the problems studied.

1.1 Dynamical Systems and Geometry

Classical Mechanics is the study of movement and equilibrium of systems composed by *not a lot* of bodies. The “not a lot” stands for the fact that it does not deal with statistical methods, in general. The main problem of Mechanics is to be able to predict the behavior of a system, something that is usually impossible. In Classical Mechanics *predict* usually means solving equations of motion, which are almost always unsolvable. Precise and sophisticated methods of approximation, however, have been developed throughout history. No matter what the method be, it will be based in one of the four main formalisms of Mechanics:

1. the Newtonian, which uses the cumbersome yet easily stated language of vectors

in $\mathbb{R}^3$;

2. the Lagrangian, which counts with a more abstract, yet less geometrical formulation using generalized coordinates on differentiable manifolds and their tangent bundles;
3. the Hamiltonian, where the tangent bundle is replaced by the cotangent one and geometrical meaning is again recovered;
4. the Hamilton-Jacobi, which in its turn forgets about finding solutions to equations of motion and focuses instead on finding special coordinate changes that, by simplifying eventual solutions, end up solving the problem indirectly.

The method used here will be mostly the Hamiltonian one. Vectors will be represented by simple characters (like a) without any sort of arrow over them, since we will not always be dealing with arrow spaces as in Newtonian Mechanics. Components of vectors will be written with a subindex no matter if they are raw vectors or 1-forms, since because we will only deal with finite dimensional vector spaces the base space and the dual are isomorphic [1]. Thus, if q is an element of an n -dimensional vector space, then $q = (q_1, q_2, \dots, q_n)$.

All previously mentioned methods have, of course, a fundamental set of equations that, if solved, tells us how to predict what will happen to a system as a function of a parameter (usually *time*). It is known since the times of Newton that an extremely small number of problems can be exactly solved in Nature, and most development in Mechanics is now focused in obtaining useful conclusions that do not depend on solving those fundamental equations. In Hamiltonian Mechanics these are *Hamilton's equations*

$$\begin{cases} \dot{q} &= \frac{\partial H(q,p;t)}{\partial p} \\ \dot{p} &= -\frac{\partial H(q,p;t)}{\partial q}, \end{cases} \quad (1.1)$$

where $\dot{q} = (\dot{q}_1, \dot{q}_2, \dots)$, $\dot{p} = (\dot{p}_1, \dot{p}_2, \dots)$ and

$$\frac{\partial H(q,p;t)}{\partial p} = \left(\frac{\partial H(q,p;t)}{\partial p_1}, \frac{\partial H(q,p;t)}{\partial p_2}, \dots \right), \quad (1.2)$$

$$\frac{\partial H(q,p;t)}{\partial q} = \left(\frac{\partial H(q,p;t)}{\partial q_1}, \frac{\partial H(q,p;t)}{\partial q_2}, \dots \right). \quad (1.3)$$

By defining $x \equiv (q_1, q_2, \dots, p_1, p_2, \dots)$ and

$$\frac{\partial}{\partial x} \equiv \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \dots, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \dots \right) \quad (1.4)$$

equations (1.1) can be further simplified and written in the compact form

$$\dot{x} = \mathcal{J} \left(\frac{\partial H(x;t)}{\partial x} \right), \quad (1.5)$$

where

$$\mathcal{J} \equiv \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}. \quad (1.6)$$

The function H is called the *Hamiltonian* and is strictly connected to the total energy of a system if its dependence on t is implicit: it is the sum of kinetic and potential energies¹. What equations (1.1) say is that each Hamiltonian function gives rise to a

¹If the Hamiltonian for the system is an explicit function of time then such analogies are no longer evident. See [2] for a presentation of the problem. In this dissertation we will only deal with autonomous Hamiltonians, that is, Hamiltonians whose dependence on t is implicit.

vector field in the cotangent bundle T^*M : first you specify a point $q \in M$, where M is a manifold (the *generalized position*), and then associate to it a 1-form $p \in T_q^*M$ (the *generalized momentum*). Such vector fields that are generated by a function give rise to what are called *Hamiltonian dynamical systems*. Obviously not all dynamical systems are Hamiltonian, but if they are, it can be proved that their flux is not only composed by diffeomorphisms, but by canonical transformations [3]. This last sentence will be addressed in the next paragraph.

A *symplectic manifold* is a pair (M, ω) of a manifold M together with a 2-form $\omega_c : T_cM \times T_cM \rightarrow \mathbb{R}$ at $c \in M$ such that $\ker \omega = \{0\}$ and $d\omega = 0$. From the closedness and antisymmetry of ω it is possible to prove that (see section 2.1)

$$\omega(x, y) = x^T \mathcal{J} y \quad , \quad x, y \in T_cM; \quad (1.7)$$

hence the important role played by $\mathcal{J}$. Also, the non-degeneracy of ω forces the dimension of M to be even [4]. If there is a linear function $f : M_1 \rightarrow M_2$ between two symplectic manifolds (M_1, ω_1) and (M_2, ω_2) such that $f^*\omega_2 = \omega_1$, then M_1 and M_2 are said to be *symplectomorphic* and f is called a *symplectomorphism*. If f is not linear, but still pullsback ω_2 into ω_1 , then it is called a *canonical transformation*.

The cotangent bundle of any $2n$ -dimensional manifold has a natural symplectic form given by (for a proof see [5])

$$\omega = \sum_{i=1}^n dq_i \wedge dp_i, \quad (1.8)$$

where $\wedge$ is the wedge product and q and p are the generalized position and momentum. If we pick a coordinate system such that the wedge product in equation (1.8) produces a

symplectic 2-form, we call it a *Darboux coordinate system*. In this work we will deal only with prototype symplectic manifolds, which are $(\mathbb{R}^{2n}, \omega)$, where $\omega = \sum_i^n dq_i \wedge dp_i$ and $\{q_1, \dots, q_n, p_1, \dots, p_n\}$ form a basis in $\mathbb{R}^{2n}$. In this way our manifold is parametrized by a single chart and we avoid the excessive use of differential geometry, but at the same time this is actually not a dramatic loss of generality: unlike Riemannian manifolds, an important theorem by Darboux states that all symplectic manifolds of the same dimension are locally symplectomorphic [4] (there is no equivalent of torsion in Symplectic Geometry). In this way, instead of compromising clarity by dealing with local coordinate systems centered at points, our coordinates will be seen as points themselves in $\mathbb{R}^{2n}$ (which will also be our prototype tangent and cotangent spaces centered at 0).

1.2 Fluxes, Maps and Normal Forms

Solutions to equation (1.5) are said to be *fluxes of H* , where H is the Hamiltonian. Those are a one parameter group of diffeomorphisms $\rho : M \times \mathbb{R} \rightarrow M$ such that at each point in M their image is tangent to the vector field generated by H . As not all vector fields are Hamiltonian, ρ is a much more general tool in the study of group actions over manifolds, since every class C^n vector field on M has an associated class C^n flux [6] (at least in compact manifolds or compact subsets of $\mathbb{R}$). However, the vast majority of Physics is built upon Hamiltonian Systems, even if non-autonomous. The reason for this is the mathematical fact that for any class C^2 autonomous Hamiltonian

$$\frac{dH(q, p; t)}{dt} = \frac{\partial H}{\partial q} \frac{dq}{dt} + \frac{\partial H}{\partial p} \frac{dp}{dt} + \frac{\partial H}{\partial t} \quad (1.9)$$

$$= 0, \quad (1.10)$$

enabling us to identify the Hamiltonian function as the total energy of an autonomous system, which must be conserved both in classical and quantum closed sys-

tems. The dynamical system associated to H is then defined as the triple (M, ω, ρ) , which is nothing but a symplectic manifold together with a Hamiltonian flux on it. It can be proved that every Hamiltonian flux is a canonical transformation [3]: $\rho_t^* \omega = \omega$ ($\forall t \in \mathbb{R}$), and it is easy to see that every canonical transformation is conservative. This means that all Hamiltonian dynamical systems are ergodic with respect to the usual Liouville (Lebesgue) measure.

Apart from *continuous* dynamical systems it is also possible to form discrete ones. To do this, we simply change ρ by some discrete mapping on M . Some maps show very desirable properties, being *conservative* or *symplectic* (preseving ω), and in the next chapter we shall come back to this in a more thorough way.

Methods for associating continuous and discrete dynamical systems exist since the 19th century, the most famous one being the *Poincaré map* of a periodic continuous system. Roughly, to obtain the Poincaré map all we have to do is to define a surface that perpendicularly crosses the image of ρ and reduce our study to the discrete mapping induced by the crossings of this surface (see figure 1.1). In this way the dimension can be reduced by one, which shows why Poincaré maps are so important: any system with 2 degrees of freedom, impossible to visualize in phase space, can be studied through its perfectly drawable three dimensional Poincaré map. For more information about Poincaré maps and proofs, see [7].

Our connection between discrete and continuous systems is very different in nature from the Poincaré map. We investigated a way to approximate the iterations of a discrete map by a continuous system. The advantage of doing so can be stated after the presentation of the concept of *normal form*, which is a strategy for simplifying a dynamical system. When dealing with Hamiltonian systems the method of *Birkhoff*

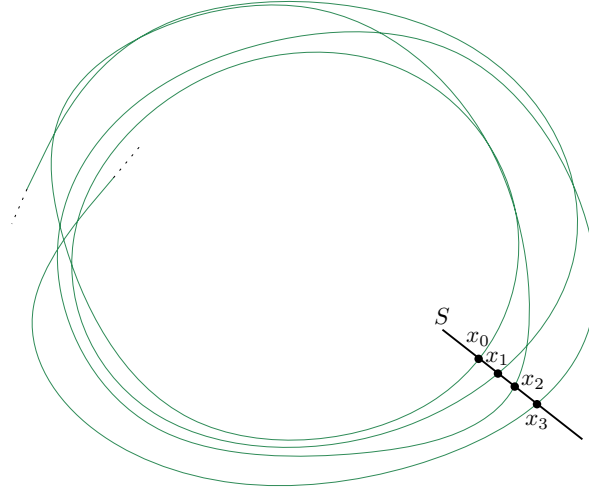


Figure 1.1: Example of a Poincaré map. The flux is presented in green and the Poincaré surface S in black. The first four crossings are depicted. The Poincaré map for this problem would be a discrete mapping $T : S \rightarrow S$ such that $x_0 = T^{-1}(x_1) = T^{-2}(x_2) = T^{-3}(x_3) = T^{-4}(x_4) = \dots$.

normal forms is based in Hamilton-Jacobi theory and it involves expanding a Hamiltonian in a series and developing strategies to eliminate as many terms from it as possible. It is roughly the act of solving the Hamilton-Jacobi equation by force. The result is a coordinate change that will bring the Hamiltonian to a simpler form in which its properties are more easily studied. The coordinate change itself can also present many important informations regarding the system, as is typical in Hamilton-Jacobi theory. For discrete systems, however, there is generally no globally defined generating function such as the Hamiltonian to be studied, which makes the implementation of the method much more difficult (although local generating functions always exist [4]). The following question then arises: is it possible to find an integrable approximation to a discrete mapping?, that is, is it possible to approximate a discrete system by a Hamiltonian one, even if only in a neighborhood of its fixed points? The method of normal forms for discrete systems works in the neighborhood of a single fixed point only, which implies that an integrable approximation that takes into account all fixed points is already likely to be useful in applications.

We start by developing a strategy to obtain maps from a special class of Hamiltonians. Our approximations will be restricted to this class of maps, which we call *separable*.

1.3 Obtaining Maps from Hamiltonians

Consider the separable autonomous Hamiltonian

$$H : \mathbb{R}^{2n} \rightarrow \mathbb{R} \quad (1.11)$$

$$(q, p) \mapsto H(q, p) \quad (1.12)$$

$$= F(p) + V(q) \quad , \quad F, V \text{ class } C^\infty, \quad (1.13)$$

with associated vector field given by Hamilton's equations:

$$\begin{cases} \dot{q} &= F'(p) \\ \dot{p} &= -V'(q), \end{cases} \quad (1.14)$$

which is a compact way of writing

$$\begin{cases} \dot{q} &= \frac{\partial F(p)}{\partial p} \\ \dot{p} &= -\frac{\partial V(q)}{\partial q} \end{cases} \iff \begin{cases} (\dot{q}_1, \dot{q}_2, \dots) &= \left(\frac{\partial F(p_1, p_2, \dots)}{\partial p_1}, \frac{\partial F(p_1, p_2, \dots)}{\partial p_2}, \dots \right) \\ (\dot{p}_1, \dot{p}_2, \dots) &= -\left(\frac{\partial V(q_1, q_2, \dots)}{\partial q_1}, \frac{\partial V(q_1, q_2, \dots)}{\partial q_2}, \dots \right) \end{cases} . \quad (1.15)$$

The resultant flow associated to this field will be, of course, continuous. We would like to obtain a discrete mapping from this continuous one, in a way that it approximates the integral curves of the continuous Hamiltonian system for a small parameter. This means that the flux generated by the Hamiltonian would be an *integrable approximation* for this discrete mapping in a small parameter regime. To start off we can write the derivatives on the left hand side in explicit form,

$$\lim_{\alpha \rightarrow 0} \left[\frac{q(t + \alpha) - q(t)}{\alpha} \right] = F'(p) \quad (1.16)$$

$$\lim_{\alpha \rightarrow 0} \left[\frac{p(t + \alpha) - p(t)}{\alpha} \right] = -V'(q); \quad (1.17)$$

now, let us define

$$Q(t, \alpha) \equiv q(t + \alpha) \quad (1.18)$$

$$P(t, \alpha) \equiv p(t + \alpha) \quad (1.19)$$

and let us simply *ignore* the limits in α . After a simple algebraic manipulation we have, for $\alpha \ll 1$,

$$Q(t, \alpha) \approx q(t) + \alpha F'(p) \quad (1.20)$$

$$P(t, \alpha) \approx p(t) - \alpha V'(q), \quad (1.21)$$

that is,

$$\begin{pmatrix} Q \\ P \end{pmatrix} \approx \begin{pmatrix} q \\ p \end{pmatrix} + \alpha \mathcal{J} \begin{pmatrix} F'(p) \\ V'(q) \end{pmatrix}. \quad (1.22)$$

Written in this way it is easy to see this transformation is *infinitesimal*, that is, it approaches the identity transformation when $\alpha \ll 1$. Now, as mentioned before, all autonomous Hamiltonian systems generate conservative fluxes, but the map in equation (1.22) is conservative iff

$$\det \begin{pmatrix} 1 & \alpha F''(p) \\ -\alpha V''(q) & 1 \end{pmatrix} = 1 \quad (1.23)$$

$$\Longleftrightarrow \alpha^2 F''(p)V''(q) = 0, \quad (1.24)$$

which is not at all a general condition since it forces $\alpha = 0$ or works only for linear Hamiltonians. In order to map *any* Hamiltonian of the form (1.13) to a conservative mapping we thus *separate* the action of each of its terms: first, the system is subject to $F(p)$, and latter to $V(q)$. This, using equations (1.22), leads to a discretization of the flux of (1.13) for small α , now taken as composed by the two systems bellow:

$$\begin{cases} Q &= q + \alpha F'(p) \\ P &= p \end{cases}, \quad \begin{cases} \bar{Q} &= Q \\ \bar{P} &= P - \alpha V'(q) \Big|_{q=Q} \end{cases}. \quad (1.25)$$

This composition of mappings solves the problem of conservation of measure, since both steps are immediately seen to be conservative and by the properties of the determinant the composition of any two conservative mappings is obviously conservative.

For small values of α , the orbits of the map in equations (1.25) must, therefore, approximate the integral curves of $H(q, p)$, but for larger values we expect different behavior since the larger the value of α the worse is the approximation given by equation (1.22). To illustrate what's being said let us analyze some 1-dimensional examples that will be studied throughout this whole dissertation.

1.3.1 Example: the Duffing Equation

The undamped and unforced Duffing Hamiltonian is given by

$$H(q, p) = \frac{p^2}{2} + \frac{\beta q^2}{2} + \frac{\gamma q^4}{4}. \quad (1.26)$$

This Hamiltonian, as all the one degree of freedom ones, *cannot* be chaotic [3].

Since H presents the same form as (1.13) we can fix $\beta = \gamma = 1$ and use equations (1.25) to derive from it the discrete mapping:

$$\begin{cases} Q &= q + \alpha p \\ P &= p \end{cases}, \quad \begin{cases} \bar{Q} &= Q \\ \bar{P} &= P - \alpha(Q + Q^3) \end{cases} \quad (1.27)$$

The level curves of (1.26) near its elliptic equilibrium point and the iterations of the map (1.27) for a small value of α are displayed in figure 1.2.

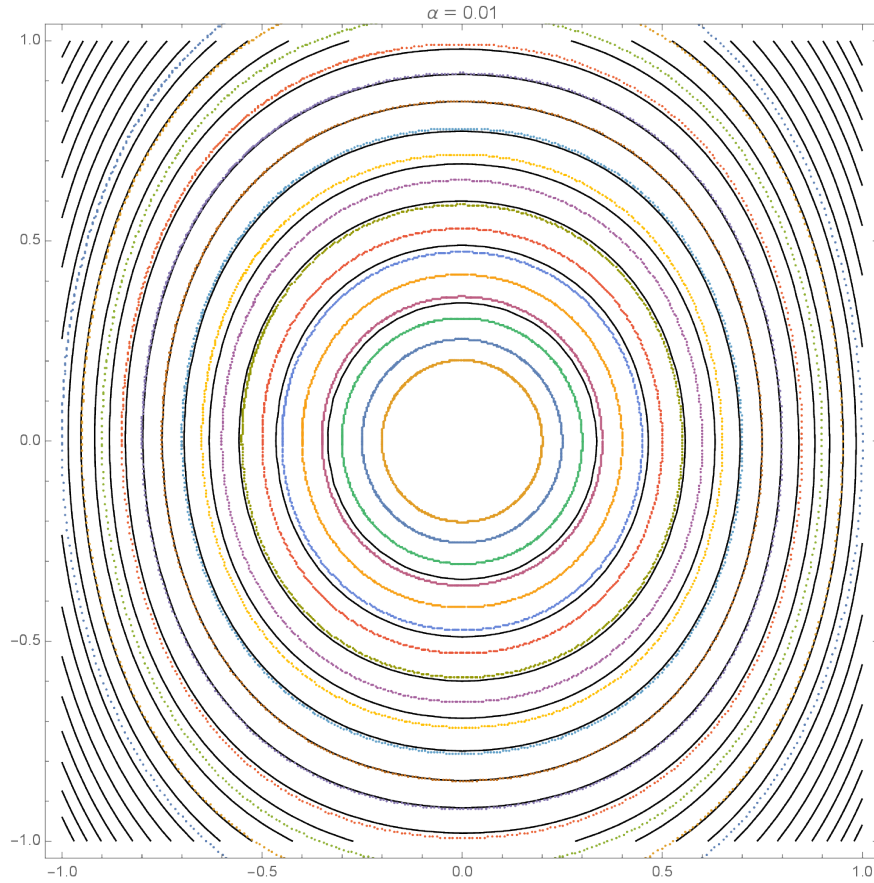


Figure 1.2: Level curves (that is, non-oriented *flux*) of the Duffing Hamiltonian (black) and 3.000 iterations of the derived map for $\alpha = 0.01$ (colored). Each color represents the map's orbit for the same initial point.

