

Geometric Tools for Global Instability of Hamiltonian Systems

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Introduction

These notes are intended as complementary support material for five lectures delivered at The University of Granada dedicated to Global Instability as part of the RTNS course of the DANCE network entitled *Geometric Tools for Global Instability of Hamiltonian Systems*. This Introduction is based upon [DG01], and Chapters 1 and 2 about Nekhoroshev and KAM theory upon [DG96a]. The part of Chapter 3 about single resonances relies on [DG01]. Chapter 4 about Global Instability is based on [DLS06a, DH09, DH11] and Chapter 5 about the Geometric Properties of the Scattering map, on [DLS08]. Chapter 6 about complete families of perturbations is based on [DS17, DS18, DGS24], Chapter 7 about the Elliptic Restricted 3-Body Problem on DelshamsKRS19, Chapter 8 about analytic genericity on [DZ25] and Chapter 9 on the Spatial restricted 3 Body Problem on [DGR26] All these papers can be found in <https://web.mat.upc.edu/amadeu.delshams/>.

0.1 Nearly-integrable Hamiltonians

The Hamiltonian dynamical systems that are close to integrable ones appear in a natural way as models of a wide class of real systems, and thus constitute a very active field of research in classical mechanics. The behavior of these systems is far from being completely understood, and one of the most relevant questions is the stability or instability of their trajectories. This problem remains unsolved for systems with more than 2 degrees of freedom.

The unperturbed rôle is played by a (completely) integrable Hamiltonian with n degrees of freedom. The Liouville–Arnold theorem (see for instance [AKN06]) establishes, under certain hypotheses, the existence on some region of the phase space of canonical *action–angle variables* $(\phi, I) = (\phi_1, \dots, \phi_n, I_1, \dots, I_n) \in \mathbb{T}^n \times G \subset \mathbb{T}^n \times \mathbb{R}^n$, in which the Hamiltonian only depends on the action variables: $h(I)$. The associated Hamiltonian equations for a trajectory $(\phi(t), I(t))$ are

$$\dot{\phi} = \omega(I), \quad \dot{I} = 0,$$

where $\omega = \partial_I h$. Hence the dynamics is very simple: every n -dimensional torus $I = \text{const}$ is invariant, with linear flow $\phi(t) = \phi(0) + \omega(I)t$, and thus all trajectories are stable. The motion on a torus is called quasiperiodic, with associated *frequencies* given by the vector $\omega(I) = (\omega_1(I), \dots, \omega_n(I))$.

Every n -dimensional invariant torus can be nonresonant or resonant, according to whether its frequencies are rationally independent or not. A nonresonant torus is densely filled by any of its trajectories. On the other hand, a resonant torus is foliated into a family of lower dimensional tori.

A *nearly-integrable* Hamiltonian can be written in the form

$$H(\phi, I) = h(I) + \varepsilon f(\phi, I), \tag{1}$$

where ε is a small perturbation parameter. Then the Hamiltonian equations are

$$\dot{\phi} = \omega(I) + \varepsilon \partial_I f(\phi, I), \quad \dot{I} = -\varepsilon \partial_\phi f(\phi, I).$$

For $\varepsilon \neq 0$, the dynamics can be very complicated: there can exist, in principle, chaotic trajectories or even unstable (in the sense that they can wander very far from their initial conditions). Note that the variation of the actions $|I(t) - I(0)|$ could grow slowly but unboundedly.

Although there may exist unstable trajectories, two very relevant results on stability have been established for nearly-integrable Hamiltonian systems. These are the *KAM theorem* and the *Nekhoroshev theorem*. We are going to give a brief description of both of them, putting emphasis on the fact that they lead to two different notions of stability.

0.2 KAM theorem

We can say that KAM (Kolmogorov–Arnold–Moser) theory is concerned with the preservation of quasi-periodic motions under small perturbations: the theorem states, under a suitable nondegeneracy condition, that most of the n -dimensional invariant tori $I = \text{const}$ of the integrable Hamiltonian h survive in (1), with some deformation, for $|\varepsilon|$ small enough. In fact, KAM theorem guarantees the preservation of the tori having “sufficiently” nonresonant frequencies, for which the influence of the *small divisors* $\langle k, \omega(I) \rangle$ can be overcome. This is expressed by means of a *Diophantine condition* on the frequency vector $\omega(I)$: for some constants τ and γ ,

$$\left| \langle k, \omega(I) \rangle \right| \geq \gamma |k|^{-\tau} \quad \forall k \in \mathbb{Z}^n \setminus \{0\},$$

where $|k| = \sum_{j=1}^n |k_j|$. The vectors satisfying this condition for given $\tau > n-1$ and $\gamma > 0$ fill a Cantorian set of relative measure $1 - O(\gamma)$ in $\mathbb{R}^n$. In this way, one obtains *perpetual stability* in the perturbed Hamiltonian, but only for initial conditions on the perturbed or *KAM tori* (the surviving ones), which form a Cantorian set not containing any open subset although its measure is large.

The KAM theorem was “discovered” in the 50’s by Kolmogorov [Kol57] constituted one of the most relevant advances about stability in nearly-integrable Hamiltonian systems. In his first theorem, Kolmogorov established the preservation of only one fixed Diophantine torus (see also [BGS84]). Some years later, Arnold [Arn63] proved, in the analytic case, the existence of a large family of invariant tori, giving an estimate for the measure of their complementary set (see also [Pös82]). Also, Moser [Mos62] proved an analogous theorem, in the differentiable case, for area-preserving maps satisfying a twist condition. As general references on KAM theory, see [Bos86, BHS96].

The nondegeneracy condition required in KAM theorem is imposed on the frequency map $\omega = \partial_I h$ to ensure that a large set of actions I have Diophantine frequencies $\omega(I)$. There are two usual types of conditions:

$$\det(\partial_I \omega(I)) \neq 0, \quad \det \begin{pmatrix} \partial_I \omega(I) & \omega(I) \\ \omega(I)^\top & 0 \end{pmatrix} \neq 0,$$

(for all $I \in G$), that can be called, respectively, *Kolmogorov nondegeneracy* and *isoenergetic nondegeneracy*. The second one is also called Arnold nondegeneracy. Under any of these conditions, for a given $\varepsilon > 0$ the invariant tori whose frequencies satisfy the Diophantine condition with $\tau > n-1$ and $\gamma = O(\sqrt{\varepsilon})$ are preserved, and the measure of the complement is small: $O(\sqrt{\varepsilon})$ (see [Pös82]).

Although the two versions (Kolmogorov and isoenergetic) of KAM theorem are known since the works by Kolmogorov, Arnold and Moser, there are only a few published proofs of the isoenergetic version. Complete proofs are given in [Dou82, BH91], indirectly from the Kolmogorov version. A direct proof of the isoenergetic KAM theorem, without using the Kolmogorov version, can be found in [DG96a].

It has to be pointed out that the isoenergetic condition is more significant from the point of view of the stability, since it ensures the existence of a large family of KAM tori on each energy level $H = \text{const}$. For $n = 2$, one deduces stability even for trajectories which do not lie on these tori, because these 2-dimensional invariant tori separate the 3-dimensional energy levels. This reasoning does not hold for $n > 2$, and one cannot guarantee stability. So in this case there could exist unstable trajectories, although it seems clear that the KAM tori should constitute stronger barriers to instability.

In these notes we will only deal with KAM and Nekhoroshev theory for Hamiltonian systems close to integrable ones written in action-angle variables. For a KAM theory without action-angle variables, see [LGJV05].

For systems violating systematically the Kolmogorov nondegeneracy, there is a *non-twist* KAM theorem, see [Sim98, DL00, GEHL14].

For general surveys on KAM theory, see [Lla01, HCF⁺16].

0.3 Nekhoroshev theorem and effective stability

The other relevant result to be commented here is Nekhoroshev theorem, which leads to the concept of *effective stability*. Nekhoroshev theorem [Nek77], first stated in 1977, establishes for all the trajectories of the system (1) that the variation of the action variables remains small for a very long time, exponentially large with respect to the parameter $\varepsilon > 0$. For every initial condition $(\phi(0), I(0))$ one has an estimate of the type

$$|I(t) - I(0)| \leq r_0 \varepsilon^b \quad \text{for } |t| \leq T_0 \exp \left\{ (\varepsilon_0 / \varepsilon)^a \right\}.$$

The constants $a, b > 0$ are called *stability exponents*.

For the validity of Nekhoroshev theorem one imposes a *steepness condition* (see [Nek77]) on the integrable Hamiltonian h . This is a very general condition, avoiding the quick escape of trajectories along certain directions related to resonances of the frequency vector $\omega(I) = \partial_I h(I)$. The simplest case is that of *quasiconvex* functions: one says h to be quasiconvex if, for any $I \in G$ and $v \in \mathbb{R}^n$,

$$\langle v, \omega(I) \rangle = 0 \implies \langle v, \partial_I^2 h(I) v \rangle \neq 0.$$

For a perturbation of a quasiconvex Hamiltonian, the estimate of Nekhoroshev theorem holds with the stability exponents

$$a = b = \frac{1}{2n}.$$

The proof of the theorem with these exponents has been given in [LN92, Pös93]. However, Chirikov [Chi79] had predicted several years before that the exponent $a = 1/2n$ should be optimal, a fact that was overlooked until it was explained in Lochak's survey [Loc92] (see also [Loc93]), where the exponent $a = 1/(2n + 1)$ was already obtained.

Comparing Nekhoroshev theorem to KAM theorem, we see that perpetual stability has been replaced by finite time stability, but on the other hand the estimates are valid for all trajectories in the phase space. Since (despite the theoretical importance of KAM theorem) it is not possible to know whether a given trajectory lies on a KAM torus, the effective stability estimates are of obvious interest from the point of view of the applications. Some recent results are intending to fill the gap between KAM and Nekhoroshev theorems. These results concern the “stickiness” of KAM tori [PW94], as well as the remarkable results about “superexponential stability” [MG95], or the existence of “quasi-invariant tori” [DG96a].

0.4 Arnold diffusion: whiskered tori, splitting, and transition chains

Nothing is said in KAM theorem about the stability of the trajectories close to unperturbed resonant invariant tori. Nekhoroshev theorem does not exclude the existence of unstable trajectories, but predicts for them an exponentially long stability time. This extremely slow phenomenon of instability is called *Arnold diffusion*, and a first description of it was given in 1964 by Arnold [Arn64] by means of his famous example. As noticed in section 0.2, diffusion can only take place for more than 2 degrees of freedom.

[Add systems studied](#)

Chapter 1

Nekhoroshev theory

1.1 Introduction to KAM and Nekhoroshev theory

We consider a *nearly-integrable Hamiltonian* written in *action-angle variables*:

$$H(\phi, I) = h(I) + f(\phi, I), \quad (1.1)$$

where $\phi = (\phi_1, \dots, \phi_n) \in \mathbb{T}^n$ and $I = (I_1, \dots, I_n) \in \mathcal{G} \subset \mathbb{R}^n$ are, respectively, the angular and action variables, and f is a small perturbation, of size ε , of the integrable Hamiltonian h . It is well-known that the dynamics associated to the unperturbed Hamiltonian h is very simple: the action $I(t)$ remains constant for all motions. Then, all n -dimensional tori $I = \text{const.}$ in phase space $\mathbb{T}^n \times \mathcal{G}$ are invariant. The flow on each torus is linear, with frequency vector $\omega(I) = \text{grad } h(I)$.

In general, for the perturbed system associated to (1.1), the dynamics can be very complicated. It is thought that there are unstable motions, and that Arnold diffusion takes place. Concerning stability, the main results are provided by Nekhoroshev and KAM (Kolmogorov–Arnold–Moser) theorems.

Nekhoroshev theorem, which was first proved in [Nek77], leads to the concept of *effective stability*. Roughly speaking, it states that an estimate of the type

$$|I(t) - I(0)| < R_0 \varepsilon^b \quad \text{for } |t| \leq T_0 \cdot \exp \left\{ \left(\frac{\varepsilon_0}{\varepsilon} \right)^a \right\},$$

holds for all initial conditions $(\phi(0), I(0)) \in \mathbb{T}^n \times \mathcal{G}$, provided *steepness* conditions are fulfilled by h . The *stability exponents* a and b are positive constants. For the case of a perturbation of a *quasiconvex* Hamiltonian (the simplest kind of steepness), these exponents have been successively improved along several papers. Thus, the exponent $a = 2/(n^2 + n)$ was found in [BGGS84]; and $a < 1/(2n + 1)$ in [Loc90b]. Finally, the exponents

$$a = b = \frac{1}{2n},$$

are stated in [LN92], [Pös93]. It has been conjectured [Chi79] that the exponent $a = 1/2n$ is *optimal*.

Estimates of an analogous type can be obtained for the case of a perturbation of a system of *harmonic oscillators*: $H(\phi, I) = \omega \cdot I + f(\phi, I)$, where ω is now a constant vector satisfying a Diophantine condition:

$$|k \cdot \omega| \geq \frac{\gamma}{|k|_1^\tau} \quad \forall k \in \mathbb{Z}^n \setminus \{0\}, \quad (1.2)$$

for some $\tau \geq n - 1$ and $\gamma > 0$ (it is well-known that, if $\tau > n - 1$, the set of vectors ω satisfying this condition for a given $\gamma > 0$ has relative measure $1 - O(\gamma)$ in $\mathbb{R}^n$). We use the notation $|k|_1 = \sum_{j=1}^n |k_j|$ for $k = (k_1, \dots, k_n)$. We say a vector ω satisfying (1.2) to be τ, γ -*Diophantine*. In this case, the optimal stability exponent seems to be $a = 1/(\tau + 1)$. This exponent has been obtained in [GDF⁺89], [Fas90] and [DG93].

KAM theorem states, under a suitable nondegeneracy condition, that most of the n -dimensional invariant tori are preserved with some deformation in the perturbed system (1.1) if the size ε of the perturbation is small enough. More precisely, this preservation is guaranteed for tori that have frequency vector $\omega(I) = \text{grad } h(I)$ satisfying a Diophantine condition. In this way, one gets *perpetual stability*, but only for initial conditions on a Cantorian set, which does not contain any open set although its measure

is large. In fact, it was first stated by Kolmogorov [Kol57] for analytic Hamiltonians, the preservation of one given torus, suitably chosen. Afterwards, Arnold proved in [Arn63] (see also [Pös82]) the existence of a large family of invariant tori and estimated the measure of the complement of the invariant set. An analogous theorem for area-preserving maps of the plane was proved by Moser [Mos62], without the hypothesis of analyticity.

Concerning the nondegeneracy condition required for the validity of KAM theorem, two sorts of conditions are usually imposed on the unperturbed frequency map $\omega = \text{grad } h$, namely the (*standard*) *nondegeneracy* and the *isoenergetic nondegeneracy* (see definitions (2.1–2.2) in section 2.1.1). There are slight differences between the statements of KAM theorem under both nondegeneracies. Indeed, in the standard case every preserved invariant torus keeps its frequency vector in the perturbation. In the isoenergetic case, the frequency vector is not usually kept but, nevertheless, every invariant torus keeps its frequency ratios and its energy and, moreover, on each fixed energy hypersurface most of the invariant tori are preserved. A well-known consequence is that, for two degrees of freedom ($n = 2$), it follows from the isoenergetic nondegeneracy the stability of the perturbed system.

The usual proofs of Nekhoroshev and KAM theorems do not allow to stress the close relationship existing between the different types of stability provided by these theorems. Actually, no use is made of the existence of the KAM tori in the proof of Nekhoroshev theorem, which gives a uniform stability time for all trajectories in phase space. These trajectories include the ones lying in KAM tori, which are the most numerous, and clearly have an infinite stability time. But one can also expect that, for a trajectory starting near a KAM torus, the stability time is much larger than the one predicted by Nekhoroshev theorem. Results concerning this “stickiness” of KAM tori, with Nekhoroshev-like estimates, have recently been obtained in [PW94], [MG95].

In these lectures we are concerned about a unified approach to Nekhoroshev and KAM theorems, already announced in [DG94]. After a preliminary part where the common method is set up, we give quantitative proofs of Nekhoroshev theorem under the assumption of quasiconvexity (theorem 1.4 in section 1.3.5) and the isoenergetic KAM theorem (theorem 2.1 in section 2.1.4). We notice that our approach to the isoenergetic theorem is direct, unlike the usual proofs where it is deduced from the standard KAM theorem (see, for example, [BH91]) or making use of the associated Poincaré map (see [Mos68]).

Moreover, under the same hypothesis of KAM theorem, we get a Nekhoroshev-like stability result (theorem 2.2 in section 2.1.5) which is slightly different from the ones of [PW94] and [MG95]. The result we prove considers the invariant tori of the unperturbed system such that their associated frequency vector satisfies approximately, up to a given precision r , a Diophantine condition. In the perturbed system, these tori survive in the form of *nearly-invariant tori*, i.e., the trajectories starting on such a torus remain near to it up to a stability time which is exponentially long in $1/r$. This result is similar to the one of [MG93] where, however, the estimates are expressed in terms of the stability time, which is previously fixed.

On the other hand, in [PW94] and [MG95] the stability estimates are expressed in terms of the distance to a given KAM torus, meaning in this way the “stickiness” of KAM tori. The stability time is then exponentially long in the inverse of this distance (or even “superexponentially” long for quasiconvex Hamiltonians [MG95]). We do not prove that KAM tori are “sticky” but we believe that our result is more useful for practical purposes, since our estimates for nearly-invariant tori do not require the existence of a KAM torus nearby.

The method we follow for the proof of Nekhoroshev and KAM theorems is standard in classical perturbation theory. It consists of seeking for a suitable canonical transformation Ψ , bringing our Hamiltonian H into a *normal form* $H^* = H \circ \Psi$, asked to depend on less angles, none if possible. The transformation Ψ is constructed iteratively as a product of successive canonical transformations $\Phi^{(1)}, \Phi^{(2)}, \dots$, near to the identity, which provide a sequence of Hamiltonians $H^{(1)}, H^{(2)}, \dots$ coming nearer and nearer to the normal form.

We construct the successive canonical transformations with the help of the well-known *Lie series formalism*, which we describe in section 1.2.1. This is a very suitable procedure for practical applications, since it allows to carry out explicit computations in concrete examples. The procedure can be directly implemented in computers, since we only use harmonics of finite order.

It is well-known that an obstruction for the construction of the normal form is found on the resonances or near them. A *resonant manifold* is characterized by a given module $\mathcal{M} \subset \mathbb{Z}^n$:

$$S_{\mathcal{M}} := \{I \in \mathcal{G} : k \cdot \omega(I) = 0 \quad \forall k \in \mathcal{M}\}. \quad (1.3)$$

The obstruction comes from the presence of the *small divisors* $k \cdot \omega(I)$, with $k \in \mathcal{M}$, which can be zero

or too small. It is because of the presence of the small divisors that one considers, near the resonance $S_{\mathcal{M}}$, a *resonant normal form*, which accepts dependence on combinations of angles $k \cdot \phi$, with $k \in \mathcal{M}$. The union of all resonances is dense in the set of frequencies, but one only needs to consider resonances up to a given suitable finite *order*: $|k|_1 \leq K$, since it turns out that the effect of higher-order resonances is exponentially small in K . Thus, we say a function $g(\phi, I)$ to be in *normal form with respect to $\mathcal{M}$ of degree K* if its Fourier series expansion in the angular variables is restricted to the form

$$g(\phi, I) = \sum_{\substack{k \in \mathcal{M} \\ |k|_1 \leq K}} g_k(I) e^{i k \cdot \phi}.$$

We express this by writing $g \in \mathbf{R}(\mathcal{M}, K)$. Note that a function is in normal form with respect to the trivial module $\mathcal{M} = 0$ if it does not depend on the angular variables.

In the first part of this lecture, we restrict ourselves to a subset $G \subset \mathcal{G}$, where the frequency vector $\omega(I)$ is allowed to satisfy resonance relations corresponding to a fixed module $\mathcal{M}$, but a neighborhood of all other resonances of order less or equal than K are excluded. For such a set we say that $\omega(G)$ is *nonresonant modulo $\mathcal{M}$ up to order K* (see definition (1.17) in section 1.2.3). On this set G we make successive reductions to the type of normal form defined above: the harmonics corresponding to integer vectors satisfying $k \notin \mathcal{M}$, $|k|_1 \leq K$, become smaller and smaller in the successive Hamiltonians, whereas the harmonics corresponding to $k \in \mathcal{M}$ or $|k|_1 > K$ have to be kept because in the set G the small divisors $k \cdot \omega(I)$ associated to these harmonics are not avoided. In this way the final Hamiltonian $H^* = H \circ \Psi$ can be written as

$$H^*(\phi, I) = h(I) + Z^*(\phi, I) + R^*(\phi, I),$$

where $Z^* \in \mathbf{R}(\mathcal{M}, K)$ and the remainder R^* is exponentially small in K .

As in [Nek77] and [BGS84], the proof of Nekhoroshev theorem is divided into two parts, usually named analytic and geometric ones. The analytic part concerns the iterative process and the estimates for the successive remainders. In the geometric part the whole action space $\mathcal{G}$ is covered by a family of sets associated to every module in order to get stability estimates for the trajectories corresponding to all initial conditions. A similar distinction may also be carried out in the proof of KAM theorem. In this case the geometric part concerns the estimates for the measure of the complement of the invariant set.

For given $\mathcal{M}$ and K , we consider a subset $G \subset \mathcal{G}$ where the nonresonance condition quoted above is satisfied. In section 1.2.1, we show how the Lie series method is applied to the construction of the iterative process, which is finite for the proof of Nekhoroshev theorem and infinite for KAM theorem. In the case of KAM theorem we always take $\mathcal{M} = 0$. The Iterative Lemma (theorem 1.1 in section 1.2.3), which is common to both proofs, provides estimates for one given step of this process. We make use of a *vectorfield norm*, introduced in section 1.2.2, which allows us to optimize the estimates of the Iterative Lemma with respect to other related papers.

From successive application of the Iterative Lemma, with a fixed K , and carrying out an appropriate number of iterative steps, we get the Normal Form Theorem (theorem 1.2 in section 1.3.1), where the estimate obtained for the remainder is exponentially small in K , and hence H^* is an approximate normal form, specific for the set G . This theorem completes the analytic part of the proof of Nekhoroshev theorem. We point out that this approach is carried out along the lines of Pöschel's proof [Pös93] of Nekhoroshev theorem, but our proof is somewhat simpler because the Iterative Lemma has been optimized.

From the Normal Form Theorem, one can deduce stability estimates for the trajectories starting in $\mathbb{T}^n \times G$, which hold up to an exponentially long time. The estimates for nonresonant ($\mathcal{M} = 0$) and resonant ($\mathcal{M} \neq 0$) regions are given in sections 1.3.2 and 1.3.3, respectively. In the resonant case we impose a quasiconvexity condition. Following [Pös93], in the geometric part of the proof, the whole domain $\mathcal{G}$ is covered by a family of sets $G = G_{\mathcal{M}}$ associated to the different modules $\mathcal{M} \subset \mathbb{Z}^n$, with suitably chosen parameters (section 1.3.4). One sees that it suffices to consider *K -modules* (a module $\mathcal{M} \subset \mathbb{Z}^n$ is said to be a K -module if it is generated by vectors of order less or equal than K). To complete the proof of Nekhoroshev theorem (section 1.3.5), with optimal exponents, we choose K as a suitable function of ε and apply the stability estimates to each set $G_{\mathcal{M}}$. In this way, we obtain estimates for all trajectories starting in $\mathbb{T}^n \times \mathcal{G}$.

As an additional application of the Normal Form Theorem, we also consider a perturbation of a system of n harmonic oscillators with a Diophantine frequency vector. The nonresonant estimates of the case $\mathcal{M} = 0$ give rise to effective stability in such a system (theorem 1.3 in section 1.3.2).

Our approach to KAM theorem is parallel, in its main lines, to the Arnold's one [Arn63]. We first prove the Inductive Lemma (proposition 2.4 in section 2.1.3), which concerns the estimates given by

the Iterative Lemma, with $\mathcal{M} = 0$, for one given step of the iterative process. In this case, it does not suffice to bring our Hamiltonian H to an approximate normal form with an exponentially small remainder. It is necessary to perform an infinite number of iterations, with orders $K_1, K_2, \dots$ increasing to infinity. Then, the resonances up to higher and higher orders are removed from the domain along the successive iterative steps. In this way, the remainders tend quickly to zero and the final Hamiltonian becomes integrable: $H^*(\phi, I) = h^*(I)$. Therefore, the domain where the transformation holds is filled with n -dimensional invariant tori with linear flow, but it shrinks to a Cantorian set corresponding to Diophantine frequencies. To finish the proof of KAM theorem, the measure of the invariant set can be estimated assuming that a suitable nondegeneracy condition is fulfilled by the unperturbed system.

In section 2.1.4, we give this direct proof of KAM theorem under the hypothesis that the unperturbed frequency map ω is isoenergetically nondegenerate. We point out that the same scheme would be useful for the standard nondegeneracy. An explanation of both nondegeneracy conditions and the technical difficulties arising in the isoenergetic case is given in section 2.1.1 (quantitative lemmas are provided in section 2.1.2). This common approach to both nondegeneracy conditions can be seen as a first step towards the proof of KAM theorem under higher-order nondegeneracy conditions. We recall that a very general condition was introduced by Rüssmann [Rüs90]. See [Sev95], [CS94], [XYQ97, XY07] for other recent results along this line.

Finally, we see in section 2.1.5 that, inside the same iterative scheme used for KAM theorem but stopping it at an appropriate step, instead of carrying it to the limit, we find that Nekhoroshev-like estimates hold for the trajectories starting in the domain at this step. This domain is then filled with nearly-invariant tori (theorem 2.2). This result is quantitatively very close to KAM theorem. Qualitatively, the perpetual stability of KAM tori is sacrificed but, on the other hand, the domain where the result holds contains inner points, and hence it is not a Cantorian set.

It is worth reminding that KAM theorem is meaningless from a practical point of view despite its theoretical importance. This is due to the fact that, from an approximation of a concrete frequency vector, one cannot decide whether this vector is Diophantine or not. The notion of nearly-invariant torus may be understood as an attempt to compensate this deficiency.

1.2 The common part

1.2.1 Normal forms via the Lie series method

We describe in this section the iterative process leading our Hamiltonian $H(\phi, I) = h(I) + f(\phi, I)$ to normal form. This setup provides a common environment for the proofs of Nekhoroshev and KAM theorems. According to the approach described in the introduction, we restrict our Hamiltonian H to a subset $G \subset \mathcal{G}$, where it is assumed that the frequency set $\omega(G)$ is nonresonant modulo $\mathcal{M}$ up to order K for given $\mathcal{M}$ and K . For notational convenience, we consider the starting Hamiltonian H written, on the set G , in the form

$$H(\phi, I) = h(I) + Z(\phi, I) + R(\phi, I), \quad (1.4)$$

with $Z \in \mathbf{R}(\mathcal{M}, K)$. For instance, we may choose $Z = 0$ and $R = f$. However, if the starting Hamiltonian is already near to the normal form, we may write it in the form (1.4), with a small R with respect to Z , and seek for a better approximation to the normal form.

The transformation Ψ leading to normal form is constructed as a product of canonical transformations $\Phi^{(1)}, \Phi^{(2)}, \dots$. We put $\Psi^{(q)} = \Phi^{(1)} \circ \dots \circ \Phi^{(q)}$. At the step q , the transformed Hamiltonian is written in the form

$$H^{(q)} = H \circ \Psi^{(q)} = h + Z^{(q)} + R^{(q)},$$

with $Z^{(q)} \in \mathbf{R}(\mathcal{M}, K)$. Obviously we start with $Z^{(0)} = Z$ and $R^{(0)} = R$.

Now, to describe a concrete iterative step, we write $H, Z, R, \tilde{Z}, \tilde{R}, \Phi$, instead of $H^{(q-1)}, Z^{(q-1)}, R^{(q-1)}, Z^{(q)}, R^{(q)}, \Phi^{(q)}$, respectively. Following the Lie series method, as in [DG93], we construct Φ as the flow at time 1 associated to a generating Hamiltonian W to be determined.

More precisely, if Φ_t denotes the flow at time t of an autonomous Hamiltonian W , it is known from the Hamiltonian theory that, for any function f , the derivative of $f \circ \Phi_t$ with respect to t can be expressed in terms of the Poisson bracket of f and W :

$$\frac{d}{dt}(f \circ \Phi_t) = \{f, W\} \circ \Phi_t.$$

So, assuming analyticity in t and taking the Taylor expansion, one has the Lie series

$$f \circ \Phi_t = \sum_{m=0}^{\infty} \frac{t^m}{m!} L_W^m f,$$

where we denote $L_W^0 f = f$ and $L_W^m f = \{L_W^{m-1} f, W\}$ for $m \geq 1$. For the remainders of the Lie series, we use the notation

$$r_m(f, W, t) := f \circ \Phi_t - \sum_{l=0}^{m-1} \frac{t^l}{l!} L_W^l f = \sum_{l=m}^{\infty} \frac{t^l}{l!} L_W^l f \quad (1.5)$$

for $m \geq 0$.

With this notation, we have for the transformed Hamiltonian the following expression:

$$H \circ \Phi = h + Z + R + \{h, W\} + r_2(h, W, 1) + r_1(Z + R, W, 1). \quad (1.6)$$

We want $\tilde{R}$ to be smaller than R in order to get $H \circ \Phi$ closer to normal form than H . Consequently W should be chosen in such a way that $R + \{h, W\}$ be in normal form. As a matter of fact, this can only be guaranteed up to order K because the nonresonance condition on $\omega(G)$ does not avoid the small divisors corresponding to higher orders. Thus, we seek for $\Delta Z \in \mathbf{R}(\mathcal{M}, K)$ and W solving the linear functional equation

$$\{W, h\} + \Delta Z = R_{\leq K}, \quad (1.7)$$

where we write $R_{\leq K}(\phi, I) = \sum_{|k|_1 \leq K} R_k(I) e^{i k \cdot \phi}$.

The resolution of equation (1.7) is standard. In terms of Fourier coefficients, we have the solution

$$\begin{aligned} W_k(I) &= \frac{R_k(I)}{i k \cdot \omega(I)}, & \Delta Z_k(I) &= 0, & \text{for } k \in \mathbb{Z}^n \setminus \mathcal{M}, |k|_1 \leq K; \\ W_k(I) &= 0, & \Delta Z_k(I) &= R_k(I), & \text{for } k \in \mathcal{M}, |k|_1 \leq K; \\ W_k(I) &= 0, & \Delta Z_k(I) &= 0, & \text{for } |k|_1 > K. \end{aligned} \quad (1.8)$$

This is the only solution of equation (1.7) if we require W to have no resonant terms with respect to $\mathcal{M}$ and to be of degree K . We denote by $\mathbf{NR}(\mathcal{M}, K)$ the set of the functions satisfying these requirements. If h and R are real functions, we see from (1.8) that ΔZ and W are also real.

The new Hamiltonian can be put as

$$H \circ \Phi = h + \tilde{Z} + \tilde{R},$$

with

$$\tilde{Z} = Z + \Delta Z \in \mathbf{R}(\mathcal{M}, K), \quad (1.9)$$

$$\tilde{R} = R_{>K} + r_2(h, W, 1) + r_1(Z + R, W, 1), \quad (1.10)$$

where we write $R_{>K} = R - R_{\leq K}$. If h , Z and R are real, then the transformation Φ preserves real domains, and the new Hamiltonian is also real. Recall that the algorithm explicited in (1.8–1.10) is just one step of the iterative process. It describes how to get $H^{(q)} = H^{(q-1)} \circ \Phi^{(q)}$.

Roughly speaking, this procedure can be considered as linear if we ignore the term $R_{>K}^{(q-1)}$. Indeed, if $Z^{(q-1)} = O(\varepsilon)$, $R^{(q-1)} = O(\varepsilon^q)$, we see from equations (1.9–1.10) that $R^{(q)} = O(\varepsilon^{q+1})$, since the generating Hamiltonian for $\Phi^{(q)}$ is taken of the same order as $R^{(q-1)}$. We use this procedure for the proof of Nekhoroshev theorem (section 1.3.5). The term $R_{>K}^{(q-1)}$ is exponentially small in K . So its influence can be overcome by choosing K large enough.

We remark that the canonical transformation $\Phi^{(q)}$ could also be constructed by means of a quadratic procedure: if $R^{(q-1)} = O(\varepsilon^{2^{q-1}})$, then $R^{(q)} = O(\varepsilon^{2^q})$. We can attain this aim by taking another term of the Lie series in (1.6), which gives rise to an alternative algorithm for the reduction to normal form. However, for an arbitrary module $\mathcal{M}$, the linear equation substituting (1.7) is not easily resolvable, and an approximate solution does not seem to improve the estimates of Nekhoroshev theorem.

In the case of KAM theorem (section 2.1), where $\mathcal{M} = 0$, the linear procedure described in (1.8–1.10) is almost quadratic, provided we take $Z^{(q-1)} = 0$ at each step (the procedure can never be strictly quadratic because of the presence of small divisors). This forces us to a little change in the algorithm: we include $\Delta Z^{(q-1)}$ in the integrable part in order to have $Z^{(q)} = 0$ for the following step. In this way, the integrable part changes at every step: we begin the step q with $H^{(q-1)}(\phi, I) = h^{(q-1)}(I) + R^{(q-1)}(\phi, I)$, and the new Hamiltonian can be written as

$$H^{(q)}(\phi, I) = h^{(q)}(I) + R^{(q)}(\phi, I), \quad (1.11)$$

where, by (1.8),

$$h^{(q)} = h^{(q-1)} + \Delta Z^{(q-1)} = h^{(q-1)} + R_0^{(q-1)} \quad (1.12)$$

(note that the function $R_0^{(q-1)}(I)$ is the angular average of $R^{(q-1)}(\phi, I)$). The new remainder $R^{(q)}$ is obtained like in (1.10), which then gives a fastly convergent procedure if the term $R_{>K}^{(q-1)}$ is ignored. To solve the difficulty caused by this term, we take increasing orders K_q , tending to infinity for $q \rightarrow \infty$. We can then see the convergence to zero of the remainders $R^{(q)}$, and hence the existence of invariant tori. However, resonances of successive higher orders have to be removed along the procedure and hence the final domain is reduced to a Cantorian set.

Another remark is that in section 2.1.4 we prove KAM theorem without showing explicitly that the remainders $R^{(q)}$ converge in a fast way, but linear. Nevertheless, we use the almost quadratic convergence of the remainders to show the existence of nearly-invariant tori, with exponential estimates (see section 2.1.5).

1.2.2 A norm for Hamiltonian vectorfields

In order to obtain rigorous estimates for the successive remainders, we need to define norms for the functions taking part in the iterative process introduced in section 1.2.1.

An important remark is that a Hamiltonian function H does not take part directly in the Hamiltonian equations, but rather its derivative

$$DH = \left(\frac{\partial H}{\partial \phi}, \frac{\partial H}{\partial I} \right) = \left(\frac{\partial H}{\partial \phi_1}, \dots, \frac{\partial H}{\partial \phi_n}, \frac{\partial H}{\partial I_1}, \dots, \frac{\partial H}{\partial I_n} \right).$$

Then, to obtain the stability estimates leading to the proof of Nekhoroshev and KAM theorems, we do not need to obtain estimates for the successive remainders provided by (1.10), but estimates for the derivatives of these remainders suffice.

Looking carefully at equations (1.9–1.10), one realizes that it is possible to bound the derivatives $D\tilde{Z}$ and $D\tilde{R}$ from the derivatives DZ and DR , since the Lie remainders r_1, r_2 have been defined in (1.5) in terms of Poisson brackets. So it would be a nice tool to work with a suitable vectorfield norm for the derivatives, which would avoid unnecessary uses of the Cauchy inequalities in estimating derivatives. This idea was suggested to us by A. I. Neishtadt, although it goes back to [Fas90], where estimates for the Lie series method for not necessarily Hamiltonian vectorfields are fully developed.