However, we can check that for some values of α the double iterations of (1.27) have more than one root. This means that the map obtained from the Hamiltonian now presents a much more complicated behavior than its predecessor: bifurcations. It is well-known that maps can present chaotic behavior in any dimension, and we have thus found a way of obtaining a chaotic map from a one dimensional Hamiltonian. General conditions for chaos will not be studied, but the presence of a homoclinic orbit in $H(q, p)$ is sufficient [8] (but, as the Duffing example shows, not essential). The behavior of the map for some large α s is shown in figure 1.3.

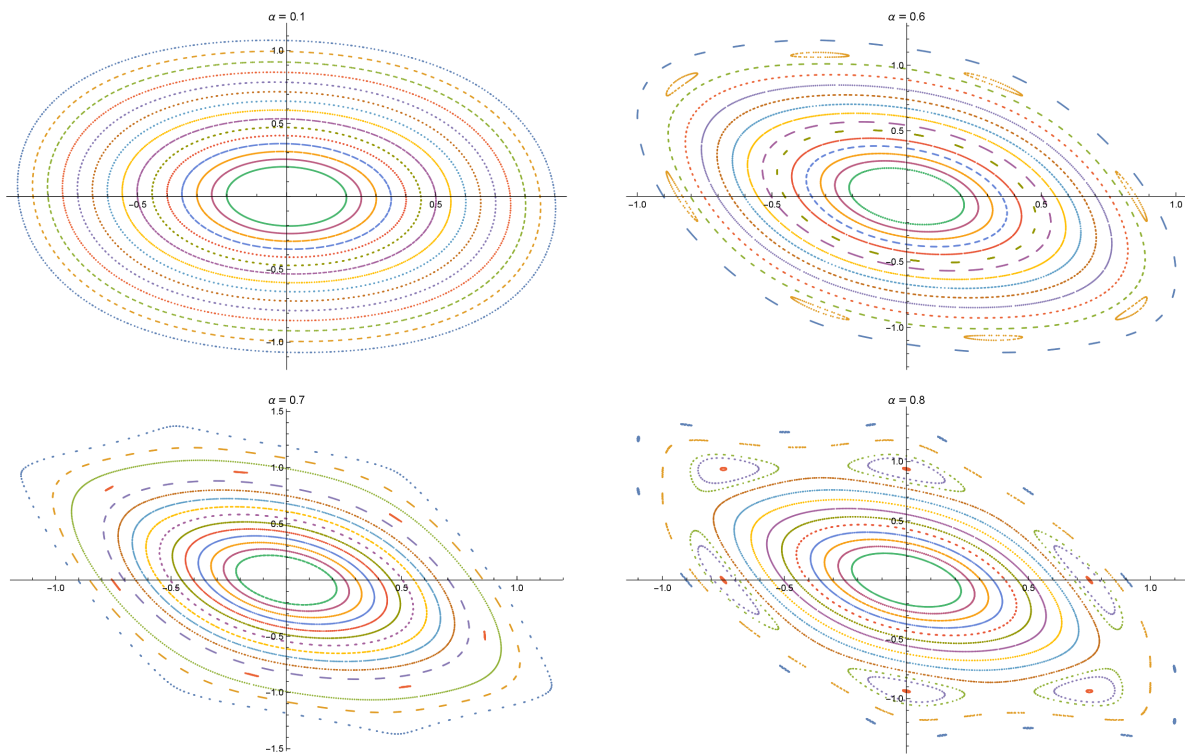


Figure 1.3: Orbits of (1.27) for different values of α show that bifurcations occur.

1.3.2 Example: the Hénon Map

The map given by

$$\begin{cases} Q = 1 - aq^2 + p \\ P = bq \end{cases} \quad (1.28)$$

has been proven to be topologically equivalent to all quadratic maps with a hyperbolic fixed point at the origin [9]. Such a map does not arise from a generating function, but because of its aforementioned generality we can easily find a quadratic symplectic mapping whose study is equivalent to studying the Hénon map itself. Thus, by taking the most general cubic Hamiltonian

$$H(q, p) = \alpha p + \beta q + \gamma p^2 + \delta q^2 + \zeta q^3 + \sigma p^3 \quad (1.29)$$

we can mimic the Hénon map. Taking $\alpha = \beta = \sigma = 0$ is by no means restrictive, since linear terms can be eliminated by a change of coordinates and the original map depends linearly on p . Also, it can be readily noticed that δ and ζ must be negative in order to make the fixed point at the origin hyperbolic. We have, then, the final Hamiltonian as

$$H(q, p) = \gamma p^2 + \delta q^2 + \zeta q^3, \quad \delta, \zeta < 0, \quad (1.30)$$

but to make it physically interesting we will fix the constants so that the final Hamiltonian is given by

$$H(q, p) = \frac{p^2}{2} - \left(\frac{q^2}{2} + \frac{q^3}{3} \right), \quad (1.31)$$

from which we obtain the discrete mapping

$$\begin{cases} Q &= q + \alpha p \\ P &= p \end{cases}, \quad \begin{cases} \bar{Q} &= Q \\ \bar{P} &= P + \alpha(Q + Q^2) \end{cases}. \quad (1.32)$$

As with the previous example we provide the level curves of the Hamiltonian and the iterations of the map (1.32) for a value of α where the original Hamiltonian is still a nice approximation in the vicinity of an elliptical equilibrium (figure 1.4), and then show how the map evolves as α grows (figure 1.5).

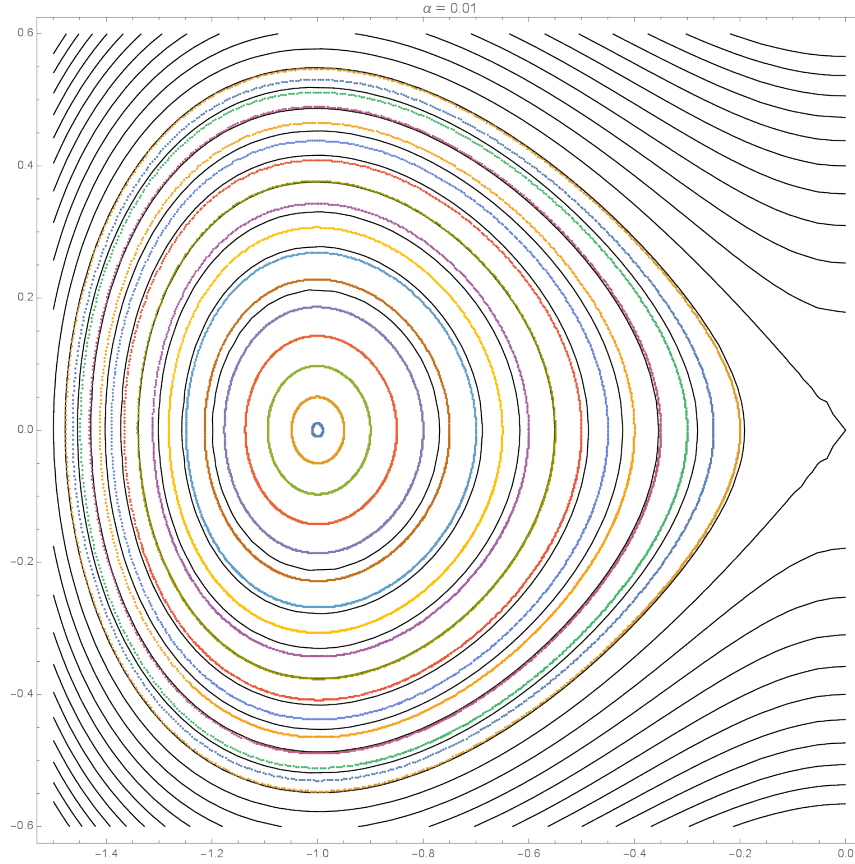


Figure 1.4: Level curves of the Hénon Hamiltonian (black) and 1000 iterations of the derived map for $\alpha = 0.01$ (colored). Iterations for each initial point still depicted in different colors.

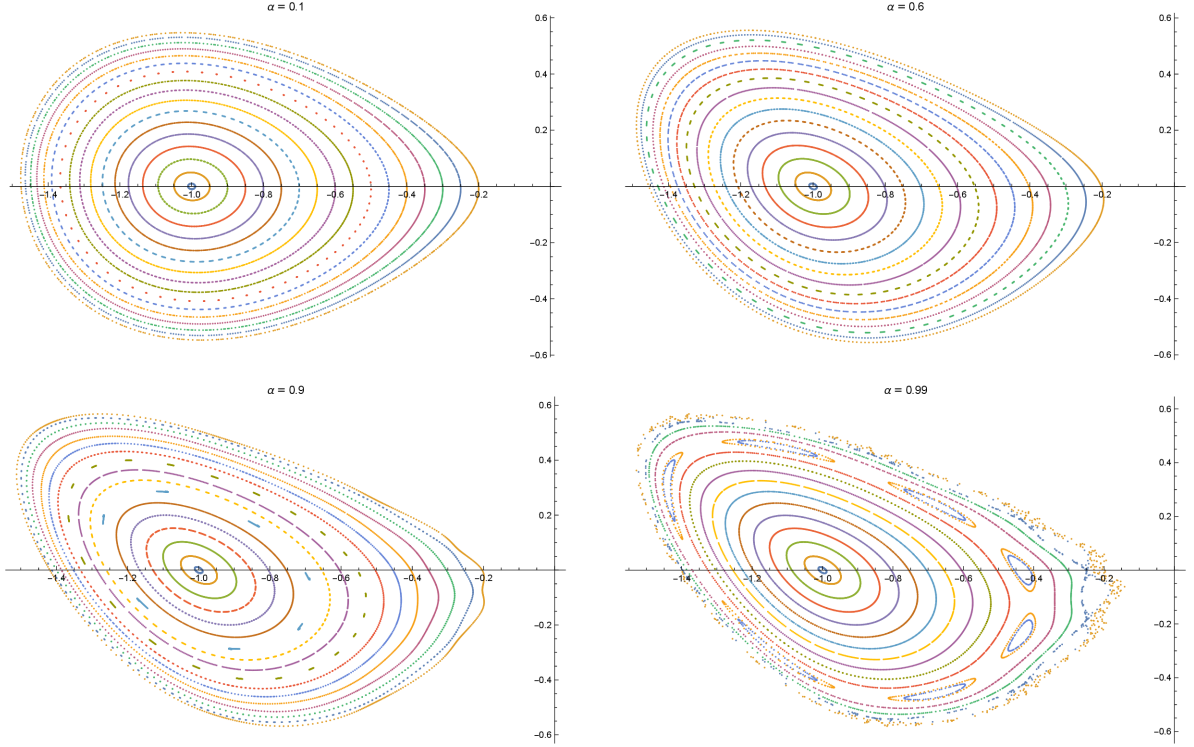


Figure 1.5: Orbits of the map derived from (1.31) for different values of α .

1.3.3 One Last Example

In the previous examples we focused on elliptic points because the hyperbolic orbits are very hard to computationally track in a map with two equilibria. The map derived from the Duffing Hamiltonian has only elliptic fixed points, but for a certain value of α suffers an order 6 bifurcation which gives rise to 6 hyperbolic points (besides the usual islands of stability around the 6 elliptic points). Those points form unstable invariant manifolds that start to complicate numerical approximations for the orbits. In order to have an example of a map that presents easy-to-track unstable orbits we chose the Hamiltonian

$$H(q, p) = \frac{p^2}{2} - q^2 - q^3 + \frac{q^4}{2}, \quad (1.33)$$

whose invariant manifolds at $(0, 0)$ are hyperbolic but at $(-0.5, 0)$ and $(2, 0)$ are elliptic. This greatly facilitates following the orbits numerically around the unstable fixed point. We present graphics equivalent to the ones of the other examples in figures 1.6 and 1.7.

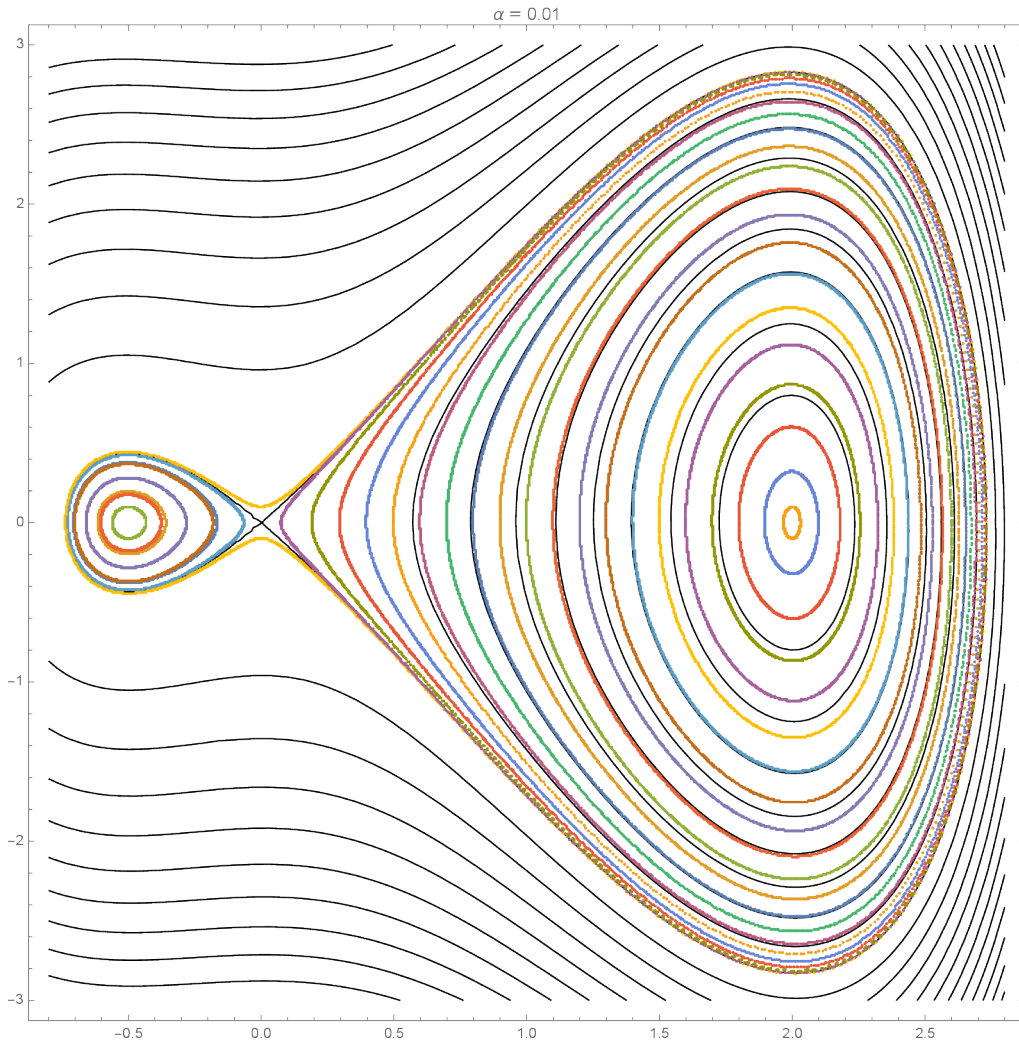


Figure 1.6: Level curves of the hamiltonian (1.33) (black) and 1000 iterations of the derived map for $\alpha = 0.01$ (colored).

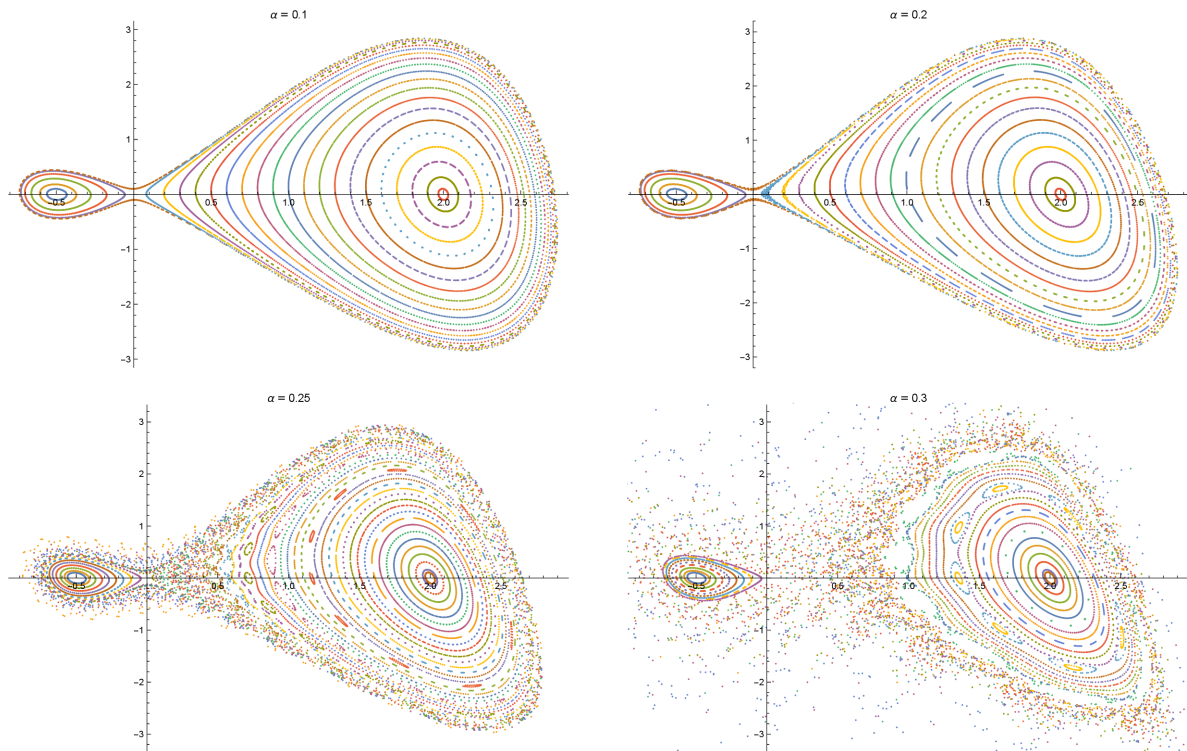


Figure 1.7: Orbits of the map derived from (1.33) for different values of α .