However, we cannot avoid all uses of the Cauchy inequalities, since the remainders r_1, r_2 in (1.10) have to be differentiated in order to estimate $D\tilde{R}$. Moreover, a differentiation has to be done before starting the first iterative step. Thus, we work with analytic functions on complex neighborhoods of the domain $\mathbb{T}^n \times G$. Given $\rho = (\rho_1, \rho_2) \geq 0$ (i.e. $\rho_j \geq 0, j = 1, 2$), we first introduce the sets:

$$\begin{aligned} \mathcal{W}_{\rho_1}(\mathbb{T}^n) &:= \{\phi : \operatorname{Re} \phi \in \mathbb{T}^n, |\operatorname{Im} \phi|_\infty \leq \rho_1\}, \\ \mathcal{V}_{\rho_2}(G) &:= \{I \in \mathbb{C}^n : |I - I'| \leq \rho_2 \text{ for some } I' \in G\}, \end{aligned}$$

where $|\cdot|_\infty$ and $|\cdot| = |\cdot|_2$ denote, respectively, the maximum norm and the Euclidean norm for vectors. We then define:

$$\mathcal{D}_\rho(G) := \mathcal{W}_{\rho_1}(\mathbb{T}^n) \times \mathcal{V}_{\rho_2}(G).$$

Several kinds of norms are used along this lectures. First, we consider functions of the n action variables. Given a (real or complex) function $f(I)$, defined on a complex neighborhood $\mathcal{V}_\eta(G)$, $\eta \geq 0$, we introduce the supremum norm:

$$|f|_{G, \eta} := \sup_{I \in \mathcal{V}_\eta(G)} |f(I)|, \quad |f|_G := |f|_{G, 0}.$$

In this way, the subscript η is removed from the notation if $\eta = 0$. This remark applies throughout this section.

In an analogous way, we consider the supremum norm for vector-valued functions, i.e. vectorfields. Given $F : \mathcal{V}_\eta(G) \rightarrow \mathbb{C}^n$ and $1 \leq p \leq \infty$, we define

$$|F|_{G,\eta,p} := \sup_{I \in \mathcal{V}_\eta(G)} |F(I)|_p, \quad |F|_{G,\eta} := |F|_{G,\eta,2}.$$

In this definition, $|\cdot|_p$ means the p -norm for vectors in $\mathbb{C}^n$, i.e.: $|v|_p = \left(\sum_{j=1}^n |v_j|^p\right)^{1/p}$ for $1 \leq p < \infty$, and $|v|_\infty = \max_{1 \leq j \leq n} |v_j|$. Note that we remove the subscript p to mean the Euclidean norm ($p = 2$).

We also define the supremum norm for matrix-valued functions or even tensor-valued functions (e.g. successive total derivatives of a function). The definition is analogous, taking for matrices and tensors the norm induced by the Euclidean norm for vectors (we only consider the case $p = 2$).

Next we consider functions of the action-angle variables. For a given complex function $f(\phi, I)$ (2π -periodic in ϕ) defined on the neighborhood $\mathcal{D}_\rho(G)$, $\rho = (\rho_1, \rho_2) \geq 0$, we may consider its supremum norm:

$$|f|_{G,\rho} := \sup_{(\phi, I) \in \mathcal{D}_\rho(G)} |f(\phi, I)|. \quad (1.13)$$

But if f is *analytic* on (a neighborhood of) the set $\mathcal{D}_\rho(G)$, we may define an exponentially weighted norm in terms of the Fourier series of f . Writing $f(\phi, I) = \sum_{k \in \mathbb{Z}^n} f_k(I) e^{i k \cdot \phi}$, we introduce

$$\|f\|_{G,\rho} := \sum_{k \in \mathbb{Z}^n} |f_k|_{G,\rho_2} \cdot e^{|k|_1 \rho_1}. \quad (1.14)$$

Note that $|f|_{G,\rho} \leq \|f\|_{G,\rho}$. This exponentially weighted norm, analogous to the one used in [Pös93], allows to carry out easily a separate control of harmonics in estimating the solution of the linear functional equation (1.7), in proposition 1.4 of section 1.2.3. This would be more difficult by using the supremum norm.

Exactly in the same way as before we may extend the definitions of the norms (1.13–1.14) to the case of vector-valued functions. Given $F : \mathcal{D}_\rho(G) \rightarrow \mathbb{C}^n$ and $1 \leq p \leq \infty$, and writing $F(\phi, I) = \sum_{k \in \mathbb{Z}^n} F_k(I) e^{i k \cdot \phi}$, where $F_k : \mathcal{V}_{\rho_2}(G) \rightarrow \mathbb{C}^n$, we define

$$\|F\|_{G,\rho,p} := \sum_{k \in \mathbb{Z}^n} |F_k|_{G,\rho_2,p} \cdot e^{|k|_1 \rho_1}, \quad \|F\|_{G,\rho} := \|F\|_{G,\rho,2}.$$

Let us recall the Cauchy inequalities for the ϕ -derivatives and the I -derivatives (see also [Pös93]). Given f analytic on $\mathcal{D}_\rho(G)$, for $0 < \delta < \rho$ (i.e. $0 < \delta_j < \rho_j$, $j = 1, 2$) one has

$$\left\| \frac{\partial f}{\partial \phi} \right\|_{G,(\rho_1-\delta_1,\rho_2),1} \leq \frac{1}{e\delta_1} \|f\|_{G,\rho}, \quad \left\| \frac{\partial f}{\partial I} \right\|_{G,(\rho_1,\rho_2-\delta_2),\infty} \leq \frac{1}{\delta_2} \|f\|_{G,\rho}.$$

To have a more compact writing and to avoid to carry out separate estimates for the ϕ -derivatives and the I -derivatives along the iterative process, we introduce for $Df = \left(\frac{\partial f}{\partial \phi}, \frac{\partial f}{\partial I} \right)$ the vectorfield norm

$$\|Df\|_{G,\rho,c} := \max \left(\left\| \frac{\partial f}{\partial \phi} \right\|_{G,\rho,1}, c \left\| \frac{\partial f}{\partial I} \right\|_{G,\rho,\infty} \right), \quad (1.15)$$

where $c > 0$ is a parameter to be fixed in subsequent sections. This parameter (having the physical dimension of the action variables) is introduced in order to compensate the difference between the Cauchy inequalities for ϕ -derivatives and I -derivatives.

Lemma 1.1. *Let f, g be analytic functions on $\mathcal{D}_\rho(G)$. For $0 < \delta = (\delta_1, \delta_2) < \rho$ and $c > 0$ given, let us denote*

$$\hat{\delta}_c := \min(c\delta_1, \delta_2).$$

Then,

- a) $\|Df\|_{G,\rho-\delta,c} \leq \frac{c}{\hat{\delta}_c} \|f\|_{G,\rho}.$
- b) $\|\{f,g\}\|_{G,\rho} \leq \frac{2}{c} \|Df\|_{G,\rho,c} \cdot \|Dg\|_{G,\rho,c}.$
- c) $\|D(f_{>K})\|_{G,(\rho_1-\delta_1,\rho_2),c} \leq e^{-K\delta_1} \cdot \|Df\|_{G,\rho,c}.$

The proof of the properties contained in this lemma is very simple. In subsequent sections, we shall see that an appropriate choice for the parameter c makes possible to obtain better estimates, even in case of very different δ_1, δ_2 .

More notation is required. At every step of the iterative process described in section 1.2.1, the canonical transformation Φ leading our Hamiltonian to normal form is constructed as a flow associated to the generating Hamiltonian W defined in (1.8). To know how near to the identity map this canonical transformation is, we need to define a norm for maps like $\Phi - \text{id}$. This map is defined in $\mathcal{D}_\rho(G)$, and we may consider it taking values in $\mathbb{C}^{2n}$. First, we take the parameter $c > 0$ of definition (1.15) and, for a $2n$ -vector $x = (\phi, I)$, we introduce its “ c -norm” as

$$|x|_c := \max(c|\phi|_\infty, |I|).$$

Then, for a map $\Upsilon : \mathcal{D}_\rho(G) \longrightarrow \mathbb{C}^{2n}$, we define the norms:

$$|\Upsilon|_{G,\rho,c} := \sup_{x \in \mathcal{D}_\rho(G)} |\Upsilon(x)|_c, \quad |D\Upsilon|_{G,\rho,c} := \sup_{x \in \mathcal{D}_\rho(G)} |D\Upsilon(x)|_c,$$

where, for the second definition, the matrix c -norm is the one induced by the c -norm for vectors. With these notations, it is easy to prove the following property: if Υ is analytic on $\mathcal{D}_\rho(G)$, then

$$|D\Upsilon|_{G,\rho-\delta,c} \leq \frac{|\Upsilon|_{G,\rho,c}}{\hat{\delta}_c}. \quad (1.16)$$

In the following lemma, the effect of the flow associated to a generating Hamiltonian is estimated in terms of the norms introduced above. Moreover, a bound for the remainder of a Lie series is found. The proof is given in section 2.2.

Lemma 1.2. *Let W be an analytic function on $\mathcal{D}_\rho(G)$, $\rho > 0$, and Φ_t its associated Hamiltonian flow at time t , $t \geq 0$. Let $\delta = (\delta_1, \delta_2) > 0$ and $c > 0$ given. Assume that $\|DW\|_{G,\rho,c} \leq \hat{\delta}_c$. Then, Φ_t maps $\mathcal{D}_{\rho-t\delta}(G)$ into $\mathcal{D}_\rho(G)$ and one has:*

- a) $|\Phi_t - \text{id}|_{G,\rho-t\delta,c} \leq t \|DW\|_{G,\rho,c}.$
- b) $\Phi_t(\mathcal{D}_{\rho'}(G)) \supset \mathcal{D}_{\rho'-t\delta}(G)$ for $\rho' \leq \rho - t\delta$.
- c) Assuming that $\|DW\|_{G,\rho,c} < \hat{\delta}_c/2e$, for any given function f , analytic on $\mathcal{D}_\rho(G)$, and for any integer $m \geq 0$, the following bound holds:

$$\begin{aligned} \|r_m(f, W, t)\|_{G,\rho-t\delta} &\leq \left[\sum_{l=0}^{\infty} \frac{1}{\binom{l+m}{m}} \cdot \left(\frac{2e \|DW\|_{G,\rho,c}}{\hat{\delta}_c} \right)^l \right] \cdot \frac{t^m}{m!} \|L_W^m f\|_{G,\rho} \\ &= \gamma_m \left(\frac{2e \|DW\|_{G,\rho,c}}{\hat{\delta}_c} \right) \cdot t^m \|L_W^m f\|_{G,\rho}, \end{aligned}$$

where, for $0 \leq x < 1$, we define

$$\gamma_m(x) := \sum_{l=0}^{\infty} \frac{l!}{(l+m)!} x^l.$$

1.2.3 The Iterative Lemma

Now we are going to obtain estimates for one step of the procedure of section 1.2.1, with the help of the norm introduced in section 1.2.2. We consider the Hamiltonian (1.4), real analytic on $\mathcal{D}_\rho(\mathcal{G})$, with $Z \in \mathbf{R}(\mathcal{M}, K)$, and we restrict it to a subset $G \subset \mathcal{G}$ such that $\omega(G)$ is nonresonant modulo $\mathcal{M}$ up to order K (see the introduction).

We first introduce, following [Pös93], a quantitative version of this nonresonance condition. Given a module $\mathcal{M}$, an integer K and $\alpha > 0$, a subset F of the n -dimensional frequency space is said to be α, K -nonresonant modulo $\mathcal{M}$ if

$$|k \cdot v| \geq \alpha \quad \forall k \in \mathbb{Z}^n \setminus \mathcal{M}, |k|_1 \leq K, \quad \forall v \in F. \quad (1.17)$$

We begin by seeing that this nonresonance condition on the set $\omega(G)$ can be extended to a complex neighborhood of small enough radius ρ_2 .

Lemma 1.3. *Let $h(I)$ be a real analytic function on $\mathcal{V}_{\rho_2}(G)$, let $\omega = \text{grad } h$, and assume that $\omega(G)$ is α, K -nonresonant modulo $\mathcal{M}$. Assume that $\left| \frac{\partial^2 h}{\partial I^2} \right|_{G, \rho_2} \leq M$. If*

$$\rho_2 \leq \frac{\alpha}{2MK}, \quad (1.18)$$

then $\omega(\mathcal{V}_{\rho_2}(G))$ is $\frac{\alpha}{2}, K$ -nonresonant modulo $\mathcal{M}$.

The proof is a simple application of the mean value theorem. We point out that, as shown in section 1.3.5, condition (1.18) on ρ_2 imposes an important restriction on the domain. An exception is the very special case of a system of harmonic oscillators, where $M = 0$ (see section 1.3.2).

The next result provides estimates for the functions ΔZ and W solving the linear functional equation (1.7).

Proposition 1.4. *Let $h(I)$, $Z(\phi, I)$, $R(\phi, I)$ be real analytic functions on $\mathcal{D}_\rho(G)$, let $\omega = \text{grad } h$, and assume that $\omega(G)$ is α, K -nonresonant modulo $\mathcal{M}$, and that $Z \in \mathbf{R}(\mathcal{M}, K)$. Assume that $\left| \frac{\partial^2 h}{\partial I^2} \right|_{G, \rho_2} \leq M$, and $\rho_2 \leq \frac{\alpha}{2MK}$. Let $c > 0$ given. Then the functions $\Delta Z \in \mathbf{R}(\mathcal{M}, K)$ and $W \in \mathbf{NR}(\mathcal{M}, K)$ given in (1.8), which solve the linear equation (1.7), are both real analytic on $\mathcal{D}_\rho(G)$, and the following bounds hold:*

$$\begin{aligned} \|D(\Delta Z)\|_{G, \rho, c} &\leq \|DR\|_{G, \rho, c}, \quad \|D(R - \Delta Z)\|_{G, \rho, c} \leq \|DR\|_{G, \rho, c}, \\ \|DW\|_{G, \rho, c} &\leq \frac{2A}{\alpha} \|DR\|_{G, \rho, c}, \end{aligned}$$

where we define

$$A := 1 + \frac{2Mc}{\alpha}. \quad (1.19)$$

Proof We obtain the estimates from the explicit solution given in (1.8), in terms of Fourier coefficients. The two first ones are clear, since ΔZ and $R - \Delta Z$ are obtained from R just removing the appropriate Fourier harmonics. To estimate DW , we bound $\frac{\partial W}{\partial \phi}$ and $\frac{\partial W}{\partial I}$. Using lemma 1.3, it is easy to see that

$$\left\| \frac{\partial W}{\partial \phi} \right\|_{G, \rho, 1} \leq \frac{2}{\alpha} \left\| \frac{\partial R}{\partial \phi} \right\|_{G, \rho, 1}.$$

Next we write, for $k \in \mathbb{Z}^n \setminus \mathcal{M}, |k|_1 \leq K$,

$$\frac{\partial W_k}{\partial I} = \frac{\frac{\partial R_k}{\partial I}}{i k \cdot \omega(I)} - \frac{R_k(I)}{(i k \cdot \omega(I))^2} \frac{\partial}{\partial I}(i k \cdot \omega(I)) = \frac{\frac{\partial R_k}{\partial I}}{i k \cdot \omega(I)} + \frac{\left[\frac{\partial R}{\partial \phi} \right]_k \cdot \frac{\partial \omega}{\partial I}}{(k \cdot \omega(I))^2},$$

where we have used that $\left[\frac{\partial R}{\partial \phi} \right]_k = i R_k(I) k$ (differentiating the Fourier expansion of R). From lemma 1.3, we obtain

$$\left| \frac{\partial W_k}{\partial I} \right|_{G, \rho_2, \infty} \leq \frac{2}{\alpha} \left| \frac{\partial R_k}{\partial I} \right|_{G, \rho_2, \infty} + \frac{4M}{\alpha^2} \left| \left[\frac{\partial R}{\partial \phi} \right]_k \right|_{G, \rho_2}.$$

Thus,

$$\left\| \frac{\partial W}{\partial I} \right\|_{G,\rho,\infty} \leq \frac{2}{\alpha} \left\| \frac{\partial R}{\partial I} \right\|_{G,\rho,\infty} + \frac{4M}{\alpha^2} \left\| \frac{\partial R}{\partial \phi} \right\|_{G,\rho}$$

and finally

$$\|DW\|_{G,\rho,c} \leq \left(\frac{2}{\alpha} + \frac{4Mc}{\alpha^2} \right) \|DR\|_{G,\rho,c} = \frac{2A}{\alpha} \|DR\|_{G,\rho,c} . \quad \square$$

Remarks

1. These estimates do not involve a reduction of the domain $\mathcal{D}_\rho(G)$. This becomes more difficult if we use a norm that does not take into account the explicit expansion in Fourier series (for example, the supremum norm). One exception is the case $\dim \mathcal{M} = n - 1$, i.e. near periodic orbits, where integral expressions for the solution of equation (1.7) are available (see [Loc90b] and also [LW04]).
2. The value of A could be big (of the order of $1/\alpha$). Therefore, it would be an obstruction to the obtainment of the optimal exponent, unless we chose c small. But we shall see in the subsequent sections that our choice of c allows to bound A by a constant not depending on α .

Theorem 1.1 (Iterative Lemma). *Let $H(\phi, I) = h(I) + Z(\phi, I) + R(\phi, I)$ real analytic on $\mathcal{D}_\rho(G)$, let $\omega = \text{grad } h$, and assume that $\omega(G)$ is α, K -nonresonant modulo $\mathcal{M}$, and that $Z \in \mathbf{R}(\mathcal{M}, K)$. Assume that $\left\| \frac{\partial^2 h}{\partial I^2} \right\|_{G,\rho_2} \leq M$. Let $\delta < \rho$ and $c > 0$ given, and let A defined as in (1.19). Assume:*

$$\rho_2 \leq \frac{\alpha}{2MK} , \quad \|DR\|_{G,\rho,c} \leq \frac{\alpha \hat{\delta}_c}{74A} . \quad (1.20)$$

Then, there exists a real analytic canonical transformation $\Phi : \mathcal{D}_{\rho-\frac{\delta}{2}}(G) \longrightarrow \mathcal{D}_\rho(G)$ such that $H \circ \Phi = h + \tilde{Z} + \tilde{R}$, with $\tilde{Z} \in \mathbf{R}(\mathcal{M}, K)$, and one has:

- a) $\|D\tilde{Z}\|_{G,\rho,c} \leq \|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} .$
- b) $\|D\tilde{R}\|_{G,\rho-\delta,c} \leq e^{-K\delta_1} \cdot \|DR\|_{G,\rho,c} + \frac{14A}{\alpha \hat{\delta}_c} \left(\|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} \right) \cdot \|DR\|_{G,\rho,c} .$
- c) $|\Phi - \text{id}|_{G,\rho-\frac{\delta}{2},c} \leq \frac{2A}{\alpha} \|DR\|_{G,\rho,c} .$
- d) $\Phi(\mathcal{D}_{\rho'}(G)) \supset \mathcal{D}_{\rho'-\frac{\delta}{2}}(G)$ for $\rho' \leq \rho - \frac{\delta}{2} .$

Proof We take ΔZ , W and Φ as constructed in section 1.2.1. Then the bounds of proposition 1.4 for $D(\Delta Z)$, $D(R - \Delta Z)$ and DW hold. In particular,

$$\|DW\|_{G,\rho,c} \leq \frac{2A}{\alpha} \|DR\|_{G,\rho,c} \leq \frac{\hat{\delta}_c}{37} < \frac{\hat{\delta}_c}{4e} ,$$

and therefore lemma 1.2 applies, with $t = 1$ and with $\delta/2$ instead of δ . We obtain $\Phi : \mathcal{D}_{\rho-\frac{\delta}{2}}(G) \longrightarrow \mathcal{D}_\rho(G)$ and expressions (1.9–1.10) hold for the transformed Hamiltonian.

From (1.9) and proposition 1.4, we easily get estimate (a). On the other hand, from (1.10) and parts (a) and (c) of lemma 1.1,

$$\|D\tilde{R}\|_{G,\rho-\delta,c} \leq e^{-K\delta_1} \cdot \|DR\|_{G,\rho,c} + \frac{2c}{\hat{\delta}_c} \left(\|r_2(h, W, 1)\|_{G,\rho-\frac{\delta}{2}} + \|r_1(Z + R, W, 1)\|_{G,\rho-\frac{\delta}{2}} \right) .$$

From part (c) of lemma 1.2,

$$\begin{aligned} \|r_2(h, W, 1)\|_{G,\rho-\frac{\delta}{2}} &\leq \gamma_2 \left(\frac{4e \|DW\|_{G,\rho,c}}{\hat{\delta}_c} \right) \cdot \left\| \{h, W\}, W \right\|_{G,\rho} , \\ \|r_1(Z + R, W, 1)\|_{G,\rho-\frac{\delta}{2}} &\leq \gamma_1 \left(\frac{4e \|DW\|_{G,\rho,c}}{\hat{\delta}_c} \right) \cdot \left\| \{Z + R, W\} \right\|_{G,\rho} . \end{aligned}$$

We estimate the Poisson brackets using part (b) of lemma 1.1:

$$\begin{aligned} \|\{Z + R, W\}\|_{G,\rho} &\leq \frac{2}{c} \left(\|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} \right) \cdot \|DW\|_{G,\rho,c} , \\ \|\{\{h, W\}, W\}\|_{G,\rho} &= \|\{\Delta Z - R_{\leq K}, W\}\|_{G,\rho} \leq \frac{2}{c} \|DR\|_{G,\rho,c} \cdot \|DW\|_{G,\rho,c} \end{aligned}$$

where, in the second estimate, we have used proposition 1.4 to ensure that

$$\|D(\Delta Z - R_{\leq K})\|_{G,\rho,c} \leq \|D(\Delta Z - R)\|_{G,\rho,c} \leq \|DR\|_{G,\rho,c} .$$

For $0 < x < 1$, one has

$$\gamma_1(x) = -\frac{\ln(1-x)}{x} , \quad \gamma_2(x) = \frac{x + (1-x)\ln(1-x)}{x^2} .$$

Using that these functions are increasing and evaluating them at $x = 4e/37$, we obtain

$$\begin{aligned} &\|r_2(h, W, 1)\|_{G,\rho-\frac{\delta}{2}} + \|r_1(Z + R, W, 1)\|_{G,\rho-\frac{\delta}{2}} \\ &\leq \frac{2}{c} \left(\gamma_2\left(\frac{4e}{37}\right) + \gamma_1\left(\frac{4e}{37}\right) \right) \cdot \left(\|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} \right) \cdot \|DW\|_{G,\rho,c} \\ &\leq \frac{7A}{c\alpha} \left(\|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} \right) \cdot \|DR\|_{G,\rho,c} . \end{aligned} \tag{1.21}$$

By putting all of these estimates together, we get (b). Finally, we deduce from lemma 1.2 (with $\delta/2$ instead of δ) the statements (c) and (d), concerning the distance from Φ to the identity. $\square$

Remarks

1. The Iterative Lemma provides a description for one step of the transformation to normal form constructed in section 1.2.1. The improvement of this result, with respect to related papers (for instance, [Pös93]), is the main contribution of the vectorfield norm (1.15). It avoids a subsequent application of the Cauchy inequalities, which would cause an extra division by $\hat{\delta}_c$ in estimate (b).
2. In the statement of the Iterative Lemma the value of the parameter c is still free. From now onwards, we shall take

$$c = \frac{\delta_2}{\delta_1} ,$$

and hence $\hat{\delta}_c = \delta_2$. This choice of c seems to be the best because it leads to the smallest possible value for the quotient

$$\frac{\|DR\|_{G,\rho,c}}{\hat{\delta}_c} ,$$

appearing implicitly in condition (1.20) and estimate (b).

1.3 Nekhoroshev estimates and related results

1.3.1 Estimates for the normal form

Now, starting with $H(\phi, I) = h(I) + Z(\phi, I) + R(\phi, I)$ on $\mathcal{D}_\rho(G)$, we apply Q times the Iterative Lemma and obtain an estimate for the remainder. By choosing $Q = Q(K)$ adequately, we get an exponentially small remainder in the next theorem.

Theorem 1.2 (Normal Form Theorem). *Let $H(\phi, I) = h(I) + Z(\phi, I) + R(\phi, I)$ real analytic on $\mathcal{D}_\rho(G)$, let $\omega = \text{grad } h$, and assume that $\omega(G)$ is α, K -nonresonant modulo $\mathcal{M}$, and that $Z \in \mathbf{R}(\mathcal{M}, K)$. Assume that $\left| \frac{\partial^2 h}{\partial I^2} \right|_{G,\rho_2} \leq M$. Let $\delta < \rho$ given, $c = \delta_2/\delta_1$, and let A the constant defined in (1.19). Assume:*

$$\rho_2 \leq \frac{\alpha}{2MK} , \quad \|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} \leq \frac{\alpha\delta_2}{61AK\delta_1} . \tag{1.22}$$

Then, there exists a real analytic canonical transformation $\Psi : \mathcal{D}_{\rho-\delta}(G) \longrightarrow \mathcal{D}_\rho(G)$ such that $H \circ \Psi = h + Z^ + R^*$, with $Z^* \in \mathbf{R}(\mathcal{M}, K)$, and one has:*

- a) $\|DZ^*\|_{G,\rho-\delta,c} + \|DR^*\|_{G,\rho-\delta,c} \leq \|DZ\|_{G,\rho,c} + 2\|DR\|_{G,\rho,c}.$
- b) $\|DR^*\|_{G,\rho-\delta,c} \leq 3e^{-\frac{K\delta_1}{2}} \cdot \|DR\|_{G,\rho,c}.$
- c) $|\Psi - \text{id}|_{G,\rho-\delta,c} \leq \frac{4A}{\alpha} \|DR\|_{G,\rho,c}.$
- d) $\Psi(\mathcal{D}_{\rho'}(G)) \supset \mathcal{D}_{\rho'-\frac{\delta}{2}}(G)$ for $\rho' \leq \rho - \delta$.

Proof Let $Q \geq 1$ be an integer to be chosen below, and let us introduce the sequence

$$\rho^{(q)} = \rho - \frac{q\delta}{Q}, \quad 0 \leq q \leq Q.$$

We take $\delta^{(q)} = \delta/Q$ for every $1 \leq q \leq Q$. Next we shall construct a sequence of real analytic canonical transformations $\Phi^{(q)} : \mathcal{D}_{\rho^{(q)}}(G) \rightarrow \mathcal{D}_{\rho^{(q-1)}}(G)$, $1 \leq q \leq Q$. Denoting $\Psi^{(q)} = \Phi^{(1)} \circ \dots \circ \Phi^{(q)}$, the successive transformed Hamiltonians will be written in the form $H^{(q)} = H \circ \Psi^{(q)} = h + Z^{(q)} + R^{(q)}$, with $Z^{(q)} \in \mathbf{R}(\mathcal{M}, K)$. Moreover, we are going to show that, if

$$K\delta_1 \geq 2Q, \tag{1.23}$$

the following statements are true for $0 \leq q \leq Q$:

- 1_q) $\|DZ^{(q)}\|_{G,\rho^{(q)},c} \leq \|DZ\|_{G,\rho,c} + \sum_{s=0}^{q-1} \|DR^{(s)}\|_{G,\rho^{(s)},c}.$
- 2_q) $\|DR^{(q)}\|_{G,\rho^{(q)},c} \leq \frac{1}{e^q} \|DR\|_{G,\rho,c}.$

We proceed by induction. The results are obviously true for $q = 0$. For $1 \leq q \leq Q$, note that, by (2_{q-1}) and condition (1.22),

$$\|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \leq \frac{1}{e^{q-1}} \|DR\|_{G,\rho,c} \leq \frac{\alpha\delta_2}{61AK\delta_1} \leq \frac{\alpha\delta_2}{122AQ}$$

and hence the Iterative Lemma applies, with δ/Q instead of δ , and we obtain the canonical transformation $\Phi^{(q)}$. We immediately get (1_q). The bound (2_q) comes from the following estimate:

$$\begin{aligned} & \|DR^{(q)}\|_{G,\rho^{(q)},c} \\ & \leq e^{-\frac{K\delta_1}{Q}} \cdot \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \\ & \quad + \frac{14AQ}{\alpha\delta_2} \left(\|DZ^{(q-1)}\|_{G,\rho^{(q-1)},c} + \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \right) \cdot \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \\ & \leq \left(\frac{1}{e^2} + \frac{28AQ}{\alpha\delta_2} \left(\|DZ\|_{G,\rho,c} + \|DR\|_{G,\rho,c} \right) \right) \cdot \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \\ & \leq \left(\frac{1}{e^2} + \frac{28}{122} \right) \cdot \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \leq \frac{1}{e} \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c}. \end{aligned}$$

Now, let us assume that $K\delta_1 \geq 2$ (if $K\delta_1 < 2$, all results are obvious if we take Ψ as the identity map). Then, we may choose $Q = Q(K)$ as the maximum integer satisfying (1.23), i.e. $Q = \left\lfloor \frac{K\delta_1}{2} \right\rfloor$. Denoting $\Psi = \Psi^{(Q)}$, $Z^* = Z^{(Q)}$, $R^* = R^{(Q)}$, we have $H \circ \Psi = h + Z^* + R^*$. Then, part (a) comes from (1_Q). For part (b), we use (2_Q):

$$\|DR^*\|_{G,\rho-\delta,c} \leq \frac{1}{e^Q} \|DR\|_{G,\rho,c} \leq \frac{1}{e^{\frac{K\delta_1}{2}-1}} \|DR\|_{G,\rho,c} \leq 3e^{-\frac{K\delta_1}{2}} \cdot \|DR\|_{G,\rho,c}.$$

The proof of (c) is very simple from the analogous bound in the Iterative Lemma and the inequalities (2_q):

$$|\Psi^{(Q)} - \text{id}|_{G,\rho-\delta,c} \leq \sum_{q=1}^Q |\Phi^{(q)} - \text{id}|_{G,\rho^{(q)},c} \leq \sum_{q=1}^Q \frac{2A}{\alpha} \|DR^{(q-1)}\|_{G,\rho^{(q-1)},c} \leq \frac{4A}{\alpha} \|DR\|_{G,\rho,c}.$$

Finally, to get (d) it suffices to prove that, for $0 \leq q \leq Q$,

$$\Psi^{(q)}(\mathcal{D}_{\rho'}(G)) \supset \mathcal{D}_{\rho' - \frac{q\delta}{2Q}}(G) \quad \text{if } \rho' \leq \rho - \frac{q\delta}{Q}.$$

Indeed, this inclusion is obvious for $q = 0$. By induction, we assume it for $q - 1$:

$$\Psi^{(q-1)}(\mathcal{D}_{\rho''}(G)) \supset \mathcal{D}_{\rho'' - \frac{(q-1)\delta}{2Q}}(G) \quad \text{if } \rho'' \leq \rho - \frac{(q-1)\delta}{Q}.$$

Then, taking $\rho'' = \rho' - \frac{\delta}{2Q}$ in this inclusion and applying part (d) of the Iterative Lemma, we get:

$$\Psi^{(q)}(\mathcal{D}_{\rho'}(G)) = \Psi^{(q-1)}\left(\Psi^{(q)}(\mathcal{D}_{\rho'}(G))\right) \supset \Psi^{(q-1)}\left(\mathcal{D}_{\rho' - \frac{\delta}{2Q}}(G)\right) \supset \mathcal{D}_{\rho' - \frac{q\delta}{2Q}}(G). \quad \square$$

Remark This result is essentially equivalent to the analogous one in [Pös93], and seems to be “optimal” in the sense that the exponent for K in the second condition of (1.22) is 1. The difference is that our proof is much simpler because the Iterative Lemma is also optimal, whereas the proof appearing in [Pös93] relies in a very careful choice of the size of the successive reductions of the domain (see also [Nei84]).

1.3.2 Nonresonant stability estimates: application to the harmonic oscillators case

From theorem 1.2, one can obtain estimates for the variation of the action variables on the set G where this theorem is applied. This is very simple in a nonresonant region ($\mathcal{M} = 0$), where no extra geometric condition on the unperturbed Hamiltonian h is required.

Lemma 1.5. *Let $H(\phi, I) = h(I) + Z(I) + R(\phi, I)$ real analytic on $\mathcal{D}_\rho(G)$, let $\omega = \text{grad } h$, and assume that $\omega(G)$ is α, K -nonresonant modulo 0. Assume that $\left|\frac{\partial^2 h}{\partial I^2}\right|_{G, \rho_2} \leq M$. Let $c = \rho_2/\rho_1$, and assume:*

$$\rho_2 \leq \frac{\alpha}{2MK}, \quad \|DZ\|_{G, \rho, c} + \|DR\|_{G, \rho, c} \leq \frac{\alpha\rho_2}{122K\rho_1}. \quad (1.24)$$

Then, for every trajectory $(\phi(t), I(t))$ of H , with $(\phi(0), I(0)) \in \mathbb{T}^n \times G$, one has

$$|I(t) - I(0)| \leq \frac{24}{\alpha} \|DR\|_{G, \rho, c} \quad \text{for } |t| \leq \frac{2}{\alpha} e^{\frac{K\rho_1}{6}}. \quad (1.25)$$

The proof is deferred to section 2.2. Now, as a simple application, we consider the case $h(I) = \omega \cdot I$, i.e. H is a perturbation of a system of n harmonic oscillators. The frequency vector $\omega \in \mathbb{R}^n$ is assumed to be τ, γ -Diophantine (see (1.2)), for $\tau \geq n - 1$ and $\gamma > 0$ given. This case, where no geometric part is required, is also considered in [GG85], [GDF⁺89], [Fas90], [Pös93] and [DG93]. We obtain, like in the last four of the quoted papers, the “optimal” stability exponent $a = 1/(\tau + 1)$. We remark that, since $M = 0$ in this case, condition (1.18) does not impose any restriction on ρ_2 .

Theorem 1.3. *Let $H(\phi, I) = \omega \cdot I + f(\phi, I)$ real analytic on $\mathcal{D}_\rho(\mathcal{G})$, and assume that the vector ω is τ, γ -Diophantine for some $\tau \geq n - 1$ and $\gamma > 0$. Assume:*

$$\varepsilon := \|f\|_{\mathcal{G}, \rho} \leq \varepsilon_0 := \frac{\gamma\rho_2}{244}.$$

Then, for every trajectory $(\phi(t), I(t))$ of H , with $(\phi(0), I(0)) \in \mathbb{T}^n \times \mathcal{G}$, one has

$$|I(t) - I(0)| \leq \frac{\rho_2}{5\rho_1} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/(\tau+1)} \quad \text{for } |t| \leq \frac{2}{\gamma} \exp\left\{\frac{\rho_1}{24} \left(\frac{\varepsilon_0}{\varepsilon}\right)^{1/(\tau+1)}\right\}.$$

Proof Let $c = \rho_2/\rho_1$. We notice that we may take $M = 0$ in lemma 1.5. For a fixed K to be chosen, the set $\{\omega\}$ is clearly $\frac{\gamma}{K^\tau}, K$ -nonresonant modulo 0. We are going to apply lemma 1.5 with $Z = 0$, $R = f$, and $\rho/2$ instead of ρ . Since

$$\|Df\|_{\mathcal{G}, \frac{\rho}{2}, c} \leq \frac{2\varepsilon}{\rho_1},$$

the second condition of (1.24) is satisfied for

$$\varepsilon \leq \frac{\gamma \rho_2}{244 K^{\tau+1}}.$$

We then choose $K = \left\lceil \left(\frac{\varepsilon_0}{\varepsilon} \right)^{1/(\tau+1)} \right\rceil$ and obtain:

$$|I(t) - I(0)| \leq \frac{24K^\tau}{\gamma} \cdot \frac{2\varepsilon}{\rho_1} \leq \frac{\rho_2}{5\rho_1} \left(\frac{\varepsilon}{\varepsilon_0} \right)^{1/(\tau+1)}.$$

Concerning the stability time, it is easily obtained from the one of lemma 1.5 if we take into account that, since $\varepsilon \leq \varepsilon_0$, we have $K \geq \frac{1}{2} \left(\frac{\varepsilon_0}{\varepsilon} \right)^{1/(\tau+1)}$. $\square$

Remarks

1. One may notice that our results in the case of a perturbation of a system of harmonic oscillators are slightly worse than the ones obtained in [Fas90]. Indeed, the stability exponent $a = 1/(\tau + 1)$ is the same but we have obtained $b = 1/(\tau + 1)$ instead of $b = 1$. This difference comes from a different performance of the iterations leading to normal form. Indeed, in [Fas90] the linear functional equation (1.7) is solved without cutting the Fourier expansions at order K (but making a reduction of the domain). This approach makes the estimates of proposition 1.4 better, but it is limited to the nonresonant case ($\mathcal{M} = 0$). Although our approach leads to worse estimates, it avoids dealing with infinitely many small divisors, and also allows to treat the resonant case.
2. Even in the harmonic oscillators case, our approach looks more significative from a practical point of view. Indeed, if we consider ε fixed (i.e. a concrete Hamiltonian), then the result of theorem 1.3 still holds if Diophantine condition (1.2) is required just for $|k|_1 \leq \left(\frac{\varepsilon_0}{\varepsilon} \right)^{1/(\tau+1)}$. For instance, if the frequency ω is known only up to a finite precision then it has no sense to check the Diophantine condition farther than a certain finite order, but our estimates could also be applied.