A note on level curves: The comparison between Hamiltonian level curves and map iterations, that is, *how well are the level curves of the Hamiltonian approximating the map's orbits*, is to be taken not as how close the continuous orbits fall to the iterations, but by a comparison of the geometry of the orbits. When Mathematica plots a level curve of a function $f(x, y)$, that is, $f(x, y) = c$, we are unable to choose efficiently which c it will use. This c is the constant that, if varied, would provide us a level curve that falls exactly over the map's orbit. Unfortunately the procedure of plotting those exact level curves is time consuming, and choosing the automatic level curve plotting provided by the function `ContourPlot` is much more effective. When searching for a comparison between the level curves and the orbits it is, therefore, sufficient to choose a curve that happens to fall over an orbit (as, for example, the

brown orbit in figure 1.2, the magenta orbit in figure 1.4 or the blue orbit in figure 1.6), or compare them by geometrical inference. In general, a nice fit is detectable by a single orbit hitting a level curve, and it is clearly visible when the map is no longer well-approximated by the Hamiltonian (this last observation refers to the approximations given in the last chapter).

Classical Generating Functions

This work uses quantum and classical methods to obtain integrable approximations for classical maps. The classical point of view is based on the center function, which is one possible “representation” of Classical Mechanics that arises after a specific symplectomorphism in a product manifold and is very rich in geometrical meaning. However, the center function’s main advantages are the existence of a center Hamiltonian that for short times approaches the position-momentum one (see [10]) and its relatively simple composition rule (which we will need, since we are dealing with the composition of two independent Hamiltonians $F(p)$ and $V(q)$). We therefore present, since the early stages, the construction of the center function and deduce its composition rule for two canonical transformations. Generalizations for any number of canonical transformations can be found in [10].

2.1 Symplectic Manifolds and Coordinate Changes

Given a symplectic manifold $(M = \mathbb{R}^{2n}, \sum_i^n dq_i \wedge dp_i)$ and a differentiable mapping $f : M \rightarrow M$, we say that f is a *canonical transformation* if

$$f^* \omega = \omega . \quad (2.1)$$

If f is linear, then it is called a *symplectomorphism*, as mentioned in the first chapter.

By defining $x_i \equiv q_i$ and $x_{i+n} = p_i$ we can write the canonical form as¹

$$\omega = \sum_{i=1}^n dx_i \wedge dx_{i+n} \quad (2.2)$$

$$= \frac{1}{2} \sum_{i,j=1}^{2n} \mathcal{J}_{ij} dx_i \wedge dx_j , \quad (2.3)$$

where $\mathcal{J}_{ij}$ is the (i, j) -element of $\mathcal{J}$. Also, the symplectic condition can be written intrinsically as (see Appendix 1)

$$\omega(f(u), f(v)) = \omega(u, v) . \quad (2.4)$$

Let u and v be vectors on $T_0 \mathbb{R}^{2n} \simeq \mathbb{R}^{2n}$ ($\simeq$ means *isomorphic to*):

¹To prove this let us start with one degree of freedom. Remembering that $\mathcal{J}_{11} = 0 = \mathcal{J}_{22}$ and $\mathcal{J}_{12} = 1 = -\mathcal{J}_{21}$ we have

$$\begin{aligned} \omega &= \frac{1}{2} \sum_{i,j=1}^2 \mathcal{J}_{ij} dx_i \wedge dx_j \\ &= \frac{1}{2} (\mathcal{J}_{12} - \mathcal{J}_{21}) dx_1 \wedge dx_2 \\ &= \sum_{i=1}^1 dx_i \wedge dx_{i+1} . \end{aligned}$$

Generalizations for higher dimensions are obtained by induction on n .

$$u = \sum_i^{2n} u_i \frac{\partial}{\partial x_i} \quad (2.5)$$

$$v = \sum_i^{2n} v_i \frac{\partial}{\partial x_i}; \quad (2.6)$$

we have

$$\omega(u, v) = \frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} dx_i \wedge dx_j \left(\sum_i^{2n} u_l \frac{\partial}{\partial x_l}, \sum_i^{2n} v_m \frac{\partial}{\partial x_m} \right) \quad (2.7)$$

$$\begin{aligned} &= \frac{1}{2} \sum_{i,l,m}^{2n} \mathcal{J}_{ij} u_l v_m \left[dx_i \left(\frac{\partial}{\partial x_l} \right) \wedge dx_j \left(\frac{\partial}{\partial x_m} \right) \right. \\ &\quad \left. - dx_i \left(\frac{\partial}{\partial x_m} \right) \wedge dx_j \left(\frac{\partial}{\partial x_l} \right) \right] \end{aligned} \quad (2.8)$$

$$= \frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} (u_i v_j - v_i u_j) \quad (2.9)$$

$$= \sum_i^n (u_i v_{i+n} - v_i u_{i+n}) \quad (2.10)$$

$$= \begin{pmatrix} u_i & u_{i+n} \end{pmatrix} \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ -\mathbb{1} & \mathbb{0} \end{pmatrix} \begin{pmatrix} v_i \\ v_{i+n} \end{pmatrix} \quad (2.11)$$

$$= u^T \mathcal{J} v, \quad (2.12)$$

where we have recovered the result highlighted in equation (1.7). Assuming f is an analytical mapping and taking its linear part $\mathcal{M}$, then, by equation (2.4),

$$\omega(f(u), f(v)) = \omega(u, v) \quad (2.13)$$

$$\iff \omega(\mathcal{M}u, \mathcal{M}v) + \mathcal{O}(2) = \omega(u, v) + \mathcal{O}(2) \quad (2.14)$$

$$\iff (\mathcal{M}u)^T \mathcal{J} (\mathcal{M}v) = u^T \mathcal{J} v \quad (2.15)$$

$$\Rightarrow \mathcal{M}^T \mathcal{J} \mathcal{M} = \mathcal{J}. \quad (2.16)$$

Our deduction is general enough to allow us to conclude that all symplectomorphisms (alongside all Jacobians of canonical transformations) satisfy Equation (2.16).

Examples of canonical transformations can be easily obtained from equations (1.8) and (2.4). Returning to coordinates (q, p) equation (2.4) reads

$$\sum_{i=1}^n [d(q_i \circ f) \wedge d(p_i \circ f) - dq_i \wedge dp_i] = 0 \quad (2.17)$$

$$\iff \sum_{i=1}^n (d[f(q_i)] \wedge d[f(p_i)] - dq_i \wedge dp_i) = 0, \quad (2.18)$$

since we are dealing² with $\mathbb{R}^{2n}$. We can simplify notation by defining $Q_i \equiv f(q_i)$, $P_i \equiv f(p_i)$. Using those definitions (2.18) becomes

$$\sum_{i=1}^n (Q_i \wedge dP_i - dq_i \wedge dp_i) = 0. \quad (2.19)$$

It is easy to see that

$$dS(P, p) \equiv \sum_{i=1}^n (Q_i dP_i - q_i dp_i) \quad (2.20)$$

²If we had not assumed that we were dealing with $\mathbb{R}^{2n}$, then we would not have the right to say, for example, that $q \circ f = f(q)$, because we would not be able to identify coordinates with points in M . Rigorously, we would have to begin by choosing a chart (U, q) around a certain point $c \in U \subset M$ and, on a vicinity of it, $(q \circ f)(U) = q[f(U)]$ would represent the local coordinates of the action of f in points belonging to U . That is why we chose to deal with Cartesian manifolds, otherwise the formalism required to deal with general manifolds, although more reaching, would obscure a great deal of this work unnecessarily. It is also worth pointing out that working with general manifolds is only useful if we are dealing with quantization in manifolds with Betti numbers different from 0, that is, non-simply connected manifolds. If we were not, Darboux theorem helps us remain general even if on $\mathbb{R}^{2n}$.

is a primitive for the 2-form in the left hand side of equation (2.19). We could have chosen dS as a function of differentials of any of the four combinations of variables (q, Q) , (q, P) , (p, Q) or (p, P) by simply using the antisymmetry of the wedge product and it would still be a primitive 1-form³. According to our choice, we see that

$$\frac{\partial S(P, p)}{\partial P_i} = Q_i \quad (2.21)$$

$$\frac{\partial S(P, p)}{\partial p_i} = -q_i. \quad (2.22)$$

S is called a *generating function* for the canonical transformation f . In most textbooks the exchange of variables between primitives is made by *Legendre transforms*, which are transformations imposed on convex 1-forms as S . In this terminology, S would be a *generating function of type 4* [2]. Nevertheless, we see that there is no need to use obscure changes of coordinates in $T_0^*\mathbb{R}^{2n}$, since it is much easier to work with the canonical 2-forms defined in $\bigwedge^2 T_0^*\mathbb{R}^{2n}$ in this case.

2.2 Poincaré Generating Functions

Using equation (2.3) the canonical condition (2.1) can be expressed as

$$\frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} [d(x_i \circ f) \wedge d(x_j \circ f) - dx_i \wedge dx_j] = 0. \quad (2.23)$$

From now on we will simplify the notation again by defining $X_i \equiv x_i \circ f = [f(x)]_i$. We might sometimes call X and x by *new* and *old* coordinates.

³What we are actually proving here is that canonical transformations give rise to *cohomologous* 1-forms.

Claim: The 1-forms

$$\phi(f) = \sum_{i,j}^{2n} \mathcal{J}_{ij} (X_i - x_i) d \left(\frac{X_j + x_j}{2} \right) \quad (2.24)$$

$$\psi(f) = - \sum_{i,j}^{2n} \mathcal{J}_{ij} \left(\frac{X_j + x_j}{2} \right) d (X_i - x_i) \quad (2.25)$$

are primitives for the left hand side of (2.23).

Proof: We will prove the claim for $\phi(f)$, since the procedure is exactly the same for $\psi(f)$. Taking the exterior derivative of (2.24) we have

$$d\phi(f) = \frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} d(X_i - x_i) \wedge d(X_j + x_j) \quad (2.26)$$

$$\begin{aligned} &= \frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} [dX_i \wedge dX_j + dX_i \wedge dx_j \\ &\quad - dx_i \wedge dX_j - dx_i \wedge dx_j] \end{aligned} \quad (2.27)$$

$$\begin{aligned} &= \frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} [dX_i \wedge dX_j - dx_i \wedge dx_j] \\ &\quad - \frac{1}{2} \sum_{i,j}^{2n} \mathcal{J}_{ij} \left[\left(\frac{\partial X_i}{\partial x_i} \right) dx_i \wedge dx_j + \left(\frac{\partial X_j}{\partial x_j} \right) dx_j \wedge dx_i \right]. \end{aligned} \quad (2.28)$$

Since the indexes are dull, we can exchange i by j in the second term of last sum in (2.28):

$$\sum_{i,j}^{2n} \mathcal{J}_{ij} \left(\frac{\partial X_i}{\partial x_i} \right) dx_i \wedge dx_j + \sum_{i,j}^{2n} \mathcal{J}_{ij} \left(\frac{\partial X_j}{\partial x_j} \right) dx_j \wedge dx_i \quad (2.29)$$

$$= \sum_{i,j}^{2n} \mathcal{J}_{ij} \left(\frac{\partial X_i}{\partial x_i} \right) dx_i \wedge dx_j + \sum_{i,j}^{2n} \mathcal{J}_{ji} \left(\frac{\partial X_i}{\partial x_i} \right) dx_i \wedge dx_j \quad (2.30)$$

$$= \sum_{i,j}^{2n} \mathcal{J}_{ij} \left[\frac{\partial X_i}{\partial x_i} \right] (dx_i \wedge dx_j - dx_i \wedge dx_j) \quad (2.31)$$

$$= 0,$$

where we have used the fact that $\mathcal{J}^T = -\mathcal{J}$. $\square$

Since both 1-forms introduced are primitives for a 2-form that equals to zero, then both are closed. Keeping in mind that we are dealing with a simply connected manifold, they are also exact⁴. This means that there are two unique functions $S(f) : \mathbb{R}^{2n} \rightarrow \mathbb{R}$ and $Z(f) : \mathbb{R}^{2n} \rightarrow \mathbb{R}$ such that $S(f)(0) = 0$, $dS(f) = \phi$ and $Z(f)(0) = 0$, $dZ(f) = \psi$. Historically $S(f)$ is called the *Poincaré generating function* for the transformation f , and $Z(f)$ receives no special name. In the next section we will define a product manifold with coordinates such that those functions gain a very simple geometrical meaning, but let us first notice that the critical points of $S(f)$ and $Z(f)$ are the zeros of $\phi(f)$ and $\psi(f)$, which, if the differentials $d\left(\frac{X_i+x_i}{2}\right)$ and $d(X_i-x_i)$ are linearly independent, occur only when

$$X_i - x_i = 0 \iff x_i \circ f = x_i \quad (2.32)$$

$$\frac{X_i + x_i}{2} = 0 \iff x_i \circ f = -x_i \quad (2.33)$$

⁴If we were dealing with general manifolds we could shrink their domain until it became locally simply connected (a lemma by Poincaré in homology theory applied to the charts states this is always possible [11]).

for $S(f)$ and $Z(f)$, respectively.

Now, stating that the differentials $d\left(\frac{X_i+x_i}{2}\right)$ and $d(X_i-x_i)$ are linearly independent is the same as saying that

$$\det \left[\frac{\partial(x_i \circ f)}{\partial x_j} + \delta_{ij} \right] \neq 0 \quad (2.34)$$

$$\det \left[\frac{\partial(x_i \circ f)}{\partial x_j} - \delta_{ij} \right] \neq 0, \quad (2.35)$$

which means that the Jacobians of the transformations should have no eigenvalue equal to -1 (or 1) in the case of $S(f)$ (or $Z(f)$). If this is true, then we can affirm that the zeros of $\phi(f)$ and $\psi(f)$ are exactly the critical points of the generating functions⁵; otherwise we have *caustics*, which will be briefly addressed afterwards.

2.3 The Product Manifold

Let $M_1 \simeq M_2 \simeq T_0^*\mathbb{R}^{2n} \simeq \mathbb{R}^{2n}$. Let us now introduce the product manifold $M_1 \times M_2$, with projections $\pi_1 : M_1 \times M_2 \rightarrow M_1$ and $\pi_2 : M_1 \times M_2 \rightarrow M_2$ into the first and second factor spaces, respectively. If $(x_1, \dots, x_{2n})$ and $(X_1, \dots, X_{2n})$ are, respectively, Darboux coordinate systems in M_1 and M_2 , then $(y_1, \dots, y_{2n}, z_1, \dots, z_{2n}) \equiv (x_1 \circ \pi_1, \dots, x_{2n} \circ \pi_1, X_1 \circ \pi_2, \dots, X_{2n} \circ \pi_2)$ is a canonical coordinate system on $M_1 \times M_2 \simeq T_0^*(\mathbb{R}^{2n} \times \mathbb{R}^{2n}) \simeq \mathbb{R}^{4n}$. If ω_0^1 and ω_0^2 are symplectic 2-forms on M_1 and M_2 , then it is easy to prove that $\omega_0^\times \equiv \lambda_1(\pi_1^*\omega_0^1) + \lambda_2(\pi_2^*\omega_0^2)$, where $\lambda_1, \lambda_2 \in \mathbb{R}$, is a symplectic 2-form on $M_1 \times M_2$ [4]. Now, if we consider the coordinates $\{z_i\}$ to be the image of some diffeomorphism f acting on $\{y_i\}$ (that is, $M_2 = f(M_1)$), then there is a submanifold of $M_1 \times M_2$ given by the embedding of the graph $\Gamma_f = \{(y_1, \dots, y_{2n}, f(y_1, \dots, y_{2n}), y_i \in M_1\}$ of f .

⁵In general manifolds, this means they also do not depend on the chart chosen.

Claim: let γ be the embedding of Γ_f into the product manifold:

$$\gamma : M_1 \rightarrow M_1 \times M_2 \quad (2.36)$$

$$x \mapsto (x, f(x)); \quad (2.37)$$

then f is a symplectomorphism iff $\lambda_1 = -\lambda_2$ and $\gamma^*\omega_0^\times = 0$.

Proof:

$$\gamma^*\omega_0^\times = \lambda_1\gamma^*\pi_1^*\omega_0^1 + \lambda_2\gamma^*\pi_2^*\omega_0^2 \quad (2.38)$$

$$= \lambda_1(\pi_1 \circ \gamma)^*\omega_0^1 + \lambda_2(\pi_2 \circ \gamma)^*\omega_0^2, \quad (2.39)$$

but

$$(\pi_1 \circ \gamma)(x) = \pi_1(x, f(x)) \quad (2.40)$$

$$= x \quad (2.41)$$

$$\Rightarrow \pi_1 \circ \gamma = \text{identity}, \quad (2.42)$$

$$(\pi_2 \circ \gamma)(x) = \pi_2(x, f(x)) \quad (2.43)$$

$$= f(x) \quad (2.44)$$

$$\Rightarrow \pi_2 \circ \gamma = f. \quad (2.45)$$

Substituting in equation (2.39),

$$\gamma^*\omega_0^\times = \lambda_1\omega_0^1 + \lambda_2f^*\omega_0^2. \quad \square \quad (2.46)$$

Picking the obvious choice $\lambda_1 = 1 = -\lambda_2$ is called *twisting* the form $\omega_0^\times$ to obtain a new 2-form $\tilde{\omega}_0^\times$. This twisting process is the basis for constructing symplectomorphisms

(and generating functions), where the existence of the so called *Lagrangian submanifolds*, which are submanifolds where the symplectic (in this case, also twisted) 2-form equals zero, is fundamental. Indeed, we have been using the fact that the symplectic condition in equation (2.4) is equivalent to the vanishing of twisted 2-forms on the product manifold since the beginning (carefully check equations (2.19) and (2.23)).

2.4 Center and Chord Functions

We now start the construction of the center and chord functions for canonical transformations. Though only the center function will be used in this work, general aspects of the chord function will also be given. We begin with the product manifold $M_1 \times M_2$, presented in the last chapter, keeping in mind that we are always restricting ourselves to a submanifold where the twisted 2-form resumes to zero.

Claim: The coordinate change

$$T : M_1 \times M_2 \rightarrow M_1 \times M_2 \tag{2.47}$$

$$\begin{pmatrix} \eta_i \\ \xi_i \end{pmatrix} \mapsto \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -1 & 1 \end{pmatrix} \begin{pmatrix} y_i \\ z_i \end{pmatrix} \tag{2.48}$$

is symplectic.

Proof: Using (2.16),

$$\begin{pmatrix} \frac{1}{2} & -1 \\ \frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \quad \square \tag{2.49}$$

Putting $y_1 \equiv x_i$, $z_i \equiv X_i (= [f(x)]_i)$ we can rewrite (2.24) and (2.25) as

$$\phi(f) = \sum_{i,j}^{2n} \mathcal{J}_{ij} (z_i - y_i) d\left(\frac{z_j + y_j}{2}\right) \quad (2.50)$$

$$\psi(f) = - \sum_{i,j}^{2n} \mathcal{J}_{ij} \left(\frac{z_j + y_j}{2}\right) d(z_i - y_i) , \quad (2.51)$$

which in the coordinates given by $T(z, y)$ become

$$\Phi(\eta) = \sum_{i,j}^{2n} \mathcal{J}_{ij} \xi_i d\eta_j \quad (2.52)$$

$$\Psi(\xi) = - \sum_{i,j}^{2n} \mathcal{J}_{ij} \eta_i d\xi_j . \quad (2.53)$$

It can be easily seen by direct computation that $d\Phi(\eta) = -d\Psi(\xi) = \tilde{\omega}_0^\times = 0$, which agrees with the theory developed in the preceding section. By the same argument used in the previous section to define $S(f)$ and $Z(f)$ we can define $\mathcal{S}(\eta)$ and $\mathcal{Z}(\xi)$ by

$$\begin{cases} \mathcal{S}(\eta)(0,0) = 0 \\ d\mathcal{S}(\eta) = \Phi(\eta) \end{cases} \quad (2.54)$$

$$\begin{cases} \mathcal{Z}(\xi)(0,0) = 0 \\ d\mathcal{Z}(\xi) = \Psi(\xi) \end{cases} , \quad (2.55)$$

which leads to

$$\xi = -\mathcal{J} \left(\frac{\partial \mathcal{S}(\eta)}{\partial \eta} \right) \quad (2.56)$$

$$\eta = \mathcal{J} \left(\frac{\partial \mathcal{Z}(\xi)}{\partial \xi} \right) \quad (2.57)$$

in the coordinates given by $(\xi_1, \dots, \xi_{2n}, \eta_1, \dots, \eta_{2n})$. Both equations above create a dynamics very close to the Hamiltonian one (compare with equation (1.5)), but this time on the product manifold. As Hamiltonian dynamics takes place in the cotangent bundle fibers or *phase spaces*, the product manifold is sometimes called *double phase space* [8, 10, 12]. Also, using the definitions we gave for ξ and η as

$$\xi = X - x \tag{2.58}$$

$$\eta = \frac{X + x}{2}, \tag{2.59}$$

we notice that if X are the coordinates for the endpoint of an iteration of f on a point x , then ξ is the *chord* joining the extremities of those vectors. We also see that η would be the midpoint of such chord, that is, its *center*. It is therefore appropriate to call $\mathcal{S}(\eta)$ and $\mathcal{Z}(\xi)$ by *center* and *chord* generating functions⁶ for f , and η and ξ by *centers* and *chords*. We can also interpret the *center representation* as seeing the action of f as a reflection around the center η , and the *chord representation* as seeing it as a translation by the chord ξ . See figure 2.1.

In the same manner as functions $S(f)$ and $Z(f)$ the center and chord functions $\mathcal{S}(\eta)$ and $\mathcal{Z}(\xi)$ present singularities for eigenvalues -1 and 1 , respectively, which we call *caustics* [10]. They occur when we cannot associate a single chord to a center or a single center to a chord. We say then that center and chord caustics happen when chords and centers *coalesce*, respectively (see figure 2.2). It is possible to show (and easy to see from equations (2.34) and (2.35)) that every time our canonical transformation f reduces locally to a reflection/translation, then we have center/chord caustics. Also, it is very clear from equation (2.35) that the chord function is unable to deal with

⁶Notice that the center and chord generating functions are nothing but the Poincaré generating function and the nameless function $Z(f)$ written in different coordinates.

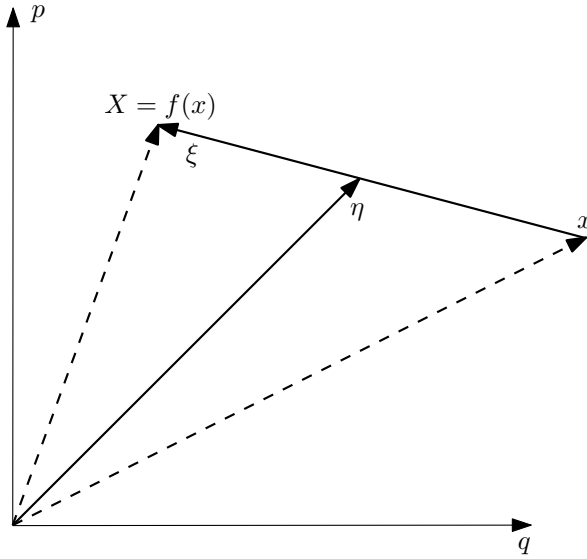


Figure 2.1: x and $f(x)$ alongside the chord ξ and the center η for f .

infinitesimal transformations, since they are perturbations of identity and have eigenvalues close to 1. This is one more reason for choosing to deal with the center function, since most of the time we will be dealing with small parameter transformations.

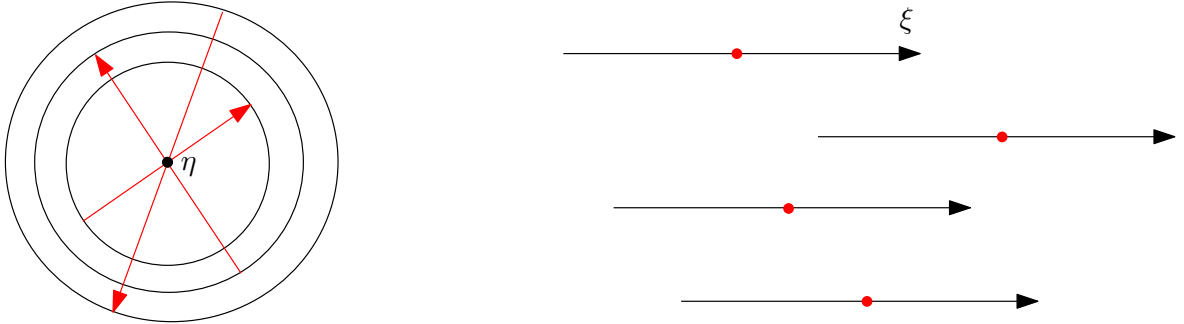


Figure 2.2: The flux of the harmonic oscillator presents a specially problematic type of caustic, where all reflections (rotations by π , shown in red) coalesce in a single center (black). Also, translations by ξ (black) will have an infinity of coalescing centers (red). We then conclude that translations must be described by center functions, and reflections by chord functions.

However, since center and chord functions do not become singular at the same sit-

uation, we can use them in pairs to analyze any system. Even better, taking a look at the singularity conditions (2.32) and (2.33) we see that when $\mathcal{S}(\eta)$ becomes singular, that is, when $X = x$, then $\mathcal{Z}(\xi)$ equals to zero, since $\xi = X - x$. The reciprocal is also true: $\mathcal{S}(\eta)$ ends up being null when $\mathcal{Z}(\xi)$ is singular.

We have therefore two functions in double phase space that present a near-Hamiltonian dynamics and that can locally describe the phase space of any system in a very simple manner. Also, these generating functions present a very desirable property: unlike general generating functions, they are invariant⁷ with respect to symplectomorphisms [5, 13, 14]. Such clean aspect (among other things) of the center and chord functions have led many authors [10, 12, 15] to make use of them after their formal discovery by Poincaré in [16]. We, on the other hand, chose center functions to analyze our problem because, for short times,

$$S(\eta, t) = -tH(\eta; t), \quad (2.60)$$

which means that we can define a center Hamiltonian associated to the center generating function (arbitrary generating functions cannot be associated to Hamiltonians in this way [10]). A presentation and proof of invariance can be found in [13], whilst a more mathematically accessible point of view can be found in the classic report [10], which also covers the remarkable heritage center and chord functions provide to the theory of Semiclassical Physics and the Wigner function.

⁷Invariant here means that if $S_x(f)$ is the center generating function for the canonical transformation f , then $S_x(f) = S_X(f)$, where $X = Tx$ and T is a symplectomorphism. We would like to include this proof here, but it is simply too long. It can be found in [13].

2.5 Quadratic Center Functions

In this section we will devote a little attention to symplectomorphisms, that is, we will study generating functions for linear symplectic mappings and quadratic Hamiltonians. We begin by noticing that any quadratic center function can be written as

$$\mathcal{S}(\eta) = \mathcal{M}_{ij}\eta_i\eta_j, \quad (2.61)$$

where we are using the Einstein summation convention. Noticing that

$$\frac{\partial \mathcal{S}(\eta)}{\partial \eta_j} = 2\mathcal{M}_{ij}\eta_i, \quad (2.62)$$

we see that

$$\mathcal{S}(\eta) = \frac{1}{2} \frac{\partial \mathcal{S}(\eta)}{\partial \eta} \cdot \eta \quad (2.63)$$

$$= \frac{1}{2} \left[(\mathcal{J}^{-1} \mathcal{J}) \frac{\mathcal{S}(\eta)}{\partial \eta} \right] \cdot \eta \quad (2.64)$$

$$= \frac{(\mathcal{J}\xi)}{2} \cdot \eta \quad (2.65)$$

$$= \frac{1}{2} \begin{pmatrix} \xi_{p_1} \\ \vdots \\ \xi_{p_n} \\ -\xi_{q_1} \\ \vdots \\ -\xi_{q_n} \end{pmatrix} \cdot \begin{pmatrix} \eta_{q_1} \\ \vdots \\ \eta_{q_n} \\ \eta_{p_1} \\ \vdots \\ \eta_{p_n} \end{pmatrix} \quad (2.66)$$

$$\Rightarrow \mathcal{S}(\eta) = \frac{1}{2} \sum_{i=1}^n (\xi_{p_i} \eta_{q_i} - \xi_{q_i} \eta_{p_i}) \quad (2.67)$$

$$= \frac{\omega(\xi, \eta)}{2}, \quad (2.68)$$

where a_q, a_p represent, from now on, the position and momentum sectors of an arbitrary vector a in phase space ($\xi_q = X_q - x_q = Q - q$, for example). This means that, for quadratic functions, $\mathcal{S}(\eta)$ can be interpreted as the symplectic *area* of the triangle spanned by ξ and η (see figure 2.1). We will next provide an example of two ways of obtaining the center function for a special class of mappings.

2.5.1 Example: Center Function for a Symplectomorphism on the Plane

Let

$$\begin{pmatrix} Q \\ P \end{pmatrix} = A \begin{pmatrix} q \\ p \end{pmatrix} \tag{2.69}$$

$$= \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}, \tag{2.70}$$

where A is a symplectomorphism. The centers are

$$\begin{aligned} \eta_q &= \frac{Q + q}{2} \\ &= \frac{(a + 1)q + bp}{2} \end{aligned} \tag{2.71}$$

$$\begin{aligned} \eta_p &= \frac{P + p}{2} \\ &= \frac{(d + 1)p + cq}{2}. \end{aligned} \tag{2.72}$$

Since the matrix A is nonsingular (otherwise it would not be a symplectomorphism) we can apply the Inverse Function Theorem to obtain

$$q = \frac{2[(d+1)\eta_q - b\eta_p]}{1 + \text{sp } A + \det A} \quad (2.73)$$

$$p = \frac{2[(a+1)\eta_p - c\eta_q]}{1 + \text{sp } A + \det A}, \quad (2.74)$$

where $\text{sp } A = a + d$ is the trace of A and, since A is symplectic, $\det A = 1$. Noticing that

$$\eta = \frac{X + x}{2} \quad (2.75)$$

$$\Rightarrow 2(\eta - x) = \xi \quad (2.76)$$

we have

$$\xi_q = \frac{2[(\text{sp } A - 2d)\eta_q - b\eta_p]}{2 + \text{sp } A} \quad (2.77)$$

$$\xi_p = \frac{2[(\text{sp } A - 2a)\eta_p - c\eta_q]}{2 + \text{sp } A}. \quad (2.78)$$

Now, from (2.56),

$$\begin{pmatrix} \xi_q \\ \xi_p \end{pmatrix} = \begin{pmatrix} -\frac{\partial S}{\partial \eta_p} \\ \frac{\partial S}{\partial \eta_q} \end{pmatrix} \quad (2.79)$$

$$\Leftrightarrow \begin{pmatrix} \frac{\partial S}{\partial \eta_q} \\ \frac{\partial S}{\partial \eta_p} \end{pmatrix} = \begin{pmatrix} \frac{2[(\text{sp } A - 2d)\eta_p - c\eta_q]}{2 + \text{sp } A} \\ -\frac{2[(\text{sp } A - 2a)\eta_q - b\eta_p]}{2 + \text{sp } A} \end{pmatrix} \quad (2.80)$$

$$= \begin{pmatrix} \frac{2[(a-d)\eta_p - c\eta_q]}{2 + \text{sp } A} \\ \frac{2[(a-d)\eta_q + b\eta_p]}{2 + \text{sp } A} \end{pmatrix}. \quad (2.81)$$

This PDE has a solution

$$S(\eta) = \frac{2(a-d)\eta_q\eta_p - c\eta_p^2 + b\eta_q^2}{2 + \text{sp } A} + C, \quad (2.82)$$

where C is a constant.

Now, instead of solving PDEs we can use (2.68) to obtain

$$S(\eta) = \frac{1}{2}(\eta_q \xi_p - \eta_p \xi_q) \quad (2.83)$$

$$= \frac{(a-d)\eta_p \eta_q - c\eta_q^2}{2 + \text{sp } A} - \left[\frac{(d-a)\eta_q \eta_p - b\eta_p^2}{2 + \text{sp } A} \right] \quad (2.84)$$

$$= \frac{2(a-d)\eta_q \eta_p - c\eta_p^2 + b\eta_q^2}{2 + \text{sp } A}, \quad (2.85)$$

which is the same as (2.82) taking $C = 0$.

2.6 Center Function for the Composition of a Pair of Mappings

We can inquire on how can the composition of two canonical transformations be described using the center generating function. Imagine the following situation: a point $p \in M = \mathbb{R}^{2n}$ is acted upon by an symplectic automorphism $f : M \rightarrow M$. Latter, $f(p)$ is acted upon by another symplectic automorphism $g : M \rightarrow M$. The process is depicted in figure 2.3.