1.3.3 Resonant stability estimates

Now we restrict ourselves to a neighborhood of the resonance associated to a given module $\mathcal{M} \subset \mathbb{Z}^n$, and afterwards the whole domain $\mathcal{G}$ will be divided in resonant and nonresonant regions corresponding to the different modules. A set of frequencies $F \subset \mathbb{R}^n$ is said to be η -close to $\mathcal{M}$ -resonances if

$$|v - \Pi_{\mathcal{M}} v| \leq \eta \quad \forall v \in F, \quad (1.26)$$

where $\Pi_{\mathcal{M}}$ denotes the orthogonal projection onto the space of exact $\mathcal{M}$ -resonant frequencies

$$\mathcal{M}^\perp = \{v \in \mathbb{R}^n : k \cdot v = 0 \quad \forall k \in \mathcal{M}\}.$$

To obtain stability estimates for the trajectories with initial condition in a set G such that $\omega(G)$ is close to a resonance, we need to impose some geometric condition on the unperturbed Hamiltonian h . In the original Nekhoroshev's proof [Nek77], a general steepness condition was imposed. But the main geometric ideas of the proof are contained in the simpler quasiconvex case, considered for instance in [BGGS84] (convex case), [Loc90b] and [Pös93]. Following [Loc90b], we say the function $h(I)$ to be m -quasiconvex on a set U if

$$\left| \frac{\partial^2 h}{\partial I^2}(I)(v, v) \right| \geq m|v|^2 \quad \forall v \in \langle \omega(I) \rangle^\perp, \quad \forall I \in U$$

(this definition is slightly different from the one given in [Pös93]). One remarks that the level hypersurfaces of h are convex if h is m -quasiconvex. Moreover, the quasiconvexity implies that, for every module $\mathcal{M}$, the resonant manifold $S_{\mathcal{M}}$ introduced in (1.3) and the vector subspace generated by $\mathcal{M}$ are always transversal.

Under this condition, the next lemma (called Resonant Stability Lemma in [Pös93]) provides stability estimates on a region $G \subset \mathcal{G}$ such that $\omega(G)$ is assumed to be close to the resonance associated to a given

module $\mathcal{M}$ and satisfying a nonresonant condition modulo $\mathcal{M}$. Our proof is standard. It follows [Loc90b] and [Pös93] in the main ideas, which go back (for convex systems) to [BG86]. The basic point is that, for a Hamiltonian in normal form with respect to $\mathcal{M}$ with an exponentially small remainder, the speed of variation of the action variables along the $\mathcal{M}^\perp$ -direction is exponentially small. On the other hand, the quasiconvexity condition forces the energy hypersurface of h passing through a point of the resonance $S_{\mathcal{M}}$ to have a contact of order two with the $\mathcal{M}$ -direction. Then, by energy conservation, one may bound the variation of the actions along the $\mathcal{M}$ -direction, giving rise to the stability estimate. It has to be noticed that this approach differs from the one of [BGGS84], where a different feature of (quasi)convex Hamiltonians is used: the transversality between the resonant manifold $S_{\mathcal{M}}$ and the $\mathcal{M}$ -direction.

We define a real neighborhood of the domain G as

$$\mathcal{U}_{\rho_2}(G) := \left\{ I \in \mathbb{R}^n : |I - I'| \leq \rho_2 \text{ for some } I' \in G \right\} = \mathcal{V}_{\rho_2}(G) \cap \mathbb{R}^n. \quad (1.27)$$

Lemma 1.6. *Let $H(\phi, I) = h(I) + Z(\phi, I) + R(\phi, I)$ real analytic on $\mathcal{D}_\rho(G)$, and let $\omega = \text{grad } h$. For a given module $\mathcal{M} \neq \mathbb{Z}^n$, assume that $\omega(G)$ is η -close to $\mathcal{M}$ -resonances (1.26, and α, K -nonresonant modulo $\mathcal{M}$, with $K \geq 1$ (1.17), and assume also that $Z \in \mathbf{R}(\mathcal{M}, K)$. Assume that*

$$\left| \frac{\partial^2 h}{\partial I^2} \right|_{G, \rho_2} \leq M, \quad |\omega|_G \leq L,$$

and that h is m -quasiconvex on $\mathcal{U}_{\rho_2}(G)$. Let $c = \rho_2/\rho_1$, and assume:

$$\rho_2 \leq \frac{m\alpha}{48M^2K}, \quad \eta \leq \frac{m\rho_2}{60}, \quad \|DZ\|_{G, \rho, c} + \|DR\|_{G, \rho, c} \leq \frac{m\sigma\rho_2^2}{350}, \quad (1.28)$$

where we write $\sigma := \min\left(1, \frac{1}{\sqrt{n}\rho_1}\right)$. Then, for every trajectory $(\phi(t), I(t))$ of H , with $(\phi(0), I(0)) \in \mathbb{T}^n \times G$, one has

$$|I(t) - I(0)| \leq \rho_2 \quad \text{for } |t| \leq \frac{m\rho_2^2}{74L\|DR\|_{G, \rho, c}} e^{\frac{mK\rho_1}{6M}}. \quad (1.29)$$

We give the proof of this result in section 2.2.

Remark If $R = 0$, this lemma implies that, if the quasiconvexity condition is fulfilled, all trajectories starting in $\mathbb{T}^n \times G$ have perpetual stability. Nevertheless, one could deduce this fact in a more direct way, because in this case the Hamiltonian $H = h + Z$ is already in normal form with respect to $\mathcal{M}$.

1.3.4 Geometry of resonances

Next we return to the Hamiltonian (1.1), which we assume real analytic on $\mathcal{D}_\rho(\mathcal{G})$. The stability estimates obtained in lemmas 1.5 and 1.6 only apply to the trajectories starting in a subset $G \subset \mathcal{G}$ where the frequencies are assumed to be close to the resonance characterized by a fixed module $\mathcal{M} \subset \mathbb{Z}^n$ and satisfying a nonresonance condition modulo $\mathcal{M}$. In order to obtain stability estimates for all trajectories starting in $\mathbb{T}^n \times \mathcal{G}$, the whole action domain $\mathcal{G}$ is covered by a family of sets $G_{\mathcal{M}}$, called resonant and nonresonant blocks (for $\mathcal{M} \neq 0$ and $\mathcal{M} = 0$, respectively). For each module $\mathcal{M}$, the frequencies on the block $G_{\mathcal{M}}$ have to be close to $\mathcal{M}$ -resonances, and to satisfy the nonresonance condition (1.17) up to a fixed order K .

A construction of such a covering is carried out in [Nek77] and [BGGS84]. The quantitative aspect was improved in [Pös93]. The Geometric Lemma stated below has been taken from [Pös93] with no changes.

Actually one may work in frequency space. We obtain for this space a covering $\{B_{\mathcal{M}}\}$, which can be pulled back by the frequency map ω to a covering $\{G_{\mathcal{M}}\}$ for $\mathcal{G}$. Before stating the Geometric Lemma we recall some concepts and terminology introduced in [Pös93].

For each module $\mathcal{M} \subset \mathbb{Z}^n$, we consider the space of $\mathcal{M}$ -resonant frequencies $\mathcal{M}^\perp$. Note that there are a lot of modules giving rise to the same resonant space. Obviously we only have to consider the *maximal* one. A module $\mathcal{M} \subset \mathbb{Z}^n$ is said to be maximal if it is not properly contained in any other module of the same dimension. See appendix 3 of the book [LM88] for an explicit characterization of the maximal modules in $\mathbb{Z}^n$.

Given a maximal d -dimensional module $\mathcal{M} \subset \mathbb{Z}^n$, the set $B_{\mathcal{M}}$ is constructed by taking a neighborhood of the space $\mathcal{M}^\perp$ and removing from it a neighborhood of the resonant spaces associated to the $(d+1)$ -dimensional modules. The set constructed in this way would not contain any open set. However, one remarks that, to satisfy the nonresonance condition (1.17) up to order K , it suffices to consider K -modules. A module $\mathcal{M} \subset \mathbb{Z}^n$ is said to be a K -module if it is generated by vectors of order less or equal than K .

To make these ideas quantitative, one requires the notion of *volume* of a module. For a d -dimensional module $\mathcal{M} \subset \mathbb{Z}^n$, $1 \leq d \leq n$, let C be the $(n \times d)$ -matrix obtained by choosing a basis of $\mathcal{M}$ and putting its vectors as columns. The volume of $\mathcal{M}$ is then defined as

$$|\mathcal{M}| := \sqrt{\det(C^\top C)},$$

i.e. the d -dimensional volume of the parallelepiped spanned by the vectors of the basis. The choice of the basis does not have influence in this definition.

Let $\lambda_d > 0$, for $1 \leq d \leq n$, be fixed parameters. For each maximal d -dimensional K -module $\mathcal{M}$, one introduces

$$\eta_{\mathcal{M}} := \frac{\lambda_d}{|\mathcal{M}|},$$

and the resonant zone associated to $\mathcal{M}$ is defined as a neighborhood of radius $\eta_{\mathcal{M}}$ around $\mathcal{M}^\perp$. Recalling that $\Pi_{\mathcal{M}}$ denotes the orthogonal projection onto $\mathcal{M}^\perp$, one defines

$$A_{\mathcal{M}} := \{v \in \mathbb{R}^n : |v - \Pi_{\mathcal{M}} v| < \eta_{\mathcal{M}}\}.$$

Then, the *resonant block* associated to $\mathcal{M}$ is defined as

$$B_{\mathcal{M}} := A_{\mathcal{M}} \setminus A_{d+1}^*,$$

where A_l^* , $1 \leq l \leq n$, stands for the union of all resonant zones corresponding to maximal l -dimensional K -modules, and $A_{n+1}^* = \emptyset$. Note that every resonant block $B_{\mathcal{M}}$ is $\eta_{\mathcal{M}}$ -close to $\mathcal{M}$ -resonances. For the trivial module one defines the *nonresonant block*:

$$B_0 := \mathbb{R}^n \setminus A_1^*.$$

It is easy to see that the whole frequency space is covered by the blocks $B_{\mathcal{M}}$.

Lemma 1.7 (Geometric Lemma). *Let us fix $K \geq 1$, $E > 0$ and $F \geq E + \sqrt{2}$. Assume:*

$$\frac{\lambda_{d+1}}{\lambda_d} \geq FK$$

for $1 \leq d < n$. Then, the blocks $B_{\mathcal{M}}$ defined above are $\alpha_{\mathcal{M}}, K$ -nonresonant modulo $\mathcal{M}$, with

$$\begin{aligned} \alpha_{\mathcal{M}} &:= EK\eta_{\mathcal{M}} \quad \text{for } \mathcal{M} \neq 0, \\ \alpha_0 &:= \lambda_1. \end{aligned}$$

For the proof, see [Pös93]. The desired covering for $\mathcal{G}$ is then obtained from this lemma by putting $G_{\mathcal{M}} = \omega^{-1}(B_{\mathcal{M}})$ for each maximal K -module $\mathcal{M}$, except for the ones giving rise to an empty set.

1.3.5 Global effective stability

Our main result on effective stability concerns estimates holding for all motions in phase space. Like in [Pös93], these estimates are obtained by considering the covering supplied by lemma 1.7 with a fixed order K (which is chosen as a suitable function of the size ε of perturbation) and then applying the stability estimates to each block of the covering.

Theorem 1.4 (Nekhoroshev Theorem). *Let $H(\phi, I) = h(I) + f(\phi, I)$ real analytic on $\mathcal{D}_\rho(\mathcal{G})$, let $\omega = \text{grad } h$, and assume that*

$$\left| \frac{\partial^2 h}{\partial I^2} \right|_{\mathcal{G}, \rho_2} \leq M, \quad |\omega|_{\mathcal{G}} \leq L.$$

Assume also that h is m -quasiconvex on $\mathcal{U}_{\rho_2}(\mathcal{G})$. Let $\lambda > 0$ given, and assume:

$$\lambda \leq \frac{23M^2\rho_2}{m}, \quad \varepsilon := \|f\|_{\mathcal{G},\rho} \leq \varepsilon_0 := \frac{m^{4n-1}\hat{\rho}\lambda^2}{2^{24n-2}M^{4n}}, \quad (1.30)$$

where we write $\hat{\rho} := \min\left(\rho_1, \frac{2}{\sqrt{n}}\right)$. Then, for every trajectory $(\phi(t), I(t))$ of H , with $(\phi(0), I(0)) \in \mathbb{T}^n \times \mathcal{G}$ and satisfying $|\omega(I(0))| \geq \lambda$, one has

$$|I(t) - I(0)| \leq \rho_2 \cdot \left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/2n} \quad \text{for } |t| \leq \frac{4}{L} \exp\left\{\frac{m\rho_1}{24M} \left(\frac{\varepsilon_0}{\varepsilon}\right)^{1/2n}\right\}. \quad (1.31)$$

Proof Fix $K \geq 1$ to be chosen below. Let

$$F = \frac{2882M^2}{m^2}, \quad E = F - \sqrt{2}.$$

For $1 \leq d \leq n$, we put:

$$\lambda_d = \frac{\lambda}{(FK)^{n-d}}.$$

Then, lemma 1.7 provides a covering $\{G_{\mathcal{M}}\}$ of $\mathcal{G}$, with $G_{\mathcal{M}} = \omega^{-1}(B_{\mathcal{M}})$, and its parameters are

$$\eta_{\mathcal{M}} = \frac{\lambda}{|\mathcal{M}|(FK)^{n-d}}, \quad \alpha_{\mathcal{M}} = \frac{E\lambda}{|\mathcal{M}|F^{n-d}K^{n-d-1}}$$

for every maximal d -dimensional K -module $\mathcal{M}$, $1 \leq d \leq n$, and

$$\alpha_0 = \frac{\lambda}{(FK)^{n-1}}$$

for the trivial module. We also put $\eta_0 = 0$.

We are going to apply lemma 1.6 with $Z = 0$ and $R = f$ on all blocks, except on the one corresponding to $\mathcal{M} = \mathbb{Z}^n$. In this way the estimates hold for all initial conditions satisfying $|\omega(I(0))| \geq \eta_{\mathbb{Z}^n} = \lambda$. Unlike the case of theorem 1.3 (harmonic oscillators), the smallness condition (1.18) on ρ_2 makes us restrict the domain. For every $\mathcal{M}$ we take $\rho^{(\mathcal{M})} = (\rho_1^{(\mathcal{M})}, \rho_2^{(\mathcal{M})})$, with

$$\rho_1^{(\mathcal{M})} = \frac{\rho_1}{2}, \quad \rho_2^{(\mathcal{M})} = \frac{m\alpha_{\mathcal{M}}}{48M^2K}, \quad c_{\mathcal{M}} = \frac{\rho_2^{(\mathcal{M})}}{\rho_1^{(\mathcal{M})}}. \quad (1.32)$$

For every d -dimensional K -module $\mathcal{M}$, $0 \leq d \leq n-1$, one has

$$\frac{60\lambda}{mF^{n-d}K^n} \leq \rho_2^{(\mathcal{M})} \leq \frac{61\lambda}{m(FK)^{n-d}} \leq \frac{\rho_2}{2},$$

where we used that $1 \leq |\mathcal{M}| \leq K^d$. We have

$$\|Df\|_{G_{\mathcal{M}}, \rho^{(\mathcal{M})}, c_{\mathcal{M}}} \leq \frac{\varepsilon}{\rho_1^{(\mathcal{M})}} \leq \frac{2\varepsilon}{\rho_1}.$$

To apply lemma 1.6 on $G_{\mathcal{M}}$, we must verify the three inequalities of (1.28). The two first ones are easily verified and the last one is fulfilled for all $\mathcal{M}$ if

$$\frac{2\varepsilon}{\rho_1} \leq \frac{2\varepsilon_0}{\rho_1 K^{2n}} \leq \frac{m\sigma}{350} \left(\frac{60\lambda}{m(FK)^n}\right)^2 \leq \frac{m\sigma}{350} \left(\rho_2^{(\mathcal{M})}\right)^2,$$

with $\sigma = \min\left(1, \frac{2}{\sqrt{n}\rho_1}\right)$. Thus, we choose $K = \left[\left(\frac{\varepsilon_0}{\varepsilon}\right)^{1/2n}\right]$. For every $\mathcal{M}$, the stability radius and the stability time for the trajectories starting in $\mathbb{T}^n \times G_{\mathcal{M}}$ are obtained from lemma 1.6:

$$\begin{aligned} \rho_2^{(\mathcal{M})} &\leq \frac{61\lambda}{mFK} \leq \frac{122\lambda}{mF} \left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/2n} \leq \rho_2 \cdot \left(\frac{\varepsilon}{\varepsilon_0}\right)^{1/2n}, \\ \frac{m\left(\rho_2^{(\mathcal{M})}\right)^2}{74L \cdot \frac{2\varepsilon}{\rho_1}} e^{\frac{mK\rho_1}{12M}} &\geq \frac{4}{L} \exp\left\{\frac{m\rho_1}{24M} \left(\frac{\varepsilon_0}{\varepsilon}\right)^{1/2n}\right\}. \quad \square \end{aligned}$$

Remarks

1. These estimates would have been a little better if, on the nonresonant block G_0 , we had used lemma 1.5 instead of lemma 1.6. But the stability exponents obtained would have been the same, so we used lemma 1.6 on all blocks for sake of simplicity.
2. We also point out that, actually, condition (1.30) on ε is not essential. It can be removed with some additional effort, but we omit the details. Note, however, that for a large ε Nekhoroshev estimate (1.31) is meaningless. The same remark holds for theorem 1.3.

In the proof of theorem 1.4, we have obtained the stability exponents

$$a = b = \frac{1}{2n}$$

by carrying out the estimates on every block $G_{\mathcal{M}}$ and always taking the worst possible case. The key point is to find greater and lower bounds for $\rho_2^{(\mathcal{M})}$, valid for all modules $\mathcal{M}$. However, the stability exponents can be improved by means of a particular analysis, if one is only interested in a given region.

In particular, one remarks the case of the nonresonant block G_0 . This case corresponds to the smallest $\rho_2^{(0)}$, which gives rise to the smallest stability radius. It is not hard to see that, as stated in theorem 2 of [Pös93] and theorem 3 of [DG93], the stability exponents obtained for this case are

$$a = \frac{1}{2n} , \quad b = \frac{1}{2} .$$

However, if lemma 1.5 were used to obtain the stability estimate, one may check that the exponents would be

$$a = \frac{1}{2n} , \quad b = \frac{n+1}{2n} .$$

It is also interesting to consider, for a fixed module $\mathcal{M}_0$, a neighborhood of the resonant manifold $S_{\mathcal{M}_0}$. This set can be covered by the blocks $G_{\mathcal{M}}$ associated to the modules $\mathcal{M}$ containing $\mathcal{M}_0$. If we restrict ourselves to these modules, the lower bound for $\rho_2^{(\mathcal{M})}$ is greater than the one obtained in theorem 1.4. This allows to choose K greater, and leads to the exponents:

$$a = b = \frac{1}{2\nu_0} ,$$

where ν_0 is the codimension of $\mathcal{M}_0$. A precise statement of this result is given in theorem 3 of [Pös93].