First off, let us define the centers

$$\eta_1 = \frac{f(x) + x}{2} \quad (2.86)$$

$$\eta_2 = \frac{(g \circ f)(x) + f(x)}{2} \quad (2.87)$$

$$\eta = \frac{(g \circ f)(x) + x}{2} \quad (2.88)$$

and the chords

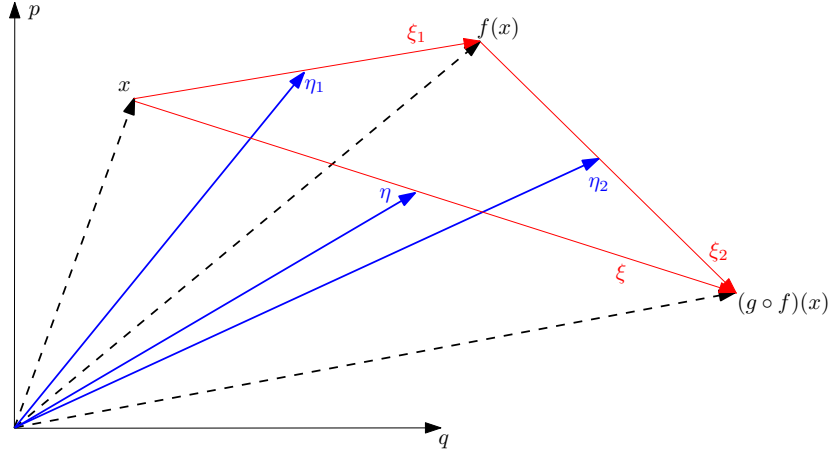


Figure 2.3: The composition of two transformations. Canonical coordinates presented in black, centers in blue and chords in red.

$$\xi_1 = f(x) - x \quad (2.89)$$

$$\xi_2 = (g \circ f)(x) - f(x) \quad (2.90)$$

$$\xi = (g \circ f)(x) - x, \quad (2.91)$$

their geometric meaning being very clear: η_1 and ξ_1 are the center and chord for the first transformation, η_2 and ξ_2 for the second and η and ξ for the whole composition. Now, since the quadratic example brought our attention to the fact that the area plays a major role, let us clean figure 2.3 by depicting only centers and chords and notice that (see figure 2.4)

$$\xi_1 = 2(\eta_2 - \eta) \quad (2.92)$$

$$\xi_2 = -2(\eta_1 - \eta), \quad (2.93)$$

with generating functions $\mathcal{S}_1(\eta_1)$ and $\mathcal{S}_2(\eta_2)$ such that, from equation (2.56),

$$\frac{\partial \mathcal{S}_1(\eta_1)}{\partial \eta_1} = \mathcal{J} \xi_1 \quad (2.94)$$

$$\frac{\partial \mathcal{S}_2(\eta_2)}{\partial \eta_2} = \mathcal{J} \xi_2 . \quad (2.95)$$

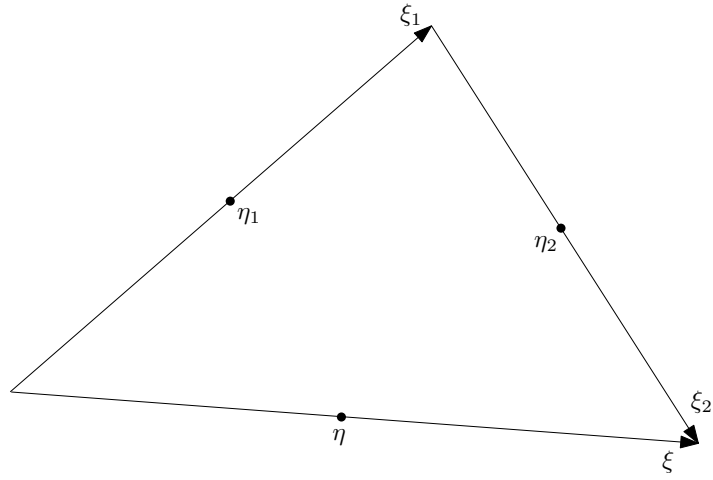


Figure 2.4: Clear view of centers and chords in figure 2.3.

We can now express the symplectic area Δ of the triangle depicted in figure 2.4 in terms of centers using the antisymmetric scalar product:

$$\Delta = \frac{\omega(\xi_1, \xi_2)}{2} \quad (2.96)$$

$$\Rightarrow \Delta(\eta, \eta_1, \eta_2) = -2\omega(\eta_2 - \eta, \eta_1 - \eta) . \quad (2.97)$$

Remembering that (see transition from equation (2.65) to equation (2.68))

$$\omega(u, v) = -\omega(v, u) \quad (2.98)$$

$$\Longleftrightarrow (\mathcal{J}u) \cdot v = -(\mathcal{J}v) \cdot u , \quad (2.99)$$

we have

$$\Delta(\eta, \eta_1, \eta_2) = -2\mathcal{J}(\eta_2 - \eta) \cdot (\eta_1 - \eta) \quad (2.100)$$

$$= 2\mathcal{J}(\eta_1 - \eta) \cdot (\eta_2 - \eta); \quad (2.101)$$

equations (2.100) and (2.101) lead us, respectively, to

$$\frac{\partial \Delta(\eta, \eta_1, \eta_2)}{\partial \eta_1} = -2\mathcal{J}(\eta_2 - \eta) \quad (2.102)$$

$$= -\mathcal{J}\xi_1, \quad (2.103)$$

$$\frac{\partial \Delta(\eta, \eta_1, \eta_2)}{\partial \eta_2} = 2\mathcal{J}(\eta_1 - \eta) \quad (2.104)$$

$$= -\mathcal{J}\xi_2, \quad (2.105)$$

which shows that the symplectic area $\Delta(\eta, \eta_1, \eta_2)$ really plays the role of a generating function for the negative of both chords. More interestingly, we see that

$$\frac{\partial \Delta(\eta, \eta_1, \eta_2)}{\partial \eta_1} + \frac{\partial \mathcal{S}_1(\eta_1)}{\partial \eta_1} = 0 \quad (2.106)$$

$$\frac{\partial \Delta(\eta, \eta_1, \eta_2)}{\partial \eta_2} + \frac{\partial \mathcal{S}_2(\eta_2)}{\partial \eta_2} = 0. \quad (2.107)$$

This means that if we define a function $\mathcal{S}(\eta_1, \eta_2, \eta)$ such that

$$\frac{\partial \mathcal{S}(\eta_1, \eta_2, \eta)}{\partial \eta_1} = \frac{\partial \mathcal{S}(\eta_1, \eta_2, \eta)}{\partial \eta_2} = 0 \quad (2.108)$$

then equations (2.106) and (2.107) can be obtained by extremizing

$$\mathcal{S}(\eta_1, \eta_2, \eta) = \mathcal{S}_1(\eta_1) + \mathcal{S}_2(\eta_2) + \Delta(\eta, \eta_1, \eta_2), \quad (2.109)$$

as can be easily checked. Adding to this the fact that, from equation (2.101),

$$\Delta(\eta, \eta_1, \eta_2) = 2 [(\mathcal{J}\eta_1) \cdot \eta_2 + (\mathcal{J}\eta_2) \cdot \eta - (\mathcal{J}\eta_1) \cdot \eta] \quad (2.110)$$

$$\Rightarrow \frac{\partial \mathcal{S}(\eta, \eta_1, \eta_2)}{\partial \eta} = \mathcal{J}(\eta_2 - \eta_1) \quad (2.111)$$

$$= \mathcal{J}\xi, \quad (2.112)$$

we see $\mathcal{S}(\eta_1, \eta_2, \eta)$ is, therefore, the desired generating function for the composition .

Chapter 3

Integrable Approximations

Having by now developed the classical point of view, in this chapter we develop the quantum one and provide the computational implementations used in this work. The quantum point of view will be drastically less systematic than the classical one, since as well observed in [10], “the formalism of Quantum Mechanics has become more familiar to physicists than the more elementary structure of Classical Mechanics”. We are therefore assuming the quantum perspective will be much more intuitive than the classical one. In the last sections Classical Mechanics comes back, since we finally calculate the composition of two canonical transformations using the center function, and then compare it to the one obtained as the classical limit of a quantum Hamiltonian. The last section is devoted to this classical limit, and a connection between quantum and classical is identified.

3.1 Quantization of Generating Functions

The solution for the Schrödinger’s equation for an autonomous Hamiltonian $\hat{H}$ is given, using the exponential mapping, by

$$|\Psi(t)\rangle = e^{-\frac{i\hat{H}t}{\hbar}}|\Psi(0)\rangle. \quad (3.1)$$

There are many ways of interpreting this solution. The most usual one is to see the exponential of the Hamiltonian operator as the *generator of time displacements*, but we can also see Schrödinger's equation as a way to find a mapping between a Lie algebra and a Lie group. The Hamiltonian operator $\hat{H}$, the momentum $\hat{p}$, the position $\hat{q}$ and all other self-adjoint operators form a Lie algebra under the identification of the commutator as the Lie bracket. Exponentiation of this algebra will give us its connected Lie group (Lie's third theorem). What Schrödinger's formula for finding this group actually does is to define the factors that multiply the operator inside the exponential: the imaginary unit must be present (otherwise the group will not be unitary and, thus, will not conserve probabilities [17]) and there must be a constant $\hbar$ that defines the quantum character of the algebra through uncertainty principles. The term $-\hat{H}t$ is nothing more than the canonical quantization of the classical generating function $S(x, t) = -tH(x)$, the short-time solution for the Hamilton-Jacobi equation for autonomous Hamiltonians [5]. Since any unitary operator defines a potential dynamics in a Hilbert space and $\hat{q}$ and $\hat{p}$ are self-adjoint, we can obtain quantum operators from the identification

$$S(q, p; t) \mapsto e^{\frac{i}{\hbar}\hat{S}(\hat{q}, \hat{p}; t)}, \quad (3.2)$$

where we have simply canonically quantized the generating function S and exponentiated it (why this makes sense can be seen most clearly in the theory of Path Integrals [18])¹. This formula is not always correct and it is still an open problem to

¹It is also necessary to chose an *ordering* of variables, otherwise the final operator will not be Hermitian (for a brief and straightforward exposition see [19]).

find a general scheme of quantization².

We will now describe how to obtain an effective Hamiltonian that approximates the maps derived in chapter 1 (as any other map associated with a separable Hamiltonian of the form (1.13)). In the same way as we divided the process of obtaining a discrete mapping from a continuous Hamiltonian flux into two steps, we will, instead of simply exponentiating the canonical quantization of (1.13) (which would lead us nowhere), separate the exponentials and use the Baker-Hausdorff-Campbell (BHC) expansion to obtain the identification

$$(S_1(q_1, p_1), S_2(q_2, p_2)) \mapsto e^{\frac{i}{\hbar} \hat{S}_2(\hat{q}_1, \hat{p}_1)} e^{\frac{i}{\hbar} \hat{S}_1(\hat{q}_2, \hat{p}_2)} \quad (3.3)$$

$$\approx e^{\frac{i}{\hbar} (S_1(q_1, p_1) + S_2(q_2, p_2) + \frac{i}{2\hbar} [S_1(q_1, p_1), S_2(q_2, p_2)] + \dots)} \quad (3.4)$$

It has been pointed out [21] that since

$$[\hat{q}, \hat{p}] = i\hbar, \quad (3.5)$$

then the expansion (3.4) will present terms of order $\hbar^{-1}$. The reason for this is the relation that defines canonical quantization. As an example, we see that, for the order -2 term

$$\left(\frac{i}{\hbar}\right)^2 [\hat{q}, \hat{p}] \propto \frac{1}{\hbar}; \quad (3.6)$$

it is easy to see this will happen in all orders: the fact that the commutators are proportional to $\hbar$ makes it possible to identify what we could see as the *emergence of*

²Whilst this quantization scheme will be exact in the case of quadratic generating functions, it will be only an approximation (a semiclassical one) in general cases (see [20] for a thorough discussion on this subject).

classical terms in the BHC expansion, since except for the $\frac{i}{\hbar}$ inherent to quantization they do not depend on $\hbar$ and are therefore essentially classical. We have, then, a possible candidate to a Hamiltonian that would approximate the maps shown in the examples of chapter 1: the *classical limit* of the quantum Hamiltonian obtained from the BHC expansion of the right hand side of (3.4)³. In terms of categories, what we are doing is $C^\infty \longrightarrow \mathfrak{g} \longrightarrow G$ and then the way back $G \longrightarrow \mathfrak{g} \longrightarrow C^\infty$, since

1. We begin with classical generating functions of class C^∞ ;
2. Canonically quantize them to obtain a Lie algebra $\mathfrak{g}$ of self-adjoint operators;
3. Use the exponential mapping $\mathfrak{g} \rightarrow G$ to access the unitary Lie group associated to this Lie algebra ;
4. Still in G we use the BHC expansion to fuse the operators into a single new unitary operator;
5. Recover a self-adjoint operator (element of $\mathfrak{g}$) from the exponential of this new operator;
6. And take its classical limit, obtaining an effective classical Hamiltonian in C^∞ .

The theory and computational procedures to evaluate BHC expansions are developed in Appendix 2.

3.2 Effective Hamiltonians

Having by now developed the theory behind the quantization of classical generating functions and the BHC series, let us summarize the process and supply examples

³We will introduce what we understand by *classical limit* latter.

which, for comparison, will be natural extensions of the ones in chapter 1.

We begin with the two maps in (1.25). They arise from the discretization of Hamiltonian fluxes generated by $F(p)$ and $V(q)$, respectively. According to the identification (3.4) we quantize such generating functions and obtain an effective Hamiltonian $\hat{H}_{eff}$ following the scheme below:

$$\begin{cases} S_1(p, t) = -tF(p) \\ S_2(q, t) = -tV(q) \end{cases} \implies (S_1(p, t), S_2(q, t)) \mapsto e^{-\frac{it}{\hbar}\hat{V}(\hat{q})}e^{-\frac{it}{\hbar}\hat{F}(\hat{p})} \approx e^{-\frac{it}{\hbar}\hat{H}_{eff}(\hat{q}, \hat{p})}, \quad (3.7)$$

where

$$\begin{aligned} \exp \left[-\frac{it}{\hbar}\hat{H}_{eff}(\hat{q}, \hat{p}) \right] &= \exp \left[-\frac{it}{\hbar} \left\{ \hat{V}(\hat{q}) + \hat{F}(\hat{p}) + \frac{1}{2} \left(-\frac{it}{\hbar} \right) [\hat{V}(\hat{q}), \hat{F}(\hat{p})] \right. \right. \\ &\quad + \frac{1}{12} \left(-\frac{it}{\hbar} \right)^2 [\hat{V}(\hat{q}) - \hat{F}(\hat{p}), [\hat{V}(\hat{q}), \hat{F}(\hat{p})]] + \\ &\quad \left. \left. + \frac{1}{24} \left(-\frac{it}{\hbar} \right)^3 [\hat{F}(\hat{p}), [\hat{V}(\hat{q}), [\hat{V}(\hat{q}), \hat{F}(\hat{p})]]] + \mathcal{O}(t^4) \right\} \right]. \quad (3.8) \end{aligned}$$

The terms that do not depend on $\hbar$ inside the curly brackets constitute the aforementioned classical terms, which in equation (3.8) are only obvious as $\hat{F}$ and $\hat{V}$. However, as mentioned before, the commutator $[\hat{V}, \hat{F}]$ might also give birth to terms that depend linearly on $\hbar$, canceling it in $\frac{it}{\hbar}$ and creating a new classical term. To exemplify let us take $\hat{F}(\hat{p}) = \frac{\hat{p}^2}{2}$ and $\hat{V}(\hat{q}) = \frac{\hat{q}^2}{2}$. The second order term will be

$$\frac{1}{2} \left(-\frac{it}{\hbar} \right) [\hat{V}(\hat{q}), \hat{F}(\hat{p})] = -\frac{it}{8\hbar} [\hat{q}^2, \hat{p}^2] \quad (3.9)$$

$$= -\frac{it}{8\hbar} (\hat{p}[\hat{q}, \hat{p}]\hat{q} + \hat{p}\hat{q}[\hat{q}, \hat{p}] + [\hat{q}, \hat{p}]\hat{q}\hat{p} + \hat{q}[\hat{q}, \hat{p}]\hat{p}) \quad (3.10)$$

$$= \frac{t}{4} (\hat{p}\hat{q} + \hat{q}\hat{p}). \quad (3.11)$$

Equation (3.11) presents the final operator in an ordered form, being therefore Hermitian and in agreement with the Weyl ordering rules. We can now see that the final result does not depend on $\hbar$, which means it can be interpreted as classical if we drop the little hat from $\hat{p}$ and $\hat{q}$ (*i.e.*, go from operators back to functions).

Taking a look at equations (1.22) or (1.25) we see that α is a time-like parameter. Also, as noticed in equation (1.22), $\alpha \rightarrow 0$ brings the map to identity. An equivalent fact is valid for $t \rightarrow 0$ in the integrable approximation: it describes the motion of the product map and the effective Hamiltonian as nothing more than the non-perturbed one (that is, it brings the *perturbation* to identity). This suggests that the approximations are a power expansion in t and that for the best fits for a map t must have the same numerical value as the map's α . We will see this is just the case.

3.2.1 Back to the Examples

In this subsection we simply provide the integrable approximations of the maps we used as examples in chapter 1 up to fourth order in t :

1. Duffing Map:

$$\begin{aligned}
H_{eff}^{class}(q, p) = & \frac{p^2}{2} + \frac{q^2}{2} + \frac{q^4}{4} + \left[\frac{p(p+q^3)}{2} \right] t + \left[\frac{p^2(3q^2+1) + (q^3+q)^2}{12} \right] t^2 \\
& + \left[\frac{pq(1+4q^2+3q^4)}{12} \right] t^3 + \left[\frac{2p^2(1+9q^2+12q^4) + 2(1+3q^2)(q+q^3)^2 - p^4}{120} \right] t^4
\end{aligned} \tag{3.12}$$

2. Hénon Map:

$$\begin{aligned}
H_{eff}^{class}(q, p) = & \frac{p^2}{2} - \left(\frac{q^2}{2} + \frac{q^3}{3} \right) - \left[\frac{pq(1+q)}{2} \right] t + \left[\frac{q^2(q+1)^2 - p^2(2q+1)}{12} \right] t^2 \\
& + \left[\frac{pq(1+3q+2q^2)}{12} \right] t^3 + \left[\frac{p^2(1+5q+5q^2) - q^2(1+q)^2(1+2q)}{60} \right] t^4
\end{aligned} \tag{3.13}$$

3. Last map:

$$\begin{aligned}
H_{eff}^{class}(q, p) = & \frac{p^2}{2} - \left(q^2 + q^3 - \frac{q^4}{4} \right) - \left[\frac{pq(2q^2 - 3q - 2)}{2} \right] t \\
& + \left[\frac{p^2(6q^2 - 6q - 2) + q^2(2 - 2q^2 + 3q)^2}{12} \right] t^2 + \left[\frac{pq(2 + 9q + q^2 - 15q^3 + 6q^4)}{6} \right] t^3 \\
& + \left[\frac{p^2(4 + 30q + 9q^2 - 96q^3 + 48q^4) + 2q^2(2 + 3q - 2q^2)^2(3q^2 - 3q - 1) - p^4}{60} \right] t^4
\end{aligned} \tag{3.14}$$

We also provide the same figures as in Chapter 1, but now fitted with the corrected Hamiltonians. We used order 5 in t for all fits. It is clear that the effective Hamiltonians are able to approximate the maps around their fixed points for large α , even though it is evident that they will not be able to approximate bifurcations⁴. The novel part of this approach is that, unlike the method of normal forms, where it is only possible to approximate maps near one of their equilibria, the effective Hamiltonian approximates the maps around *all* of their equilibria at the same time. This is most clearly seen in the last map example.