Chapter 2

KAM theory

2.1 KAM theorem and nearly-invariant tori

2.1.1 Nondegeneracy conditions

Now our aim is to prove that, for a nearly-integrable Hamiltonian $H(\phi, I) = h(I) + f(\phi, I)$, analytic on $\mathcal{D}_\rho(\mathcal{G})$, most orbits lie in n -dimensional invariant tori if the perturbation f is small enough. To reach this result, a suitable nondegeneracy condition has to be fulfilled by unperturbed system. In the usual statements of KAM theorem, two sorts of nondegeneracy conditions are imposed on $\omega = \text{grad } h$. These are the *(standard) nondegeneracy* and the *isoenergetic nondegeneracy*. The frequency map ω is said to be nondegenerate if

$$\det \left(\frac{\partial \omega}{\partial I}(I) \right) \neq 0 \quad \forall I \in \mathcal{G}, \quad (2.1)$$

and isoenergetically nondegenerate if

$$\det \begin{pmatrix} \frac{\partial \omega}{\partial I}(I) & \omega(I) \\ \omega(I)^\top & 0 \end{pmatrix} \neq 0 \quad \forall I \in \mathcal{G}. \quad (2.2)$$

An equivalent formulation for the isoenergetic nondegeneracy is to require that ω is nonvanishing on $\mathcal{G}$ and

$$\frac{\partial \omega}{\partial I}(I) v + \lambda \omega(I) \neq 0 \quad \forall v \in \langle \omega(I) \rangle^\perp \setminus \{0\}, \quad \forall \lambda \in \mathbb{R}, \quad \forall I \in \mathcal{G}, \quad (2.3)$$

In action space, condition (2.3) can be interpreted as transversality, at every point, between any energy level $M_E = h^{-1}(E)$ and the hypersurfaces $\omega(I) \cdot v = 0$ (which include the resonant ones). The interpretation in frequency space is that the image $\omega(M_E)$ of any energy level and the subspace $\langle \omega(I) \rangle^\perp$ are always transversal.

It is easy to construct examples showing that conditions (2.1) and (2.2) are independent:

$$h(I_1, I_2) = \ln \frac{I_2}{I_1}, \quad h(I_1, I_2) = \frac{1}{2} I_1^2 + I_2. \quad (2.4)$$

The first one is only nondegenerate on its whole domain, and the second one is only isoenergetically nondegenerate.

We give in the next sections a direct and quantitative proof of KAM theorem under the assumption of isoenergetic nondegeneracy, although the same approach holds for the standard nondegeneracy. Our setup differs from the one which can be found in [Dou82], [BH91], where the isoenergetic KAM theorem is proved from the standard one.

We first remind that the standard version of KAM theorem (under the standard condition (2.1)) states that, given $\tau > n - 1$ and $\gamma > 0$ previously fixed, and assuming for the size of the perturbation f a smallness condition of the type

$$\varepsilon = O(\gamma^2), \quad (2.5)$$

then every invariant torus of the unperturbed Hamiltonian h having τ, γ -Diophantine frequency (i.e. satisfying (1.2)) is preserved in the perturbed system with the same frequency vector. Moreover, the measure of the complement of the set filled with the invariant tori is $O(\gamma)$. In proving this statement

it is crucial to use that, under condition (2.1), the map ω is a local diffeomorphism and therefore the unperturbed invariant tori can be locally parametrized by their frequency vector.

The preservation of the invariant tori with the same frequency vector can be false under the isoenergetic condition (2.2). Indeed, it suffices to consider $h(I)$ as in the second example of (2.4), where the frequency map $\omega(I_1, I_2) = (I_1, 1)$ maps the whole plane into a straight line, and $f(\phi, I) = \varepsilon h(I)$ as a perturbation.

Nevertheless, it is known that in the isoenergetic case the unperturbed invariant tori can be locally parametrized on each energy level M_E by their frequency ratios. More precisely, if we assume, with no loss of generality, that the component ω_n does not vanish on $\mathcal{G}$, then the isoenergetic condition is equivalent to requiring that the map

$$\Omega(I) := \left(\frac{\bar{\omega}(I)}{\omega_n(I)}, h(I) \right) = \left(\frac{\omega_1(I)}{\omega_n(I)}, \dots, \frac{\omega_{n-1}(I)}{\omega_n(I)}, h(I) \right) \quad (2.6)$$

is a local diffeomorphism on $\mathcal{G}$. We use, in this section and in the subsequent ones, the notation $\bar{v} = (v_1, \dots, v_{n-1})$ for $v = (v_1, \dots, v_{n-1}, v_n)$. Note that, including the last component $h(I)$ in the definition of Ω , we avoid to consider each energy level separately. Using the nondegeneracy of the map Ω , we are able to state that, if a smallness condition on ε like (2.5) is fulfilled, then for every τ, γ -Diophantine torus of the unperturbed Hamiltonian there exists an invariant torus of the perturbation, with the same frequency ratios (though the frequency itself can vary) and the same energy. Moreover, like in the standard case, we get that the measure of the complement of the invariant set can be estimated as $O(\gamma)$. One deduces that in the isoenergetic case most of the invariant tori on any energy level are preserved under the perturbation. Indeed, since $\omega_n(I) \neq 0$ for $I \in \mathcal{G}$, the frequency vector $\omega(I)$ associated to a given torus is Diophantine if the vector $\left(\frac{\bar{\omega}(I)}{\omega_n(I)}, 1 \right)$ is also Diophantine. This occurs for most of the unperturbed tori on a fixed energy level, since these tori can always be parametrized by their frequency ratios.

It is worth noting that the isoenergetic version of KAM theorem is more significative from the point of view of stability, because in this case the existence of a large family of invariant tori is ensured on every fixed energy level. For two degrees of freedom ($n = 2$), it follows the stability of the system (in the sense that all motions are bounded), since a given energy level is always separated by the invariant tori. Under the standard nondegeneracy condition, one cannot deduce from KAM theorem that on a given energy level any invariant tori is preserved. On the other hand, for more than two degrees of freedom, stability cannot be guaranteed under any nondegeneracy condition but in the isoenergetic case the preserved tori seem to be stronger barriers to Arnold diffusion.

Another remark is that the isoenergetic KAM theorem can eventually be applied to periodic nonautonomous Hamiltonians, by taking the time variable as an additional angular variable.

Let us make an outline of the method we use for the proof of KAM theorem and the main technical problems found. As established in section 1.2.1, we use an iterative procedure leading to successive Hamiltonians of the form $H^{(q)} = h^{(q)} + R^{(q)}$, with the integrable part $h^{(q)}$ changing from every step to the next one. The domain is restricted by removing at every step resonant strips up to successive orders K_q increasing to infinity. A first problem is that we need to guarantee the nondegeneracy condition for the frequency map $\omega^{(q)} = \text{grad } h^{(q)}$ at every iteration. Hence the analytic part and the geometric part cannot be separated and must be carried out simultaneously along the proof.

Another technical problem is that, to move the bounds of the measure of the resonant zones from frequency space to phase space, we need to estimate from below the Jacobian determinant of a suitable diffeomorphism. In the standard case, the frequency map ω itself is a local diffeomorphism, and one can see that the successive maps $\omega^{(q)}$ are still diffeomorphisms on their domains. One can assume the starting map ω to be one-to-one (restricting the domain if necessary). To guarantee the perturbed maps $\omega^{(q)}$ to be also one-to-one, their domains still have to be slightly restricted after having removed resonances.

The isoenergetic case is, in this aspect, more cumbersome. As showed above, the frequency map ω is not necessarily a local diffeomorphism, but we may use the map Ω introduced in (2.6), which we shall assume to be one-to-one on $\mathcal{G}$. Then, like one would do in the standard case, successive perturbations $\Omega^{(q)}$ of this map will be guaranteed to be also one-to-one provided their domain is slightly restricted.

We notice that the resonant strips to be removed along the successive iterations are better expressed in the image space $\omega(\mathcal{G})$ or $\Omega(\mathcal{G})$. Indeed, the strips can then be taken as linear and are thus easier to handle. To be more precise, in the isoenergetic case we remove from $\Omega(\mathcal{G})$ resonant strips of the form

$$\Delta(k, \alpha) := \left\{ J \in \mathbb{R}^n : \left| \bar{k} \cdot \bar{J} + k_n \right| < \alpha \right\}, \quad (2.7)$$

with $\alpha > 0$. This is very appropriate for the isoenergetic case since Ω maps every resonant zone $|k \cdot \omega(I)| < \delta$ into such a linear strip. The only exception is the case $k = (0, \dots, 0, 1)$, since $\Delta(k, \alpha)$ is then empty if $\alpha < 1$, but this integer vector corresponds to the resonance $\omega_n(I) = 0$, which has previously been excluded from the domain. We also remark that it is easy to bound the measure of a linear strip like (2.7), and that this bound can be pulled back to action space by estimating from below the Jacobian determinant of the diffeomorphism.

It is possible to construct a common environment for both the standard and the isoenergetic nondegeneracy conditions. Indeed, let us consider the condition:

$$\frac{\partial \omega}{\partial I}(I) v \neq 0 \quad \forall v \in \langle \omega(I) \rangle^\perp \setminus \{0\}, \quad \forall I \in \mathcal{G}, \quad (2.8)$$

which means that the restriction of ω to each energy level M_E is a local diffeomorphism. It is not hard to check that this condition is equivalent to that, at every point $I \in \mathcal{G}$, the standard or the isoenergetic condition holds.

It is known that the measure of the set of vectors which do not satisfy Diophantine condition (1.2), with given $\tau > n - 1$ and γ , is $O(\gamma)$. Note also that the nondegeneracy condition (2.8) implies that every resonance $k \cdot \omega(I) = 0$, with $k \neq 0$, is a regular hypersurface. Then, the measure of the complement of the invariant set is also $O(\gamma)$, since this estimate is obtained by pulling back to action space the measure of every resonant strip removed along the iterative process. This is the idea of the measure estimates for both nondegeneracy conditions (2.1) and (2.2), and the only reason for carrying out the proofs separately is the technical problem concerning the appropriate diffeomorphisms described above.

A higher-order nondegeneracy condition was introduced by Rüssmann [Rüs90]: the Taylor expansion of ω at a point I is required to contain n linearly independent coefficients. As a matter of fact, it is easy to see (using that $\frac{\partial \omega}{\partial I}(I)$ is a symmetric matrix) that condition (2.8) is equivalent to imposing that n of the vectors $\omega(I), \frac{\partial \omega}{\partial I_1}(I), \dots, \frac{\partial \omega}{\partial I_n}(I)$ are linearly independent, namely Rüssmann's condition at order 1. As said in [Rüs90], KAM theorem remains true even under the most general Rüssmann's condition. However, the estimate one would get for the measure of the complement of the invariant set would then be larger: $O(\gamma^b)$, with $b < 1$. Related results along these lines can be found in [Sev95], [CS94] and [XYQ97, XY07].

2.1.2 Isoenergetic nondegeneracy: quantitative results

We give in this section several quantitative results related to the isoenergetic nondegeneracy. All proofs are technical and we postpone them to section 2.2.

We need to work with a quantitative version of the isoenergetic nondegeneracy in its form (2.3). If $h(I)$ is defined on a set $G \subset \mathbb{R}^n$, we say the frequency map $\omega = \text{grad } h$ to be μ -isoenergetically nondegenerate if ω does not vanish on G and

$$\left| \frac{\partial \omega}{\partial I}(I) v + \lambda \omega(I) \right| \geq \mu |v| \quad \forall v \in \langle \omega(I) \rangle^\perp, \quad \forall \lambda \in \mathbb{R}, \quad \forall I \in G.$$

Moreover, we modify slightly the map defined in (2.6). For a fixed constant $a > 0$, we define

$$\Omega_{\omega, h, a}(I) := \left(\frac{\bar{\omega}(I)}{\omega_n(I)}, a h(I) \right), \quad I \in G. \quad (2.9)$$

The constant a is introduced for quantitative reasons. It has the appropriate dimensions to make the components of the map (2.9) dimensionally coherent. But its main motivation is that the estimates given in the next lemma are better with a good choice of a .

Lemma 2.1. *Let h be a real function of class $\mathcal{C}^3$ on $G \subset \mathbb{R}^n$, and $\omega = \text{grad } h$. Assume the bounds:*

$$\left| \frac{\partial^2 h}{\partial I^2} \right|_G \leq M, \quad \left| \frac{\partial^3 h}{\partial I^3} \right|_G \leq M', \quad |\omega|_G \leq L \quad \text{and} \quad |\omega_n(I)| \geq l \quad \forall I \in G.$$

Assume also that ω is μ -isoenergetically nondegenerate on G . Let $a \geq 2M/l^2$ be a fixed constant, and denote $\Omega = \Omega_{\omega, h, a}$. One has:

$$\text{a) } \left| \frac{\partial \Omega}{\partial I} \right|_G \leq 2La.$$

- b) $\left| \frac{\partial \Omega}{\partial I}(I) v \right| \geq \frac{\mu}{2L} |v| \quad \forall v \in \mathbb{R}^n, \forall I \in G.$
- c) $\left| \det \left(\frac{\partial \Omega}{\partial I}(I) \right) \right| \geq \frac{\mu^{n-1} a}{L^{n-2}} \quad \forall I \in G.$
- d) $\left| \frac{\partial^2 \Omega}{\partial I^2} \right|_G \leq \left(\frac{M'}{2M} + \frac{3M}{l} \right) La.$

Next we state how a slight variation of the frequency map affects the constant μ of the isoenergetic nondegeneracy condition. This result may be expressed in terms of vectors and matrices.

Lemma 2.2. *Let $\omega, \tilde{\omega} \in \mathbb{R}^n$, and let $A, \tilde{A}$ be $(n \times n)$ -matrices. Let $\varepsilon = |\tilde{\omega} - \omega|$, $\varepsilon' = |\tilde{A} - A|$, and define $l = \min(|\omega|, |\tilde{\omega}|)$, $M = \max(|A|, |\tilde{A}|)$. For some $\mu > 0$, assume that*

$$|Av + \lambda\omega| \geq \mu|v| \quad \forall v \in \langle \omega \rangle^\perp, \quad \forall \lambda \in \mathbb{R}.$$

Then,

$$|\tilde{A}v + \lambda\tilde{\omega}| \geq \left(\mu - \frac{4M\varepsilon}{l} - \varepsilon' \right) |v| \quad \forall v \in \langle \tilde{\omega} \rangle^\perp, \quad \forall \lambda \in \mathbb{R}.$$

Finally, we see that a small perturbation of a one-to-one map is still one-to-one provided the domain is slightly restricted. Previously, for $b \geq 0$ we define the set

$$G - b := \{I \in G : \mathcal{U}_b(I) \subset G\},$$

where $\mathcal{U}_b(I)$ means the closed ball of radius b centered at I , according to (1.27).

Lemma 2.3. *Let $G \subset \mathbb{R}^n$ a compact, and let $\Omega, \tilde{\Omega} : G \rightarrow \mathbb{R}^n$ maps of class $\mathcal{C}^2$, with $|\tilde{\Omega} - \Omega|_G \leq \varepsilon$. Assume that Ω is one-to-one on G , and let $F = \Omega(G)$. Assume the bounds:*

$$\begin{aligned} \left| \frac{\partial \Omega}{\partial I} \right|_G &\leq M, & \left| \frac{\partial \tilde{\Omega}}{\partial I} \right|_G &\leq \tilde{M}, & \left| \frac{\partial^2 \tilde{\Omega}}{\partial I^2} \right|_G &\leq \tilde{M}', \\ \left| \frac{\partial \Omega}{\partial I}(I) v \right| &\geq m|v|, & \left| \frac{\partial \tilde{\Omega}}{\partial I}(I) v \right| &\geq \tilde{m}|v| & \forall v \in \mathbb{R}^n, \forall I \in G, \end{aligned}$$

with $0 < \tilde{m} < m$, $\tilde{M} > M$. Assume also that

$$\varepsilon \leq \frac{\tilde{m}^2}{4\tilde{M}'} . \tag{2.10}$$

Then, given a subset $\tilde{F} \subset F - \frac{4M\varepsilon}{\tilde{m}}$ and writing $\tilde{G} = \left(\tilde{\Omega} \right)^{-1}(\tilde{F})$, the map $\tilde{\Omega}$ is one-to-one from $\tilde{G}$ to $\tilde{F}$, and one has the inclusions

$$\tilde{G} \subset G - \frac{2\varepsilon}{\tilde{m}}, \quad \Omega(\tilde{G}) \supset \tilde{F} - \varepsilon.$$

Moreover, the following estimate holds:

$$\left| \left(\tilde{\Omega} \right)^{-1} - \Omega^{-1} \right|_{\tilde{F}} \leq \frac{\varepsilon}{m} .$$

2.1.3 Analytic and geometric estimates for one step

We provide in proposition 2.4 below quantitative estimates for one concrete step of the iterative process described in section 1.2.1 for the isoenergetic KAM theorem. A parallel result for the standard theorem is called Inductive Lemma in [Arn63].

Let us outline what we call the “analytic part”. If the starting Hamiltonian in a step of the iterative process is written in the form $H(\phi, I) = h(I) + R(\phi, I)$, we get, from the Iterative Lemma (section 1.2.3), estimates for the new Hamiltonian $\tilde{H}(\phi, I) = \tilde{h}(I) + \tilde{R}(\phi, I)$. Assuming the starting frequencies $\omega(I)$ to be Diophantine up to a given order K , we ensure the Iterative Lemma to apply with $\mathcal{M} = 0$. To be more precise, the Diophantine condition up to order K is slightly modified (see condition (2.11) below) in view of the resonant strips introduced in (2.7). In this way, we obtain the estimates of parts (a–e) of proposition 2.4, which could be stated without the hypothesis of isoenergetic nondegeneracy.

On the other hand, some “geometric part” is required. Indeed, assuming that ω is isoenergetically nondegenerate on the domain G , we need to guarantee that the new frequency map $\tilde{\omega} = \text{grad } \tilde{h}$ is also isoenergetically nondegenerate, with a new parameter, in order to allow further iterations. This is established in part (f) of proposition 2.4. Moreover, if the map $\Omega_{\omega, h, a}$ introduced in (2.9) is one-to-one, we see in part (g) that the new map $\Omega_{\tilde{\omega}, \tilde{h}, a}$ is also one-to-one on a new domain $\tilde{G} \subset G$.