⁴To approximate bifurcations those Hamiltonians would need to be chaotic, but they represent 1-dimensional systems - this is impossible.

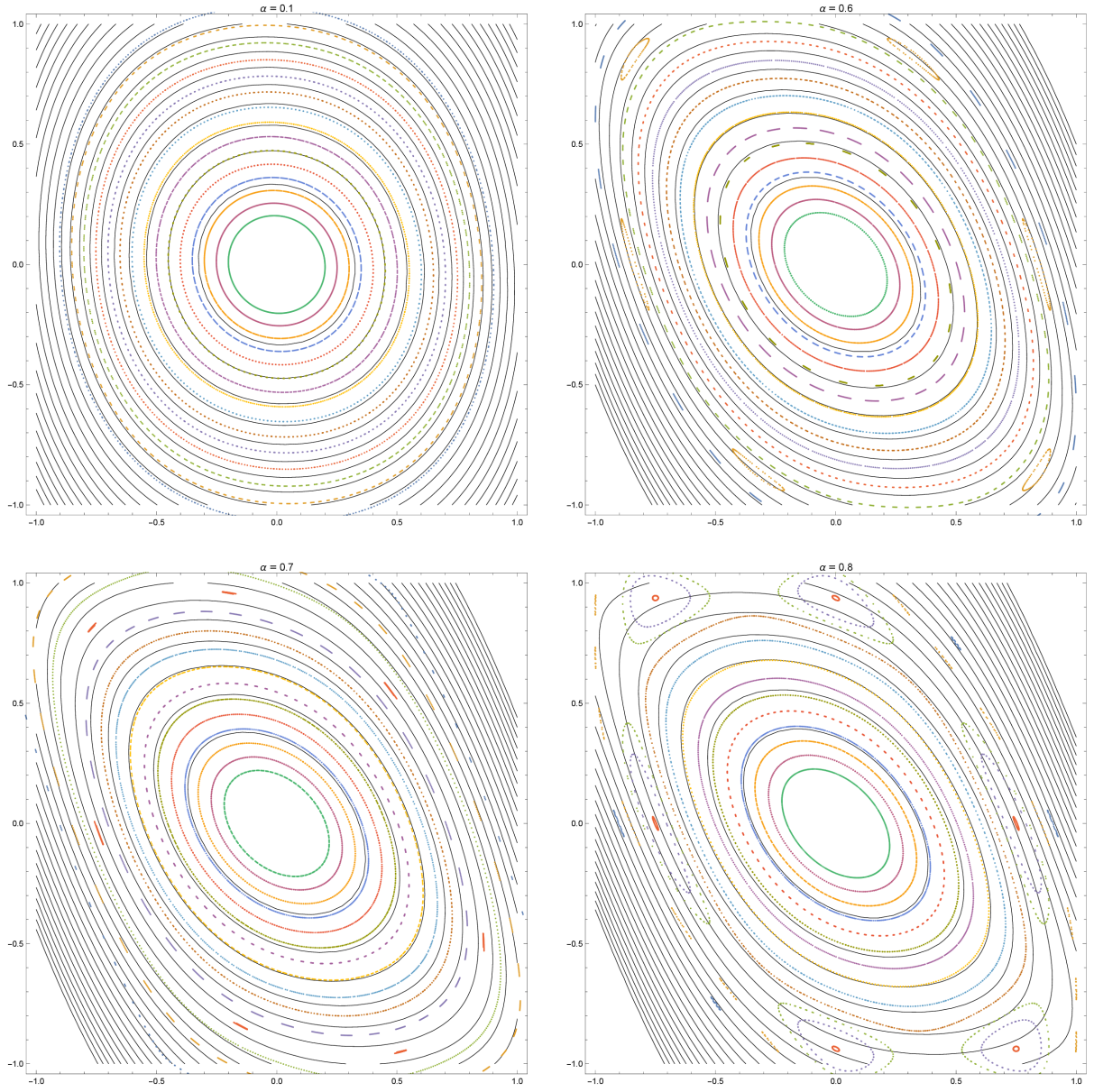


Figure 3.1: Level curves of the effective Duffing Hamiltonian (black) fitted to the orbits of the chaotic map obtained from duffing equation (colored).

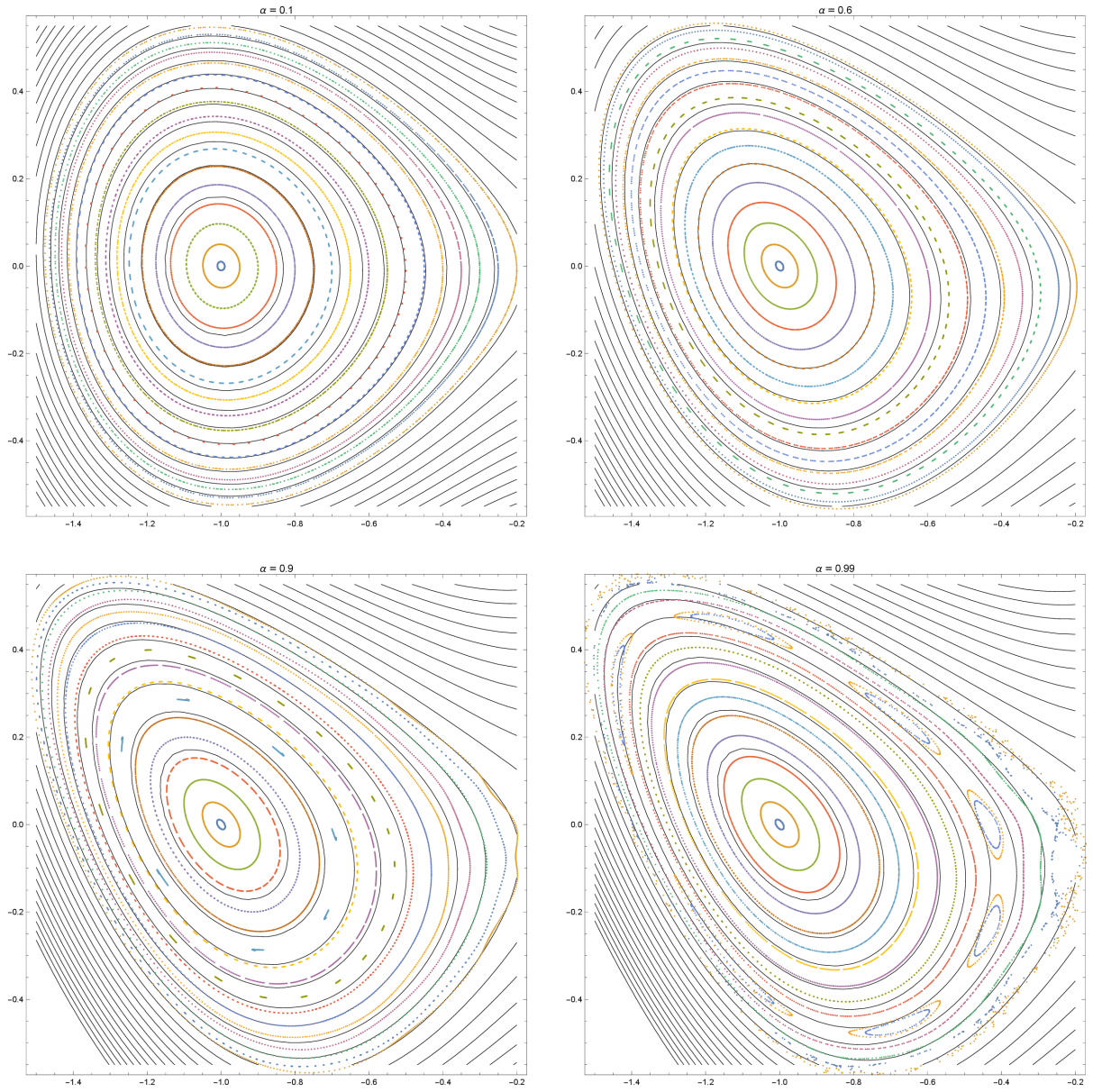


Figure 3.2: The same, but for Hénon's map.

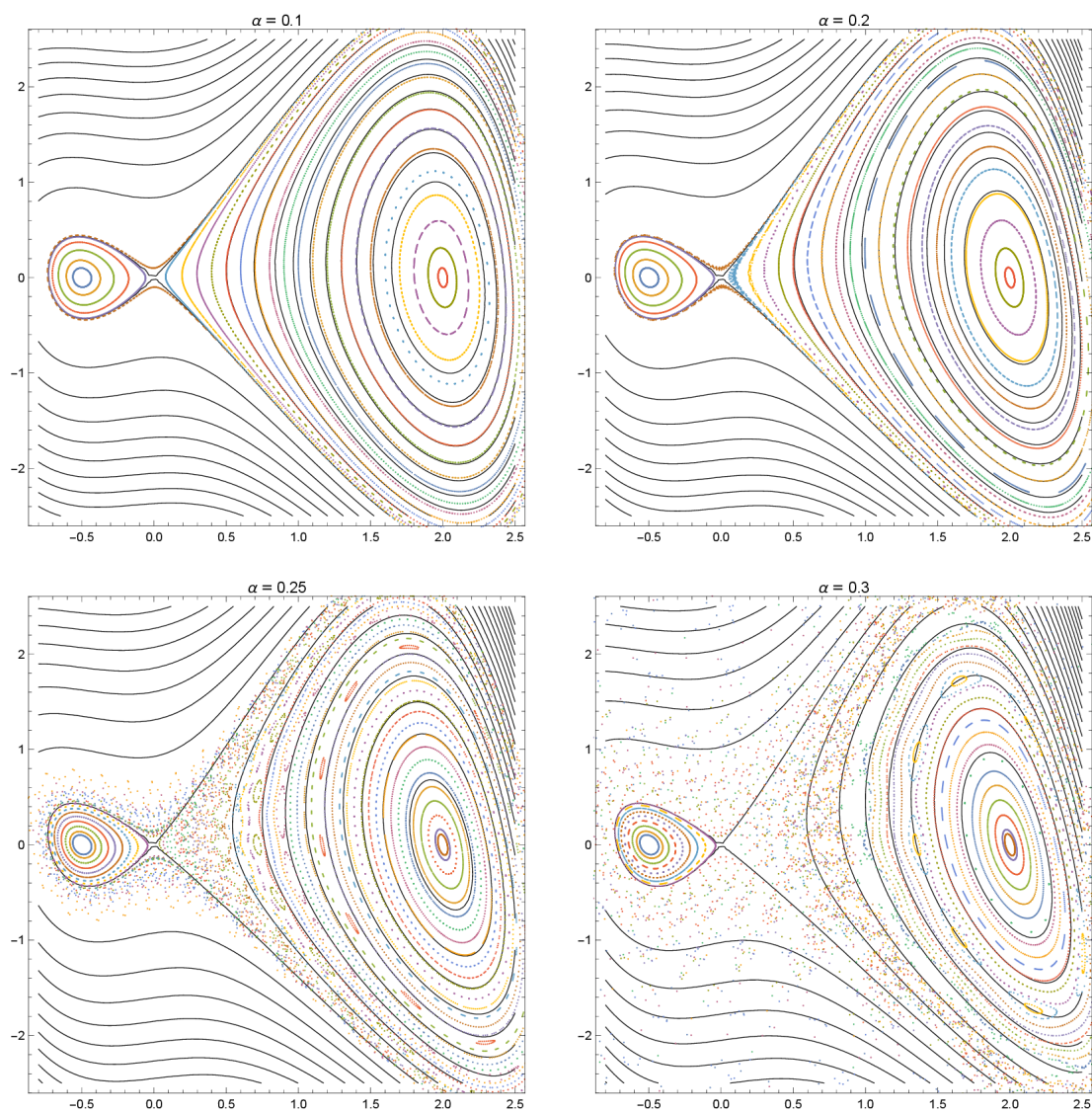


Figure 3.3: The same, but for the last map in the chapter 1 examples.

3.3 The Center Approach

It is also possible to try and describe the map's iterations through the use of the center generating functions deduced in chapter 2. For that we first notice that in the case of two independent generating functions that depend either on ps or qs separately the centers and the chords are quite evident, since each step is vertical or horizontal (see figure 3.4).

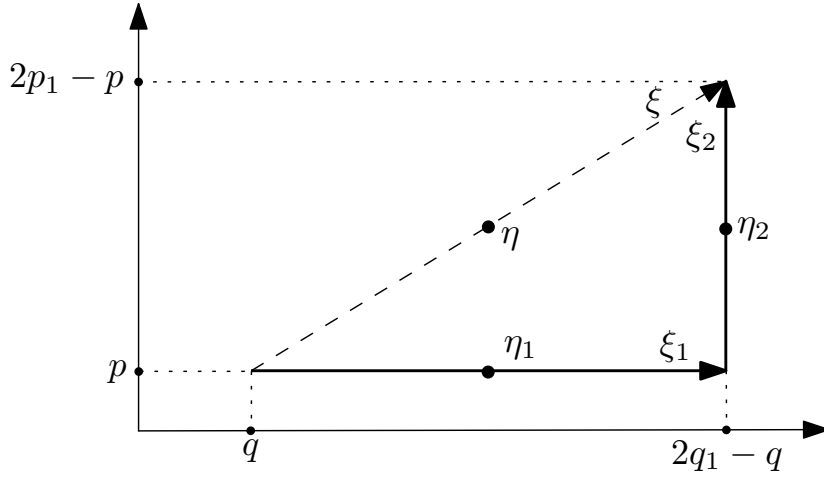


Figure 3.4: The system is brought from (q, p) to $(2q_1 - q, p)$ by the action of H_1 and from $(2q_1 - q, p)$ to $(2q_1 - q, 2p_1 - p)$ by the action of H_2 . The reason for this choice of initial and final points will be made clear when we define the centers for the problem.

From the properties of the center function we know that, for short times [10],

$$S(\eta, t) = -tH(\eta; t), \quad (3.15)$$

and that in this limit $H(\eta) \rightarrow H(q, p)$ ⁵. For our example we will have the composition of the Hamiltonians $H_1(p) = F(p)$ and $H_2 = V(q)$ (see figure 3.4), from which we

⁵This last property is why we are using the center generating functions in the first place, and it is easy to prove from the definition of η and ξ .

will define centers and chords. We will consider that one time interval consists of one iteration of an individual Hamiltonian, which means we will be actually calculating the generating function for two time intervals (one on q axis and one in p axis).

It is readily seen that if we keep the definitions as seen in figure 3.4 the centers are given simply by

$$\eta_1 \equiv \begin{pmatrix} q_1 \\ p \end{pmatrix} \quad , \quad \eta_2 \equiv \begin{pmatrix} q_1 \\ p_2 \end{pmatrix} \quad , \quad (3.16)$$

justifying our choice of initial and final points. The fact that each Hamiltonian has its action confined to a single axis means that each generating functions will depend on either position or momentum projections one at a time:

$$(q, p) \xrightarrow{S_1(\eta_p, t)} (q_1, p) \xrightarrow{S_2(\eta_q, t)} (q_1, p_2) \quad , \quad (3.17)$$

since the generating function that depends on the momenta will act on the position axis and vice versa (see equation (1.1)). Using equation (3.15) we have, therefore, the chords

$$\begin{cases} S_1(\eta_p, t) = S_1(p_2, t) &= -tF(p_2) \\ S_2(\eta_q, t) = S_2(q_1, t) &= -tV(q_1), \end{cases} \implies \begin{cases} \xi_1 = t \begin{pmatrix} 0 \\ F'(p_2) \end{pmatrix} \\ \xi_2 = -t \begin{pmatrix} V'(q_1) \\ 0 \end{pmatrix} \end{cases} \quad , \quad (3.18)$$

and from equations (2.109) and (2.96),

$$S(q, p, 2t) = -tF(p_2) - tV(q_1) + \frac{t^2}{2}F'(p_2)V'(q_1) \quad (3.19)$$

$$= -t \left[F(p_2) + V(q_1) - \frac{t}{2}F'(p_2)V'(q_1) \right], \quad (3.20)$$

where we used $t \rightarrow 2t$ because, as mentioned before, we are considering each Hamiltonian acting during t units of time. Also, from equation (3.15) we see that the object between brackets is our new Hamiltonian for the composition of center functions, which we will call $H(q_1, p_2; 2t)$; notice also that we are seeing q_1 and p_2 as centers.

From figure 3.4 it is easy to see that

$$\xi_{1q} = 2(q_1 - q) = tF'(p_2) \implies q_1 = q + \frac{t}{2}F'(p_2) \quad (3.21)$$

$$\xi_{2p} = 2(p_2 - p) = tV'(q_1) \implies p_2 = p + \frac{t}{2}V'(q_1), \quad (3.22)$$

where the sub-indexes refer to momentum and position projections. This allows us to write q_1 and p_2 as two series in q and p :

$$q_1 = q + \frac{t}{2}V'(p_2) \quad (3.23)$$

$$= q + \frac{t}{2}V' \left(p + \frac{t}{2}F' \left(p + \frac{t}{2}V' \left(\dots \right. \right. \right. \quad (3.24)$$

$$p_2 = p + \frac{t}{2}F'(q_1) \quad (3.25)$$

$$= p + \frac{t}{2}F' \left(q + \frac{t}{2}V' \left(q + \frac{t}{2}F' \left(\dots \right. \right. \right. \quad (3.26)$$

Substituting the above expressions for q_1 and p_2 in $H(q_1, p_2; 2t)$ will give us the center Hamiltonian for the composition of two generating functions up to first order in t . A fourth order correction to the center function (corresponding to a third order

correction to the Hamiltonian) was calculated in one of the appendices of [10] and is given by

$$S(\eta, t) = -tH(\eta) - \frac{t^3}{24} \left[\dot{\eta}^T \left(\frac{\partial^2 H(\eta; t)}{\partial \eta^2} \right) \dot{\eta} \right], \quad (3.27)$$

where

$$\dot{\eta} = \mathcal{J} \left(\frac{\partial H(\eta; t)}{\partial \eta} \right). \quad (3.28)$$

Interpreting the third order correction is simple: in first order we are approximating the initial and final points by a line segment (*i.e.*, the chord itself), and in third by a quadratic arc segment. Higher order corrections result in higher order polynomial approximations. Notice also that since $S(-t, q, p) = tH(q, p)$, even powers of t must vanish.

Using then the correction (3.27) for $H(q_1, p_2, 2t)$ (where we substitute q_1 and p_2 using equations (3.24) and (3.26)) we obtain the third order approximation for the center generating function, from which we can recover the center Hamiltonian in an entirely classical way. The center generating functions for the Hamiltonians presented in the last section are

1. Duffing Hamiltonian:

$$\begin{aligned} S(q, p, 2t) = & -\frac{t}{4} [2p^2 + q^2(2 + q^2)] - \frac{t^2}{2} [pq(1 + 3q^2)] - \frac{t^3}{12} [p^2(1 + 3q^2) + (q + q^3)^2] \\ & - \frac{t^4}{12} [pq(1 + 4q^2 + 3q^4)] \end{aligned} \quad (3.29)$$

2. Hénon Map:

$$\begin{aligned} S(q, p, 2t) = & -\frac{t}{6} [-3p^2 + q^3(3 + 2q)] + \frac{t^2}{2} [pq(1 + q)] - \frac{t^3}{12} [q^2(1 + q)^2 - p^2(1 + 2q)] \\ & - \frac{t^4}{12} [pq(1 + 3q + 2q^2)] \end{aligned} \quad (3.30)$$

3. Last map:

$$\begin{aligned}
S(q, p, 2t) = & t \left[\frac{p^2}{2} - q^2 + q^3 - \frac{q^4}{4} \right] + \frac{t^2}{2} [pq(2 + 3q - 2q^2)] \\
& + \frac{t^3}{12} [p^2(2 + 6q - 6q^2) - q^2(2 + 3q - 2q^2)^2] \\
& - \frac{t^4}{6} [pq(2 + 9q + q^2 - 15q^3 + 6q^4)]
\end{aligned} \tag{3.31}$$

It is easy to see that using equation (3.15) we recover the classical effective Hamiltonians provided in the end of the last section, confirming that the center generating function approach worked.

3.4 The Deformation of Lie Brackets

Taking a closer look at the effective Hamiltonians we can analyze what happens to the commutators in the classical limit, which we will finally define. We will consider the Hénon map as an example in this section, but the conclusions are valid for all maps.

The classical limit of the quantum effective Hamiltonian for the Hénon map up to second order was found to be

$$H_{eff}^{class}(q, p) = \frac{p^2}{2} - \left(\frac{q^2}{2} + \frac{q^3}{3} \right) - \frac{t pq(1 + q)}{2} + \frac{t^2 [q^2(q + 1)^2 - p^2(2q + 1)]}{12}. \tag{3.32}$$

Notice, however, that since

$$F(p) = \frac{p^2}{2} \tag{3.33}$$

$$V(q) = - \left(\frac{q^2}{2} + \frac{q^3}{3} \right), \tag{3.34}$$

then

$$\{V(q), F(p)\} = -pq(1+q) \quad (3.35)$$

$$\{V(q) - F(p), \{V(q), F(p)\}\} = q^2(q+1)^2 - p^2(2q+1), \quad (3.36)$$

where the curly brackets denote the usual Poisson bracket between functions, defined by

$$\{f, g\} = \omega \left(\frac{\partial f}{\partial x}, \frac{\partial g}{\partial x} \right) \quad (3.37)$$

$$= \begin{pmatrix} \frac{\partial f}{\partial q} \\ \frac{\partial f}{\partial p} \end{pmatrix}^T \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial g}{\partial q} \\ \frac{\partial g}{\partial p} \end{pmatrix}. \quad (3.38)$$

Also,

$$\frac{1}{2} \left(-\frac{it}{\hbar} \right) [\hat{V}(\hat{q}), \hat{F}(\hat{p})] = -\frac{it\hbar}{2} \left(\frac{1}{2} + \hat{q} \right) - \frac{t}{2} [\hat{p}\hat{q}(1+\hat{q})] \quad (3.39)$$

$$\frac{1}{12} \left(-\frac{it}{\hbar} \right)^2 [\hat{V}(\hat{q}) - \hat{F}(\hat{p}), [\hat{V}(\hat{q}), \hat{F}(\hat{p})]] = \frac{t^2 [\hat{q}^2(\hat{q}+1)^2 - \hat{p}^2(2\hat{q}+1) - 2i\hbar\hat{p}]}{12}. \quad (3.40)$$

This means that if we take $\hbar \rightarrow 0$ and consider that, in this limit, $\mathfrak{g} \rightarrow C^\infty$,

$$\lim_{\hbar \rightarrow 0} \left\{ \left(-\frac{i}{\hbar} \right) [\hat{V}(\hat{q}), \hat{F}(\hat{p})] \right\} = \{V(q), F(p)\} \quad (3.41)$$

$$\lim_{\hbar \rightarrow 0} \left\{ \left(-\frac{i}{\hbar} \right)^2 [\hat{V}(\hat{q}) - \hat{F}(\hat{p}), [\hat{V}(\hat{q}), \hat{F}(\hat{p})]] \right\} = \{V(q) - F(p), \{V(q), F(p)\}\}, \quad (3.42)$$

and this is what we meant when we said *classical limit* before. It is very important to notice that if we had not used the BHC expansion, then taking the limit $\hbar \rightarrow 0$ would bring us to undefined expressions (divisions by zero would appear). The quantization factors $\frac{i}{\hbar}$ that naturally arise in the BHC series are responsible for removing non-nuclear

expressions from the commutators, as can be noticed in the last calculations.

In Quantum Mechanics the Lie algebra of self-adjoint operators has as its Lie bracket the commutator, and in Classical Mechanics the Lie Bracket is given by the Poisson bracket on the Lie algebra of Hamiltonian functions. We have then found that if the classical limit of the effective Hamiltonian is taken as previously defined, then the commutator *deforms* into the usual Poisson bracket. The classical limit of the quantum effective Hamiltonian can thus be obtained from

$$\begin{aligned}
H_{eff}^{class}(q, p) = & V(q) + F(p) + \frac{t}{2}\{V(q), F(p)\} \\
& + \frac{t^2}{12}\left(\{V(q) - F(p), \{V(q), F(p)\}\}\right) \\
& - \frac{t^3}{24}\{F(p), \{V(q), \{V(q), F(p)\}\}\} + \mathcal{O}(t^4), \quad (3.43)
\end{aligned}$$

which is a Baker-Hausdorff-Campbell equivalent for the Lie algebra of Hamiltonian functions. When dealing with the Lie algebra of operators, however, the Lie group is non-Abelian, but the Lie algebra of Hamiltonian functions comes from an Abelian group [5]. This means that it makes total sense to start from the Lie algebra of self-adjoint operators and map it to its Lie group using the BHC series, but since the Lie algebra of Hamiltonian functions is commutative there is no equivalent of the BHC series for Classical Mechanics when one considers the space of C^∞ functions as the Lie algebra. Even though, exponentiation of $H_{eff}^{class}(q, p)$ will play the same role as the BHC expansion does to non-Abelian Lie groups: it will provide us a Hamiltonian from the Lie algebra generated by $V(q)$ and $F(p)$.

Conclusion

In this work we have studied integral approximations of a special class of discrete mappings, which are obtainable from separable Hamiltonians. In short:

1. We started with a separable Hamiltonian $H(q, p) = F(p) + V(q)$;
2. Separated the action of $F(p)$ and $V(q)$, as if the system were subjected to each at a time, and discretized the flux of those actions;
3. The resulting discretized flux provides us with a discrete composition mapping that, in a small parameter regime, approximates the continuous flux from which it is derived, but when this parameter is increased new phenomena occur;
4. Using canonical quantization we separately quantized two generating functions, an analog of separating the action of each term in the classical Hamiltonian, and exponentiated them to obtain two unitary operators;
5. The Baker-Hausdorff-Campbell expansion was used to unite those two operators in a single effective quantum Hamiltonian;
6. Due to canonical commutation relations, terms that can be considered as classical emerged in this effective Hamiltonian. By defining the classical limit to be $\hbar \rightarrow 0$

and $\mathfrak{g} \rightarrow C^\infty$ we recovered a classical Hamiltonian that was shown to approximate the map of item 3 in any pre-bifurcation regime.

Besides being successful in the integral approximation, we could also draw a couple more observations from this work. First, we point out that a great deal of this dissertation was related to the center function, and we have used it to obtain the exact same approximation we got when using Quantum Mechanics. This was at the same time a test of their consistency and a way to see what was happening geometrically: the center function has a very easy composition rule, from which we extracted some of the geometry Quantum Mechanics hides. As a second observation, the fact that commutators deform into Poisson brackets is a very desirable one, since Quantum Mechanics has been build upon canonical quantization. Nevertheless, taking $\hbar \rightarrow 0$ in relations such as $[\hat{q}, \hat{p}] \rightarrow i\hbar\{q, p\}$ doesn't mean much, whilst the effective Hamiltonian provides us a valid classical rule in this limit.

Future perspectives include the study of:

1. A method for obtaining integral approximations in bifurcation situations:

It might be possible to extract integral approximations from the double iterations of a map; the fixed points in period 2 bifurcations would then be traceable in a projected integrable approximation. If successful, higher period bifurcations should present no difficulties either.

2. Higher order correction for the center function for short times:

Until now the third order correction given by equation (3.27) is the highest one we have, since third order generating functions come from linear vector fields and are, therefore, easy to calculate. Higher order corrections would be more challenging, but we would already have the right answer to compare to (obtained from the BHC expansion).

3. Group-theoretical point of view:

Keeping in mind that taking the classical limit of the effective quantum Hamiltonian is intrinsically mapping a Lie algebra of a non-Abelian Lie group (the Lie algebra of self-adjoint operators) to an Abelian one (the Lie algebra of C^∞ Hamiltonians), the study of such a transition from a group-theoretical point of view might bring us to new results and generalizations.

4. Experimental Physics:

A huge number of Accelerator Physics phenomena are modeled by symplectic maps or Hamiltonians (to name a few, [22–25]). The method here developed might be of great help to experimentalists to analyze the behavior of accelerator beams.

After the writing of the present dissertation, a previous employment of the BHC identity to obtain approximate effective Hamiltonians in classical and quantum mechanics was found [26]. The method used in [26] has a very different computational implementation than the one developed here. The general framework is also slightly different, since there is no analogy between composite maps and quantization. The BHC expansion is developed separately for classical and quantum systems using the Lie algebra of operators and the Lie algebra of Hamiltonian vector fields, not Hamiltonian functions. The Lie algebra of vector fields is non-commutative, which means the BHC expansion arises as naturally as in Quantum Mechanics. The different approach devised in [26] clarified many things about our approach itself and supported our general idea, since this article is cited by many others that use the BHC method to analyze theoretical models and experimental data⁶. We can thus focus on the differences between approaches and find out

⁶One article that should be explicitly mentioned is [27], which uses integrable approximations to explore the Poincaré-Birkhoff theorem in Quantum Mechanics.

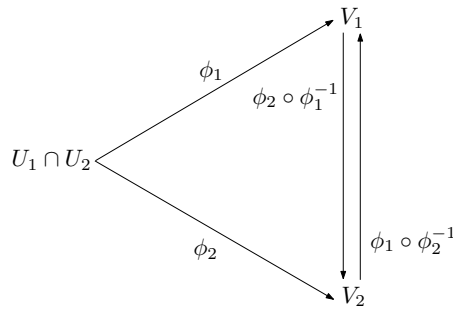
what is really new about our work: no article was found to explore the classical limit of the quantum effective Hamiltonian before.

Appendix A

Differentiable Manifolds

Let $(M, \mathcal{T})$ be a Hausdorff space equipped with a topology $\mathcal{T}$, which from now on we will omit. A *chart* is a pair $\mathcal{C} = (U, x)$ such that $x : M \supset U \rightarrow V \subset \mathbb{R}^n$, where U and V are open sets and ϕ is a homeomorphism. x is usually called a *local coordinate system on M* .

Let $\mathcal{C}_1 = (U_1, \phi_1)$ and $\mathcal{C}_2 = (U_2, \phi_2)$ be charts over M such that $U_1 \cap U_2 \neq \emptyset$. This means that there is a subset of M that belongs both to the domains of ϕ_1 and ϕ_2 . It is then necessary to be sure that such a subset is mapped equally, and this means to assure that $\phi_2 \circ \phi_1^{-1}$ and $\phi_1 \circ \phi_2^{-1}$ are isomorphisms. For differentiable manifolds it is required that those compositions be actually C^k -diffeomorphisms, and we'll take $k = \infty$. The diagram below is, therefore, commutative.



The compositions in the above diagram are called *transition functions* or *coordinate changes*.

Let us now come back to the topological space M . A Hausdorff space is said to be *second countable* if, roughly, it can be decomposed as a countable union of open sets. Let us assume this is the case. Let us then say that

$$M \subseteq \bigcup_{i \in \mathbb{N}} U_i,$$

each U_i being an open set. By equipping each U_i with a homeomorphism ϕ_i , we're saying that each neighborhood of M is locally homeomorphic to a subset of an euclidean space. The collection of all (U_i, ϕ_i) is called an *atlas*, and of course there are many ways of covering M by open sets. Second countability, nevertheless, restricts the ways M can be covered, and we define the *maximal atlas* to be the atlas that contains all other atlases, $\mathcal{A} = \bigcup_{i \in \mathbb{N}} (U_i, \phi_i)$. Finally, we call the pair $(M, \mathcal{A})$ a *differential manifold* or simply *manifold*, in our context. If all the ϕ_i map on an euclidean space of dimension n , then the manifold M (we'll omit the atlas from now on) is said to be n -dimensional.

$T_p M$, that is, the *tangent space to M at p* can now be defined. Pick a chart $x : U \rightarrow \mathbb{R}^n$ and let $\gamma : \mathbb{R} \supset I \rightarrow U \subseteq M$ be a curve such that $\gamma(0) = p$ and $x \circ \gamma$ is differentiable at p . Then $(x \circ \gamma)'(p)$ gives a tangent vector to M at p . There are clearly an infinity of curves that have the same derivative at p , and we form an equivalence class of such derivatives. $T_p M$ is then defined as the space composed of all equivalence classes of derivatives of curves at p and easily proven to be a vector space with the same dimension as M [28]. If x_i are the components of a local coordinate system at p , then the associated basis of $T_p M$ is proven to be $\frac{\partial}{\partial x_i}(p)$, and in this way vectors in $T_p M$ can be obtained from curves in M , *i.e.*, vectors can be seen as *operators* acting on

the space of smooth functions over M . Naturally, as a vector space, $T_p M$ has a dual space $T_p^* M$ called *cotangent space to M at p* , whose dual basis is proven to be $dx_i(p)$. As we are considering only finite-dimensional manifolds, $T_p M \simeq T_p^* M$. We can also define *tangent TM* and *cotangent bundles $T^* M$ of M* as being the union of all tangent and cotangent spaces at all points in M .

Let $f : M \rightarrow N$ be a smooth (class C^∞) mapping from a manifold M to a manifold N . Taking $p \in M$ and $f(p) \in N$, a mapping $df_p : T_p M \rightarrow T_{f(p)} N$ is also induced by f and called its *pushforward* at p . What this function does is to associate a vector in $T_p M$ to a vector in $T_{f(p)} N$: if $(x \circ \gamma)'(0)$ is a tangent vector to M at p in a coordinate system x , then $(y \circ f \circ \gamma)'(0)$ is a vector tangent to N at $f(p)$ in the coordinate system y (this definition is clearly coordinate free). The transpose of the pushforward is called *pullback*, and is a function $f_p^* : T_{f(p)}^* N \rightarrow T_p^* M$ defined by

$$(f^* \alpha)_p(X) = \alpha_{f(p)}(df_p(X)), \quad (\text{A.1})$$

where α_p is a 1-form in $T_p^* N$ and X is a vector in $T_p N$. Taking $\alpha_p \equiv d\beta_p$, then (A.1) becomes

$$(f^* d\beta)_p(X) = d\beta_{f(p)}(df_p(X)) \quad (\text{A.2})$$

$$= d(\beta \circ f)_p(X) \quad (\text{A.3})$$

$$\iff f^*(d\beta) = d(\beta \circ f), \quad (\text{A.4})$$

where we have omitted the point p and used the chain rule. This identification will be extensively used in this dissertation, though we will often simplify this notation.

Implementing the BHC Series

It is well-known that starting with a Lie algebra $\mathfrak{g}$ it is possible to access its Lie group G through the *exponential map*¹ $\exp : \mathfrak{g} \rightarrow G$. In the case of matrix Lie groups, then the exponential map reduces to the exponential of a matrix, defined by

$$\exp A = \sum_{k=0}^{\infty} \frac{A^k}{k!} . \quad (\text{B.1})$$

The Baker-Hausdorff-Campbell (BHC) formula allows one to obtain elements of a Lie algebra from exponentials, *i.e.*, elements of a Lie group. Its formula for two operators is widely used in Quantum Mechanics²:

$$Z = \log (\exp A \exp B) \quad (\text{B.2})$$

$$= \log \left\{ \exp \left[A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A - B, [A, B]] + \dots \right] \right\} , \quad (\text{B.3})$$

¹Every Lie group is associated to a Lie algebra, but the opposite is not always true. For existence, uniqueness and conditions imposed on the Baker-Hausdorff-Campbell formula see [29].