Proposition 2.4 (Inductive Lemma). *Let $G \subset \mathbb{R}^n$ a compact, and $H(\phi, I) = h(I) + R(\phi, I)$ real analytic on $\mathcal{D}_\rho(G)$. Let $\omega = \text{grad } h$, and assume the bounds:*

$$\left| \frac{\partial^2 h}{\partial I^2} \right|_{G, \rho_2} \leq M, \quad |\omega|_G \leq L \quad \text{and} \quad |\omega_n(I)| \geq l \quad \forall I \in G.$$

Assume also that ω is μ -isoenergetically nondegenerate on G . Let $\tilde{M} > M$, $\tilde{L} > L$, $\tilde{l} < l$ and $\tilde{\mu} < \mu$ given. For a fixed constant $a \geq 2\tilde{M}/\tilde{l}^2$, assume that the map $\Omega = \Omega_{\omega, h, a}$ is one-to-one on G , and let $F = \Omega(G)$. For $\tau > 0$, $0 < \beta \leq 1$ and K given, K an integer, assume the nonresonance condition:

$$F \cap \Delta \left(k, \frac{\beta}{|k|_1^\tau} \right) = \emptyset \quad \forall k = (\bar{k}, k_n) \in \mathbb{Z}^n, |k|_1 \leq K, \bar{k} \neq 0. \quad (2.11)$$

Let $\delta < \rho$ given, $c = \delta_2/\delta_1$ and

$$A = 1 + \frac{2McK^\tau}{l\beta}.$$

Let $\varepsilon := \|DR\|_{G, \rho, c}$, $\eta := |R_0|_{G, \rho_2}$ and $\xi := \left| \frac{\partial R_0}{\partial I} \right|_{G, \rho_2}$ (where $R_0(I)$ is the angular average of $R(\phi, I)$), and assume:

$$\rho_2 \leq \frac{\tilde{l}\beta}{2\tilde{M}K^{\tau+1}}, \quad (2.12)$$

$$\varepsilon \leq \frac{l\beta\delta_2}{74AK^\tau}, \quad \xi \leq \min \left((\tilde{M} - M) \delta_2, \tilde{L} - L, l - \tilde{l}, \frac{(\mu - \tilde{\mu})\rho_2}{3} \right), \quad (2.13)$$

$$\eta' := \frac{L\xi}{2\tilde{M}} + \eta \leq \frac{\tilde{\mu}^2(\rho_2 - \delta_2)}{32\tilde{L}^3a^2}. \quad (2.14)$$

Then, there exists a real analytic canonical transformation $\Phi : \mathcal{D}_{\rho - \frac{\delta}{2}}(G) \longrightarrow \mathcal{D}_\rho(G)$ and a decomposition $H \circ \Phi = \tilde{h}(I) + \tilde{R}(\phi, I)$ such that, writing $\tilde{\omega} = \text{grad } \tilde{h}$ and $\tilde{\Omega} = \Omega_{\tilde{\omega}, \tilde{h}, a}$, one has:

- a) $|\tilde{\omega} - \omega|_{G, \rho_2} = \xi, \quad \left| \tilde{h} - h \right|_{G, \rho_2} = \eta.$
- b) $\tilde{\varepsilon} := \|D\tilde{R}\|_{G, \rho - \delta, c} \leq e^{-K\delta_1} \cdot \varepsilon + \frac{14AK^\tau}{l\beta\delta_2} \cdot \varepsilon^2.$
- c) $\tilde{\eta} := \left| \tilde{R}_0 \right|_{G, \rho_2 - \frac{\delta_2}{2}} \leq \frac{7AK^\tau}{cl\beta} \cdot \varepsilon^2.$
- d) $|\Phi - \text{id}|_{G, \rho - \frac{\delta}{2}, c} \leq \frac{2AK^\tau}{l\beta} \cdot \varepsilon.$

- e) $\left| \frac{\partial^2 \tilde{h}}{\partial I^2} \right|_{G, \rho_2 - \delta_2} \leq \tilde{M}, \quad |\tilde{\omega}|_G \leq \tilde{L} \quad \text{and} \quad |\tilde{\omega}_n(I)| \geq \tilde{l} \quad \forall I \in G.$
- f) $\tilde{\omega}$ is $\tilde{\mu}$ -isoenergetically nondegenerate on G .
- g) Given a subset $\tilde{F} \subset F - \frac{16L\tilde{L}a^2\eta'}{\tilde{\mu}}$ and writing $\tilde{G} = (\tilde{\Omega})^{-1}(\tilde{F})$, the map $\tilde{\Omega}$ is one-to-one from $\tilde{G}$ to $\tilde{F}$, and one has the inclusions

$$\tilde{G} \subset G - \frac{4\tilde{L}a\eta'}{\tilde{\mu}}, \quad \Omega(\tilde{G}) \supset \tilde{F} - a\eta'.$$

Moreover, the following estimates hold:

$$\left| \tilde{\Omega} - \Omega \right|_G \leq a\eta', \quad \left| (\tilde{\Omega})^{-1} - \Omega^{-1} \right|_{\tilde{F}} \leq \frac{2La\eta'}{\mu}.$$

Proof By condition (2.11) we have, for every $I \in G$ and $0 < |k|_1 \leq K, \bar{k} \neq 0$,

$$|k \cdot \omega(I)| \geq \frac{\beta}{|k|_1^\tau} |\omega_n(I)| \geq \frac{l\beta}{K^\tau}.$$

This estimate holds even if $\bar{k} = 0$ since $|\omega_n(I)| \geq l$ and $\beta \leq 1$. Then, the set $\omega(G)$ is $\frac{l\beta}{K^\tau}, K$ -nonresonant modulo 0. This fact and conditions (2.12) and (2.13) on ρ_2 and ε allow to apply the Iterative Lemma (theorem 1.1 with $Z = 0, \mathcal{M} = 0$ and $\alpha = \frac{l\beta}{K^\tau}$). We obtain the canonical transformation Φ and, according to (1.11–1.12), the new Hamiltonian may be written as $H \circ \Phi = \tilde{h} + \tilde{R}$, where $\tilde{h} = h + \tilde{Z}$, and we have $\tilde{Z} = R_0$. One sees the estimates of (a) using that

$$|\tilde{\omega} - \omega|_{G, \rho_2} = \left| \frac{\partial R_0}{\partial I} \right|_{G, \rho_2} = \xi. \quad (2.15)$$

The estimates of (b) and (d) are provided directly by the Iterative Lemma. The bound (c) comes from the inequality (1.21) in the Iterative Lemma. The estimates of part (e) come from (2.15), condition (2.13) on ξ and the Cauchy inequality

$$\left| \frac{\partial^2 \tilde{h}}{\partial I^2} - \frac{\partial^2 h}{\partial I^2} \right|_{G, \rho_2 - \delta_2} \leq \frac{\xi}{\delta_2}.$$

We prove (f) using lemma 2.2, which tells us that $\tilde{\omega}$ is μ' -isoenergetically nondegenerate on G , where

$$\mu' = \mu - \frac{4\tilde{M}}{\tilde{l}} |\tilde{\omega} - \omega|_G - \left| \frac{\partial^2 \tilde{h}}{\partial I^2} - \frac{\partial^2 h}{\partial I^2} \right|_G \geq \mu - \frac{4\tilde{M}}{\tilde{l}} \cdot \xi - \frac{\xi}{\rho_2} \geq \mu - \frac{3\xi}{\rho_2} \geq \tilde{\mu}.$$

We have used (2.15), condition (2.13) on ξ , the inequality

$$\left| \frac{\partial^2 \tilde{h}}{\partial I^2} - \frac{\partial^2 h}{\partial I^2} \right|_G \leq \frac{\xi}{\rho_2}$$

and the inequality $\rho_2 \leq \tilde{l}/2\tilde{M}$, deduced from (2.12).

Before going on, we remark that the bounds on the derivatives of Ω given in lemma 2.1 are also valid for $\tilde{\Omega}$, on G , provided one replaces M, L, l, μ , by $\tilde{M}, \tilde{L}, \tilde{l}, \tilde{\mu}$, respectively. We do not need to change the constant a because we are assuming that $a \geq 2\tilde{M}/\tilde{l}^2$. We shall now apply lemma 2.3 but we have to take, instead of the parameters of that lemma $M, m, \tilde{M}, \tilde{m}$, the values obtained applying lemma 2.1 to Ω and to $\tilde{\Omega}$. We first find the value which will replace ε in lemma 2.3, i.e. an estimate for $\left| \tilde{\Omega} - \Omega \right|_G$. We have

$$\begin{aligned} \left| \tilde{\Omega}(I) - \Omega(I) \right| &\leq \frac{|\tilde{\omega}_n(I) - \omega_n(I)| \cdot |\tilde{\omega}(I)| + |\tilde{\omega}(I) - \omega(I)| \cdot |\omega_n(I)|}{|\omega_n(I)| \cdot |\tilde{\omega}_n(I)|} \\ &\leq \frac{|\tilde{\omega}(I) - \omega(I)| \cdot |\omega(I)|}{|\omega_n(I)| \cdot |\tilde{\omega}_n(I)|} \leq \frac{L\xi}{\tilde{l}}, \\ \left| \tilde{\Omega}_n(I) - \Omega_n(I) \right| &\leq a \left| \tilde{h}(I) - h(I) \right| \leq a\eta. \end{aligned}$$

Therefore,

$$\left| \tilde{\Omega} - \Omega \right|_G \leq \sqrt{\left(\frac{L\xi}{\tilde{l}} \right)^2 + (a\eta)^2} \leq a\eta',$$

where the condition on a has been used. Then, lemma 2.3 applies if the next inequality (which replaces (2.10) of that lemma) is fulfilled:

$$a\eta' \leq \frac{\left(\frac{\tilde{\mu}}{2\tilde{L}} \right)^2}{4 \left(\frac{\tilde{M}'}{2\tilde{M}} + \frac{3\tilde{M}}{\tilde{l}} \right) \tilde{L}a}, \quad (2.16)$$

where we have taken into account the inequality

$$\left| \frac{\partial^3 \tilde{h}}{\partial I^3} \right|_G \leq \tilde{M}' := \frac{\tilde{M}}{\rho_2 - \delta_2}.$$

It is easy to check that the inequality (2.16) is guaranteed by condition (2.14) on η' . Then, lemma 2.3 gives part (g). $\square$

2.1.4 Invariant tori

In order to estimate the measure of the resonant strips which we remove along the successive steps, a reasonable condition has to be imposed on the domain. Given $F \subset \mathbb{R}^n$ and $D > 0$ we say F to be a D -set if, for any $0 \leq b_1 < b_2$,

$$\text{mes} \left[(F - b_1) \setminus (F - b_2) \right] \leq D(b_2 - b_1).$$

We remark that the constant D is a rough upper bound of the “area” of the boundary of F , which is forced to be finite.

The next technical lemma provides the necessary estimates for the measure when resonant strips of the type introduced in (2.7) are removed from F . We point out that it suffices to remove resonant strips corresponding to integer vectors $k = (\bar{k}, k_n) \in \mathbb{Z}^n$ with $\bar{k} \neq 0$, since it is assumed that $\omega_n(I) \neq 0$ throughout the domain. The proof of this result is deferred to section 2.2.

Lemma 2.5. *Let $F \subset \mathbb{R}^n$ a D -set. For $d \geq 0$, $\tau > 0$, $\beta \geq 0$ and $K \geq 0$ given, K an integer, let us denote*

$$F(d, \beta, K) := (F - d) \setminus \bigcup_{\substack{|k|_1 \leq K \\ \bar{k} \neq 0}} \Delta \left(k, \frac{\beta}{|k|_1^\tau} \right).$$

One has:

a) *Given $d' \geq d$, $\beta' \geq \beta$ and $K' \geq K$,*

$$\begin{aligned} & \text{mes} \left[F(d, \beta, K) \setminus F(d', \beta', K') \right] \\ & \leq D(d' - d) + 2(\text{diam } F)^{n-1} \left(\sum_{\substack{|k|_1 \leq K \\ \bar{k} \neq 0}} \frac{\beta' - \beta}{|k|_1^\tau \cdot |\bar{k}|} + \sum_{\substack{K < |k|_1 \leq K' \\ \bar{k} \neq 0}} \frac{\beta'}{|k|_1^\tau \cdot |\bar{k}|} \right). \end{aligned}$$

b) *For every $b \geq 0$,*

$$\text{mes} \left[F(d, \beta, K) \setminus (F(d, \beta, K) - b) \right] \leq \left(D + 2^{n+1}(\text{diam } F)^{n-1} K^n \right) b.$$

Next we give the proof of KAM theorem under the assumption of isoenergetic nondegeneracy. We remark that the basic scheme of the proof would be the same for the standard nondegeneracy.

Our approach consists, like the original Arnold’s proof [Arn63], of iterating the estimates of the Inductive Lemma, which give rise to a rapidly convergent (i.e. more than linear) procedure. However,

conversely to [Arn63], for the proof of KAM theorem we only need to show explicitly that the remainders decrease in a linear way. This approach already appears in [Pös82]. However, in the next section (on nearly-invariant tori) we show the rapid convergence in order to obtain exponential stability estimates.

A comment has to be made on the parameter ν appearing in theorem 2.1 below. Our statement and its proof have been slightly complicated because of the presence of this parameter. Actually, the freedom on the choice of ν is not strictly necessary but we make use of it in the next section, where it is shown that a small ν gives rise to an almost quadratic procedure (with exponent $2^{1-\nu}$) and hence to better stability estimates. It is not possible to choose $\nu = 0$, which would actually provide a quadratic procedure.

Theorem 2.1 (Isoenergetic KAM Theorem). *Let $\mathcal{G} \subset \mathbb{R}^n$, $n \geq 2$, a compact, and let $H(\phi, I) = h(I) + f(\phi, I)$ real analytic on $\mathcal{D}_\rho(\mathcal{G})$. Let $\omega = \text{grad } h$, and assume the bounds:*

$$\left| \frac{\partial^2 h}{\partial I^2} \right|_{\mathcal{G}, \rho_2} \leq M, \quad |\omega|_{\mathcal{G}} \leq L \quad \text{and} \quad |\omega_n(I)| \geq l \quad \forall I \in \mathcal{G}.$$

Assume also that ω is μ -isoenergetically nondegenerate on $\mathcal{G}$. For $a = 16M/l^2$, assume that the map $\Omega = \Omega_{\omega, h, a}$ is one-to-one on $\mathcal{G}$, and that its range $F = \Omega(\mathcal{G})$ is a D -set. Let $\tau > n - 1$, $\gamma > 0$ and $0 < \nu < 1$ given, and assume:

$$\varepsilon := \|f\|_{\mathcal{G}, \rho} \leq \frac{\nu^2 l^6 \mu^2 \hat{\rho}^{2\tau+2}}{2^{4\tau+32} L^6 M^3} \cdot \gamma^2, \quad \gamma \leq \min \left(\frac{8LM\rho_2}{\nu l \hat{\rho}^{\tau+1}}, l \right), \quad (2.17)$$

where we write $\hat{\rho} := \min \left(\frac{\nu \rho_1}{12(\tau+2)}, 1 \right)$. Define the set

$$\widehat{G} = \widehat{G}_\gamma := \left\{ I \in \mathcal{G} - \frac{2\gamma}{\mu} : \omega(I) \text{ is } \tau, \gamma\text{-Diophantine} \right\}.$$

Then, there exists a real continuous map $\mathcal{T} : \mathcal{W}_{\frac{\rho_1}{4}}(\mathbb{T}^n) \times \widehat{G} \rightarrow \mathcal{D}_\rho(\mathcal{G})$, analytic with respect to the angular variables, such that:

- a) For every $I \in \widehat{G}$, the set $\mathcal{T}(\mathbb{T}^n \times \{I\})$ is an invariant torus of H , its frequency vector is colinear to $\omega(I)$ and its energy is $h(I)$.
- b) Writing

$$\mathcal{T}(\phi, I) = (\phi + \mathcal{T}_\phi(\phi, I), I + \mathcal{T}_I(\phi, I)),$$

one has the estimates

$$|\mathcal{T}_\phi|_{\widehat{G}, (\frac{\rho_1}{4}, 0), \infty} \leq \frac{2^{2\tau+15} L^2 M}{\nu^2 l^2 \hat{\rho}^{2\tau+1}} \cdot \frac{\varepsilon}{\gamma^2}, \quad |\mathcal{T}_I|_{\widehat{G}, (\frac{\rho_1}{4}, 0)} \leq \frac{2^{\tau+16} L^3 M}{\nu l^3 \mu \hat{\rho}^{\tau+1}} \cdot \frac{\varepsilon}{\gamma}.$$

- c) $\text{mes} \left[(\mathbb{T}^n \times \mathcal{G}) \setminus \mathcal{T}(\mathbb{T}^n \times \widehat{G}) \right] \leq C \gamma$, where C is a (very complicated) constant depending on $n, \tau, \text{diam } F, D, \hat{\rho}, M, L, l, \mu$.