²Especially when $A = \hat{q}$ and $B = \hat{p}$, which provides us a finite BHC series since $[\hat{q}, [\hat{q}, \hat{p}]] = [\hat{p}, [\hat{q}, \hat{p}]] = 0$, avoiding the usual difficulties of proving this series converges (much to the like of Physicists).

where $\log$ here indicates the logarithm of a matrix. Since the BHC expansion gives us only elements of the Lie algebra generated by A and B , it is easy to see that the generalization

$$Z = \log (\exp A_1 \exp A_2 \dots \exp A_n) , \quad (\text{B.4})$$

where $A_n \in \mathfrak{g}$, is also valid. To calculate those terms the procedure is the same as in (B.3): we expand the exponential series, aggregate terms in powers and compute the logarithm (if it exists). In ramifications of this work we had the need to use the BHC formula with three, sometimes five A_n , and the computational time required for each order quickly increases if we simply express matrices as power series. Based in [30]³, however, we devised a Mathematica function that can return any order of a BHC expression involving any number of matrices much faster than using power series. Also, since Mathematica (as all other algebraic manipulators known to the author) is not prepared to deal with non-commutative algebra in an effective way, we also used the package `Quantum Mathematica v2.3.0`, devised by José Luis Gómez-Muñoz and Francisco Delgado, to simplify and manipulate expressions involving commutators.

We will here give an introduction to this method. Let us start by calculating the BHC terms for two matrices X and Y . Define the matrices

$$F \equiv \exp \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix} , \quad G \equiv \exp \begin{pmatrix} 0 & \sigma_1 & 0 & \dots & 0 \\ 0 & 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \sigma_n \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix} , \quad (\text{B.5})$$

³We refer to this article in case any demonstrations are sought.

and our expression for the n th order of the BHC series for two operators will be given by (see [30])

$$z_n = T(\log FG)_{1,1+n}, \quad (\text{B.6})$$

where T is what we shall call the *vocabulary operator*. Mathematically, T is a vector space isomorphism from the space of polynomials in σ_i -variables to the space of polynomials of operators X and Y , but let us not delve into details about T right now; they will become much clearer further on. Evaluating the exponentials we have

$$F = \begin{pmatrix} 1 & 1 & \frac{1}{2} & \frac{1}{6} & \dots \\ 0 & 1 & 1 & \frac{1}{2} & \dots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & 1 & 1 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}, \quad G = \begin{pmatrix} 1 & \sigma_1 & \frac{\sigma_1\sigma_2}{2} & \frac{\sigma_1\sigma_2\sigma_3}{3} & \dots \\ 0 & 1 & \sigma_2 & \frac{\sigma_2\sigma_3}{2} & \dots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & \sigma_n \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}, \quad (\text{B.7})$$

Which shows F and G are upper triangular with diagonal elements equal to unity. Since all their eigenvalues are 1 it can be proved that, in this case, the logarithm of FG will be finite and unique [31]. In our case we have

$$\log FG = - \sum_{i=1}^n \frac{(-1)^i}{i} (FG - \mathbb{1})^i, \quad (\text{B.8})$$

as proved in [30]. The first three orders of z are, therefore,

$$z_1 = T \left[\log \begin{pmatrix} 1 & 1 + \sigma_1 \\ 0 & 1 \end{pmatrix} \right]_{1,2} = T(\sigma_1^0 + \sigma_1^1) \quad (\text{B.9})$$

$$z_2 = T \left[\log \begin{pmatrix} 1 & 1 + \sigma_1 & \frac{1}{2} + \sigma_2 + \frac{1}{2}\sigma_1\sigma_2 \\ 0 & 1 & 1 + \sigma_2 \\ 0 & 0 & 1 \end{pmatrix} \right]_{1,3} = T \left(\frac{1}{2}\sigma_1^0\sigma_2^1 - \frac{1}{2}\sigma_1^1\sigma_2^0 \right) \quad (\text{B.10})$$

$$z_3 = T \left(\frac{1}{12}\sigma_1^1\sigma_2^0\sigma_3^0 - \frac{1}{6}\sigma_1^0\sigma_2^1\sigma_3^0 + \frac{1}{12}\sigma_1^0\sigma_2^0\sigma_3^1 + \frac{1}{12}\sigma_1^1\sigma_2^1\sigma_3^0 \right. \quad (\text{B.11})$$

$$\left. - \frac{1}{6}\sigma_1^1\sigma_2^0\sigma_3^1 + \frac{1}{12}\sigma_1^0\sigma_2^1\sigma_3^1 \right). \quad (\text{B.12})$$

Now, to each order n we define the n -word to be n times the operator X . What the vocabulary operator T effectively does is to substitute an X for a Y in position i in the n -word for each σ_i ($\sigma^0 \equiv 1$). For example, if we are dealing with order 2 and we have $\sigma_1^1\sigma_2^0 + \sigma_2^1$, then the 2-word is XX and $T(\sigma_1^1\sigma_2^0 + \sigma_2^1) = T(\sigma_1 + \sigma_2) = YX + XY$. This reasoning leads us to

$$z_1 = T(1 + \sigma_1) \quad (\text{B.13})$$

$$= X + Y, \quad (\text{B.14})$$

$$z_2 = T \left(\frac{1}{2}\sigma_2 - \frac{1}{2}\sigma_1 \right) \quad (\text{B.15})$$

$$= \frac{1}{2}(XY - YX) \quad (\text{B.16})$$

$$= \frac{1}{2}[X, Y], \quad (\text{B.17})$$

$$z_3 = T \left(\frac{1}{12}\sigma_1 - \frac{1}{6}\sigma_2 + \frac{1}{12}\sigma_3 + \frac{1}{12}\sigma_1\sigma_2 - \frac{1}{6}\sigma_1\sigma_3 + \frac{1}{12}\sigma_2\sigma_3 \right) \quad (\text{B.18})$$

$$= \frac{YXX}{12} - \frac{XYX}{6} + \frac{XXY}{12} + \frac{YYX}{12} - \frac{YXY}{6} + \frac{XY Y}{12} \quad (\text{B.19})$$

$$= \frac{1}{12}([X - Y, [X, Y]]), \quad (\text{B.20})$$

which is what we would expect by comparison with (B.3). This finishes the example.

In order to find BHC terms for (B.4) we need to define $n - 1$ matrices like (B.7), but using different commuting symbols instead of more σ s. We can show by inspection that such a method works, as we did for two matrices, but a proof is sketched in [30].

Our Mathematica function is composed of two main parts, the first being a routine to form expressions like (B.6) for any number of operators and the second being an implementation of the vocabulary operator. The simplification of expressions like (B.19) to commutators as in (B.20) becomes cumbersome with higher order terms and is done using the aforementioned `Quantum Mathematica` package; it is the most computationally involved step of the process and we couldn't go beyond seventh order. Our needs, however, did not require us to go further than fifth.

Appendix C

Zoom in Some Figures

In this appendix we simply provide some zooms of the integrable approximations for high αs . It might be hard to see the fits in the pictures presented in Chapter 3.

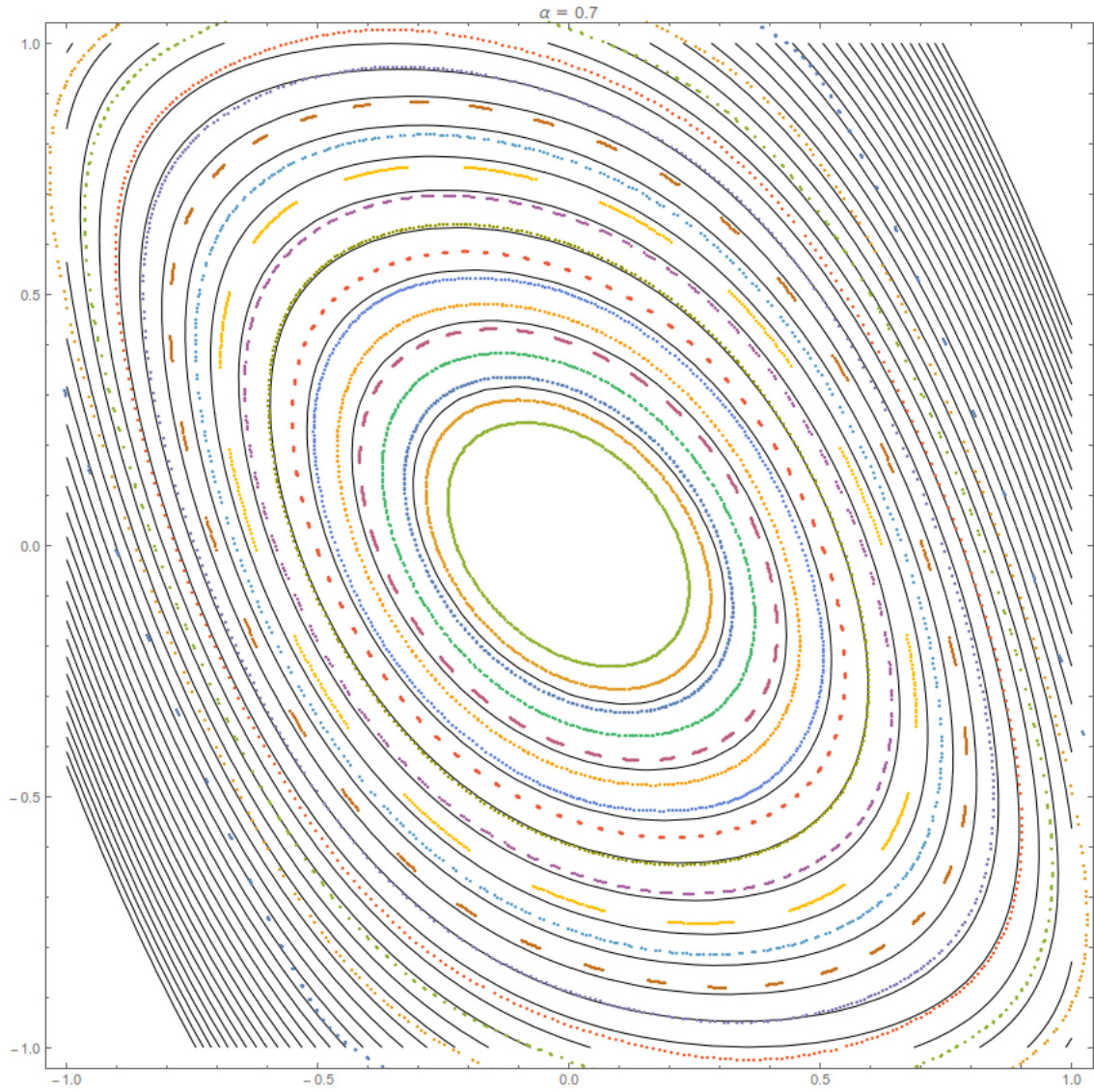


Figure C.1: Zoom in Duffing's Map for $\alpha = 0.7$.

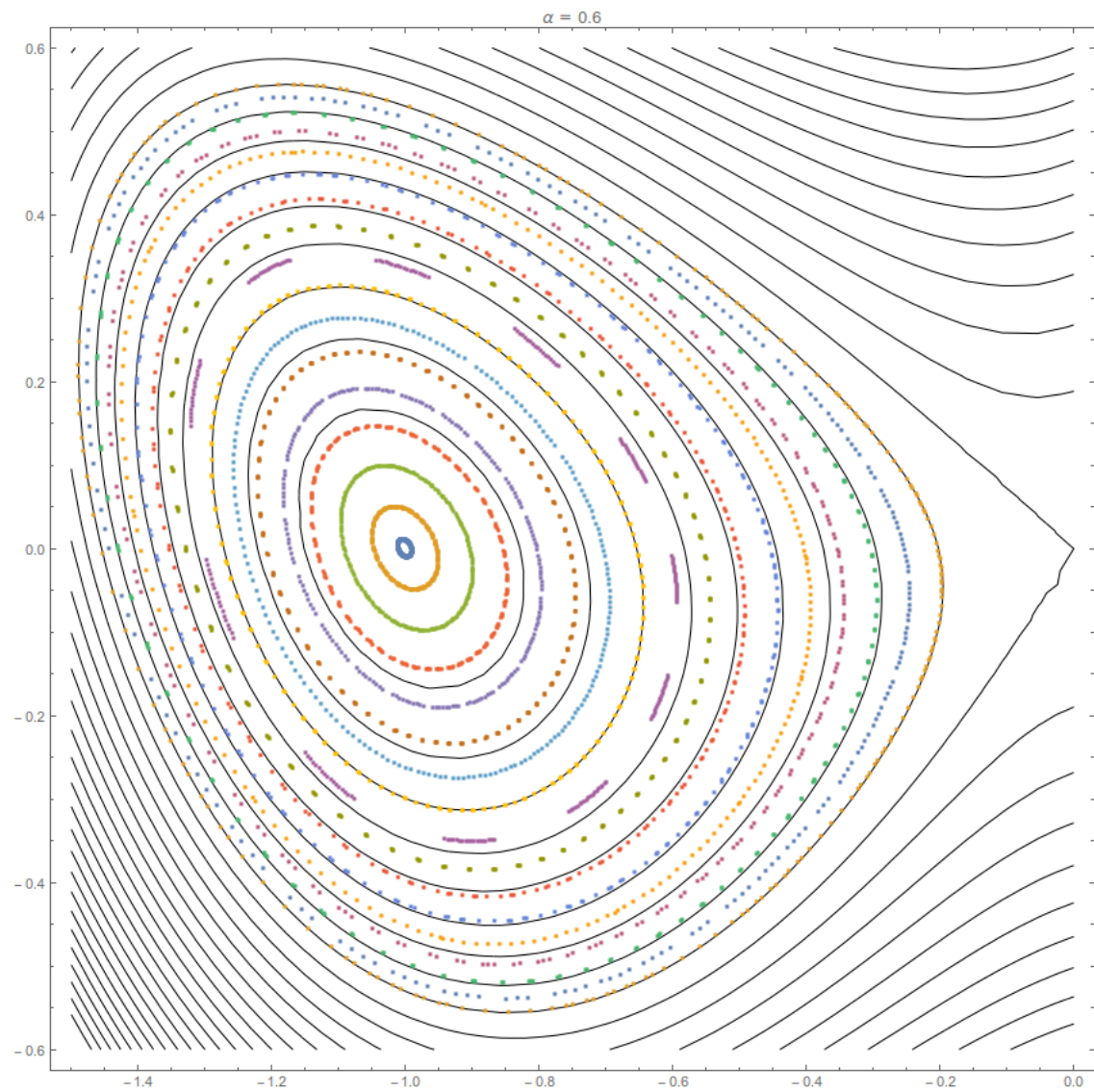


Figure C.2: Zoom in Henon's map for $\alpha = 0.6$.

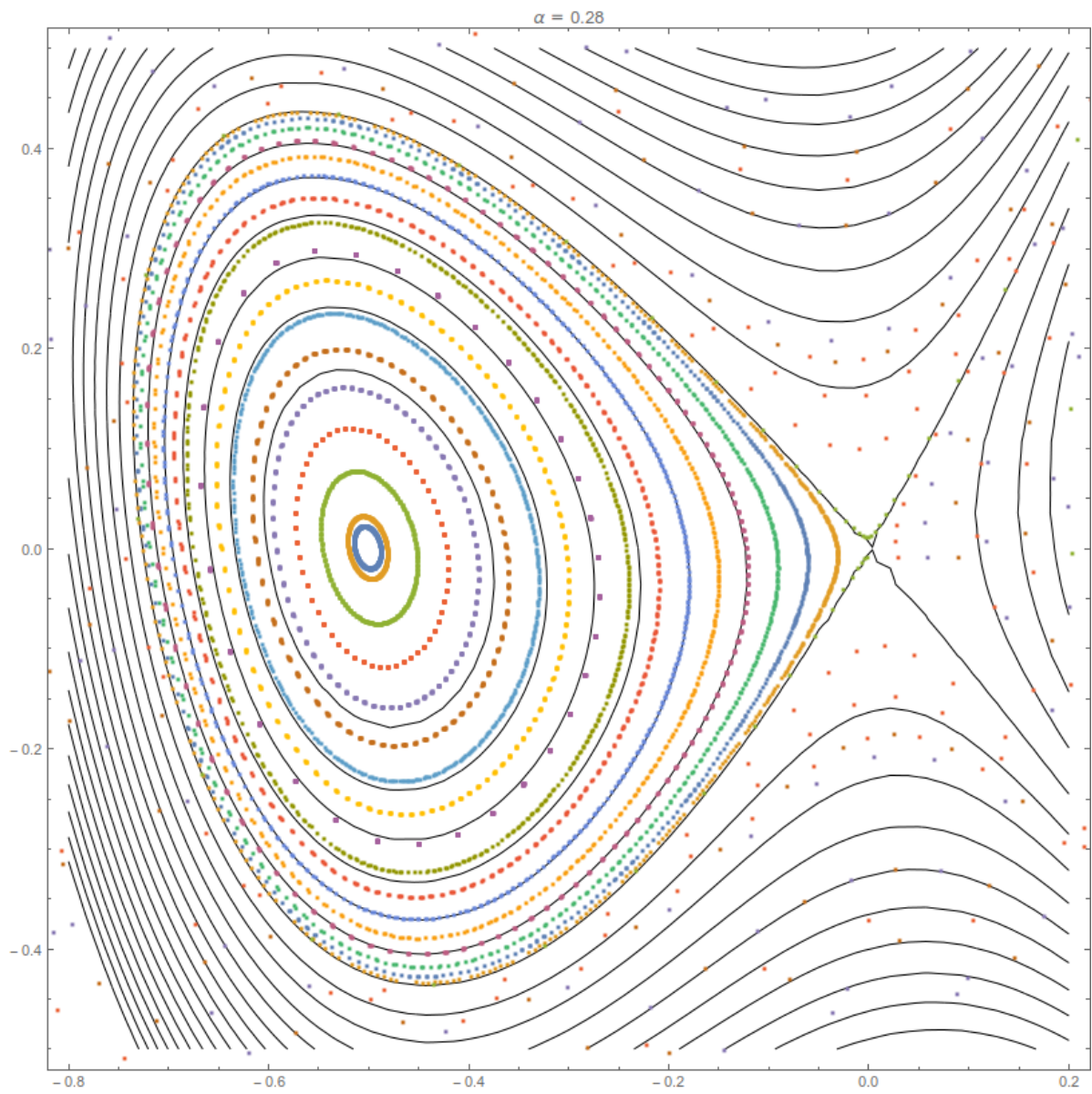


Figure C.3: Zoom in last map's first (elliptic) and second (hyperbolic) fixed points for $\alpha = 0.28$. Notice the external green dots, which falls on the homoclinic orbit.

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