Proof

A. Choice of the parameters. Since we make iterative use of proposition 2.4, we first introduce appropriate sequences of parameters to replace the constants of that proposition. For $q \geq 0$, we define

$$M_q = \left(2 - \frac{1}{2^q}\right) M, \quad L_q = \left(2 - \frac{1}{2^q}\right) L, \quad l_q = \left(1 + \frac{1}{2^q}\right) \frac{l}{2}, \quad \mu_q = \left(1 + \frac{1}{2^q}\right) \frac{\mu}{2}.$$

Note that M_q, L_q increase from M, l to $2M, 2L$, respectively, for $q \rightarrow \infty$, and that l_q, μ_q decrease from l, μ to $l/2, \mu/2$. We also put

$$K_0 = 0, \quad K_q = K \cdot 2^{q-1}, \quad q \geq 1,$$

where $K \geq 1$ is an integer to be fixed below. Moreover, we define

$$\beta := \frac{\gamma}{L} \leq 1$$

and, for $q \geq 0$, we put $\rho^{(q)} = (\rho_1^{(q)}, \rho_2^{(q)})$, with

$$\rho_1^{(q)} = \left(1 + \frac{1}{2^{\nu q}}\right) \frac{\rho_1}{4}, \quad \rho_2^{(q)} = \frac{\nu l \beta}{32 M K_{q+1}^{\tau+1}}.$$

We notice that $\rho_1^{(q)}$ decreases from $\rho_1/2$ to $\rho_1/4$, and that $\rho_2^{(q)}$ decreases to 0. We also write

$$\delta_1^{(q)} = \rho_1^{(q-1)} - \rho_1^{(q)}, \quad \delta_2^{(q)} = \rho_2^{(q-1)} - \rho_2^{(q)}, \quad c_q = \frac{\delta_2^{(q)}}{\delta_1^{(q)}}.$$

Taking into account that the inequalities $\frac{\nu}{2} \leq 1 - \frac{1}{2^\nu} \leq \nu$ and $1 - \frac{1}{2^{\tau+1}} \geq \frac{1}{2}$, hold for $0 < \nu < 1$ and $\tau > 0$ respectively, it is easy to see that, for every $q \geq 1$,

$$\frac{\nu \rho_1}{8 \cdot 2^{\nu(q-1)}} \leq \delta_1^{(q)} \leq \frac{\nu \rho_1}{4 \cdot 2^{\nu(q-1)}}, \quad \delta_2^{(q)} \geq \frac{\nu l \beta}{64 M K_q^{\tau+1}}, \quad (2.18)$$

$$\frac{l \beta \cdot 2^{\nu(q-1)}}{16 M K_q^{\tau+1} \rho_1} \leq c_q \leq \frac{l \beta \cdot 2^{\nu(q-1)}}{4 M K_q^{\tau+1} \rho_1}. \quad (2.19)$$

Finally, we define

$$\beta_q = \left(1 - \frac{1}{2^{\nu q}}\right) \beta, \quad \beta'_q = \frac{\beta_q + \beta_{q+1}}{2},$$

which are both increasing with limit β . It is also easy to check that $\beta'_q \geq \nu \beta / 4$ for every $q \geq 0$.

We choose K as the minimum integer such that $K \hat{\rho} \geq 1$. Then, one has $K \leq 2/\hat{\rho}$. Using this inequality, our choice $\beta = \gamma/L$ and the inequality $\hat{\rho} \leq \nu \rho_1$, we deduce from conditions (2.17) the inequalities

$$\varepsilon \leq \min \left(\frac{\nu^3 l^2 \rho_1 \beta^2}{2^{2\tau+20} M K^{2\tau+1}}, \frac{\nu^2 l^6 \mu^2 \beta^2}{2^{\tau+30} L^4 M^3 K^{2\tau+2}} \right), \quad \beta \leq \frac{8 M K^{\tau+1} \rho_2}{\nu l}. \quad (2.20)$$

B. Induction. Starting with $G_0 = \mathcal{G}$, we shall now construct a decreasing sequence of compacts $G_q \subset \mathcal{G}$ and a sequence of real analytic canonical transformations $\Phi^{(q)} : \mathcal{D}_{\rho^{(q)}}(G_q) \rightarrow \mathcal{D}_{\rho^{(q-1)}}(G_{q-1})$, $q \geq 1$. Denoting $\Psi^{(q)} = \Phi^{(1)} \circ \dots \circ \Phi^{(q)}$, the transformed Hamiltonians will be written in the form $H^{(q)} = H \circ \Psi^{(q)} = h^{(q)}(I) + R^{(q)}(\phi, I)$. Moreover, we write $\omega^{(q)} = \text{grad } h^{(q)}$ and $\Omega^{(q)} = \Omega_{\omega^{(q)}, h^{(q)}, a}$. We are going to show that the following statements hold for every $q \geq 0$:

$$1_q) \quad \varepsilon_q := \|DR^{(q)}\|_{G_q, \rho^{(q)}, c_{q+1}} \leq \frac{8\varepsilon}{\nu \rho_1 \cdot 2^{(2\tau+2)q}}.$$

$$2_q) \quad \eta_q := |R_0^{(q)}|_{G_q, \rho_2^{(q)}} \leq \frac{\varepsilon}{2^{(2\tau+3)q}}, \quad \xi_q := \left| \frac{\partial R_0^{(q)}}{\partial I} \right|_{G_q, \rho_2^{(q)}} \leq \frac{2^6 M K^{\tau+1} \varepsilon}{\nu l \beta \cdot 2^{(\tau+2)q}}.$$

$$3_q) \quad \left| \frac{\partial^2 h^{(q)}}{\partial I^2} \right|_{G_q, \rho_2^{(q)}} \leq M_q, \quad |\omega^{(q)}|_{G_q} \leq L_q \quad \text{and} \quad |\omega^{(q)}(I)| \geq l_q \quad \forall I \in G_q.$$

$$4_q) \quad \omega^{(q)} \text{ is } \mu_q\text{-isoenergetically nondegenerate on } G_q.$$

$$5_q) \quad \Omega^{(q)} \text{ is one-to-one on } G_q, \text{ and } \Omega^{(q)}(G_q) = F_q, \text{ where we define}$$

$$F_q := (F - \beta_q) \setminus \bigcup_{\substack{|k|_1 \leq K_q \\ \bar{k} \neq 0}} \Delta \left(k, \frac{\beta_q}{|k|_1^\tau} \right). \quad (2.21)$$

We proceed by induction. For $q = 0$, we choose $G_0 = \mathcal{G}$, $h^{(0)} = h$, $R^{(0)} = f$. Note that

$$\rho_1^{(0)} = \frac{\rho_1}{2}, \quad \rho_2^{(0)} = \frac{\nu l \beta}{32 M K^{\tau+1}} \leq \frac{\rho_2}{2}$$

by (2.20). Then,

$$\varepsilon_0 = \|Df\|_{\mathcal{G}, \rho^{(0)}, c_1} \leq \frac{\varepsilon}{\delta_1^{(1)}} \leq \frac{8\varepsilon}{\nu \rho_1}, \quad (2.22)$$

namely (1_0) . The first estimate of (2_0) is obvious, and the second one comes from the Cauchy inequality

$$\xi_0 \leq \frac{2}{\rho_2} \left| R_0^{(0)} \right|_{\mathcal{G}, \rho_2} \leq \frac{2\varepsilon}{\rho_2} \leq \frac{\varepsilon}{\rho_2^{(0)}}.$$

The remaining statements (3_0-5_0) are clear.

For $q \geq 1$, we assume the statements true for $q-1$ and we prove them for q . We attain this aim by applying proposition 2.4 to $H^{(q-1)} = h^{(q-1)} + R^{(q-1)}$, with K_q instead of K . However, in order to fulfil condition (2.11), we must replace the domains G_{q-1} and F_{q-1} by suitable subsets where the resonances from order $K_{q-1} + 1$ to order K_q have been removed. More precisely, we define

$$F'_{q-1} := (F - \beta_{q-1}) \setminus \bigcup_{\substack{|k|_1 \leq K_q \\ \bar{k} \neq 0}} \Delta \left(k, \frac{\beta'_{q-1}}{|k|_1^\tau} \right), \quad G'_{q-1} := \left(\Omega^{(q-1)} \right)^{-1} \left(F'_{q-1} \right). \quad (2.23)$$

The nonresonance condition (2.11) is then fulfilled by F'_{q-1} , β'_{q-1} and K_q instead of F , β and K , respectively (taking β'_{q-1} instead of β_{q-1} , we avoid to apply proposition 2.4 with $\beta_0 = 0$ for $q = 1$). The remaining parameters taking part in proposition 2.4 are M_{q-1} , L_{q-1} , l_{q-1} , μ_{q-1} , $\rho^{(q-1)}$, $\delta^{(q)}$, c_q , M_q , L_q , l_q , μ_q , replacing M , L , l , μ , ρ , δ , c , $\tilde{M}$, $\tilde{L}$, $\tilde{l}$, $\tilde{\mu}$, respectively, and

$$a = \frac{16M}{l^2} \geq \frac{2M_q}{l_q^2}.$$

It is clear that condition (2.12) on $\rho_2^{(q-1)}$ is satisfied with our choice of the parameters. Concerning condition (2.13) on ε_{q-1} , we first notice that, by (2.19) and our choice of K ,

$$A_q := 1 + \frac{2M_{q-1}c_qK_q^\tau}{l_{q-1}\beta'_{q-1}} \leq 1 + \frac{32M}{\nu l \beta} \cdot \frac{l\beta}{4MK\rho_1} = 1 + \frac{8}{\nu K\rho_1} \leq 2.$$

Then, to see that condition (2.13) is fulfilled we have to check the inequality

$$\varepsilon_{q-1} \leq \frac{l_{q-1}\beta'_{q-1}\delta_2^{(q)}}{148K_q^\tau}.$$

Indeed, recalling the definitions of the parameters and applying (1_{q-1}) and (2.18), it suffices to check that

$$\frac{8\varepsilon}{\nu\rho_1} \leq \frac{\nu l \beta}{2^{11}K^\tau} \cdot \frac{\nu l \beta}{64MK^{\tau+1}},$$

which can be deduced from (2.20). Let us verify the second condition of (2.13), namely

$$\xi_{q-1} \leq \min \left((M_q - M_{q-1})\delta_2^{(q)}, L_q - L_{q-1}, l_{q-1} - l_q, \frac{(\mu_{q-1} - \mu_q)\rho_2^{(q-1)}}{3} \right).$$

By (2_{q-1}) and (2.18), this condition holds, since we may deduce from (2.20) the inequality

$$\frac{2^6MK^{\tau+1}\varepsilon}{\nu l \beta} \leq \min \left(\frac{M}{2} \cdot \frac{\nu l \beta}{64MK^{\tau+1}}, \frac{L}{2}, \frac{l}{4}, \frac{\mu}{12} \cdot \frac{\nu l \beta}{32MK^{\tau+1}} \right).$$

Finally, we have to check condition (2.14):

$$\eta'_{q-1} := \frac{L_{q-1}\xi_{q-1}}{2M_q} + \eta_{q-1} \leq \frac{\mu_q^2\rho_2^{(q)}}{32L_q^3a^2}. \quad (2.24)$$

By (2_{q-1}) , we have the estimate

$$\eta'_{q-1} \leq \frac{L}{2M} \cdot \frac{2^6MK^{\tau+1}\varepsilon}{\nu l \beta \cdot 2^{(\tau+2)(q-1)}} + \frac{\varepsilon}{2^{(2\tau+3)(q-1)}} \leq \frac{2^6LK^{\tau+1}\varepsilon}{\nu l \beta \cdot 2^{(\tau+2)(q-1)}}. \quad (2.25)$$

Taking into account the value of a , the inequality (2.24) holds, since

$$\frac{2^6LK^{\tau+1}\varepsilon}{\nu l \beta} \leq \frac{l^4\mu^2}{2^{18}L^3M^2} \cdot \frac{\nu l \beta}{2^{\tau+6}MK^{\tau+1}},$$

as deduced from (2.20).

Applying proposition 2.4 with the parameters considered above, we obtain a canonical transformation $\Phi^{(q)}$ and a new Hamiltonian $H^{(q)} = h^{(q)} + R^{(q)}$. The new domain $G_q \subset G'_{q-1}$ is chosen below. First, we prove (1_q-4_q) . By the bound (b) of proposition 2.4 and the inequality $c_{q+1} \leq c_q$,

$$\varepsilon_q \leq \left\| DR^{(q)} \right\|_{G_q, \rho^{(q)}, c_q} \leq e^{-K_q \delta_1^{(q)}} \cdot \varepsilon_{q-1} + \frac{14A_q K_q^\tau}{l_{q-1} \beta'_{q-1} \delta_2^{(q)}} \cdot \varepsilon_{q-1}^2. \quad (2.26)$$

Let us bound the terms of this sum. By (2.18) and the inequality $K\hat{\rho} \geq 1$,

$$K_q \delta_1^{(q)} \geq \frac{\nu K \rho_1}{8} \cdot 2^{(1-\nu)(q-1)} \geq (2\tau + 3) \ln 2, \quad (2.27)$$

and therefore

$$e^{-K_q \delta_1^{(q)}} \leq \frac{1}{2^{2\tau+3}}.$$

Moreover, applying (2.18), (1_{q-1}) and (2.20),

$$\frac{14A_q K_q^\tau}{l_{q-1} \beta'_{q-1} \delta_2^{(q)}} \cdot \varepsilon_{q-1} \leq \frac{2^8 K_q^\tau}{\nu l \beta} \cdot \frac{64M K_q^{\tau+1}}{\nu l \beta} \cdot \frac{8\varepsilon}{\nu \rho_1 \cdot 2^{(2\tau+2)(q-1)}} \leq \frac{1}{2^{2\tau+3} \cdot 2^{q-1}}. \quad (2.28)$$

Then, we deduce from (2.26) that

$$\varepsilon_q \leq \frac{\varepsilon_{q-1}}{2^{2\tau+2}},$$

which gives (1_q) . For (2_q) , we use part (c) of proposition 2.4. Writing $\sigma_2^{(q)} = \rho_2^{(q-1)} - \delta_2^{(q)}/2$, we have:

$$\eta_q \leq \left| R_0^{(q)} \right|_{G_q, \sigma_2^{(q)}} \leq \frac{7A_q K_q^\tau}{c_q l_{q-1} \beta'_{q-1}} \cdot \varepsilon_{q-1}^2 \leq \frac{\delta_1^{(q)} \varepsilon_{q-1}}{2} \cdot \frac{1}{2^{2\tau+3} \cdot 2^{q-1}} \leq \frac{\varepsilon}{2^{(2\tau+3)q}}, \quad (2.29)$$

where we have used the inequalities (2.28), (2.18) and (1_{q-1}) . We obtain the other estimate of (2_q) using the Cauchy inequality and (2.18):

$$\xi_q \leq \frac{2}{\delta_2^{(q)}} \left| R_0^{(q)} \right|_{G_q, \sigma_2^{(q)}} \leq \frac{2}{\delta_2^{(q)}} \cdot \frac{\varepsilon}{2^{(2\tau+3)q}}.$$

The statements (3_q-4_q) are clear from proposition 2.4. For (5_q) , we apply part (g) of proposition 2.4 to the subset F_q . We have to check that

$$F_q \subset F'_{q-1} - \frac{16L_{q-1}L_q a^2 \eta'_{q-1}}{\mu_q}. \quad (2.30)$$

Defining

$$d_q := \frac{\beta_q - \beta_{q-1}}{2K_q^{\tau+1}}$$

and looking at (2.23) and (2.21), we have

$$F'_{q-1} - d_q \supset (F - (\beta_{q-1} + d_q)) \setminus \bigcup_{\substack{|k|_1 \leq K_q \\ \bar{k} \neq 0}} \Delta \left(k, \frac{\beta'_{q-1}}{|k|_1^\tau} + |\bar{k}| d_q \right) \supset F_q, \quad (2.31)$$

where we have used the inequalities

$$\beta_{q-1} + d_q \leq \beta_q, \quad \frac{\beta'_{q-1}}{|k|_1^\tau} + |\bar{k}| d_q \leq \frac{\beta_q}{|k|_1^\tau}.$$

Moreover, applying estimate (2.25) for η'_{q-1} and (2.20),

$$\frac{16L_{q-1}L_q a^2 \eta'_{q-1}}{\mu_q} \leq \frac{2^{15} L^2 M^2}{l^4 \mu} \cdot \frac{2^6 L K^{\tau+1} \varepsilon}{\nu l \beta \cdot 2^{(\tau+2)(q-1)}} \leq \frac{\nu \beta}{4 \cdot 2^{\nu(q-1)} K_q^{\tau+1}} \leq d_q.$$

This bound and the inclusion (2.31) imply (2.30). Hence, part (g) of proposition 2.4 says that $\Omega^{(q)}$ is one-to-one on $G_q = \left(\Omega^{(q)}\right)^{-1}(F_q)$. This gives (5_q), and the induction is completed.

C. Convergence of the diffeomorphisms. We now see the convergence of the successive maps $\Omega^{(q)} : G_q \rightarrow F_q$. Applying part (g) of proposition 2.4 again, we obtain for $q \geq 1$ the estimates

$$\left| \Omega^{(q)} - \Omega^{(q-1)} \right|_{G_q} \leq a\eta'_{q-1}, \quad \left| \left(\Omega^{(q)}\right)^{-1} - \left(\Omega^{(q-1)}\right)^{-1} \right|_{F_q} \leq \frac{2L_{q-1}a\eta'_{q-1}}{\mu_{q-1}}. \quad (2.32)$$

Therefore, by the bound (2.25) on η'_{q-1} , the sequences $\Omega^{(q)}$ and $\left(\Omega^{(q)}\right)^{-1}$ converge respectively to maps which we name Ω^* and Υ , defined on the sets

$$G^* := \bigcap_{q \geq 0} G_q, \quad F^* := \bigcap_{q \geq 0} F_q = (F - \beta) \setminus \bigcup_{\substack{k \in \mathbb{Z}^n \\ k \neq 0}} \Delta \left(k, \frac{\beta}{|k|_1^\tau} \right). \quad (2.33)$$

Note that the compacity of F^* has been used to establish the second equality. From (2.32) we deduce:

$$\left| \Omega^* - \Omega^{(q)} \right|_{G^*} \leq \sum_{s \geq q} a\eta'_s, \quad \left| \Upsilon - \left(\Omega^{(q)}\right)^{-1} \right|_{F^*} \leq \sum_{s \geq q} \frac{2L_s a\eta'_s}{\mu_s}. \quad (2.34)$$

Note also that, for every q ,

$$G_q \subset G_{q-1} - \frac{4L_q a\eta'_{q-1}}{\mu_q}, \quad F_q \subset F_{q-1} - \frac{16L_{q-1}L_q a^2\eta'_{q-1}}{\mu_q}.$$

Iterating these inclusions we deduce the following two ones:

$$G^* \subset G_q - \sum_{s \geq q} \frac{4L_{s+1}a\eta'_s}{\mu_{s+1}}, \quad F^* \subset F_q - \sum_{s \geq q} \frac{16L_s L_{s+1} a^2 \eta'_s}{\mu_{s+1}}, \quad (2.35)$$

to be used below. We are now going to see that Ω^* is one-to-one on G^* and that $\Omega^*(G^*) = F^*$. Given $I \in G^*$, we have $\Omega^{(q)}(I) \in F_q$ for every q . Hence $\Omega^*(I) \in F^*$, and we deduce that $\Omega^*(G^*) \subset F^*$. Analogously, we have $\Upsilon(F^*) \subset G^*$. Moreover, we prove that $\Upsilon(\Omega^*(I)) = I$ for every $I \in G^*$. Indeed, for every q ,

$$\begin{aligned} & \left| \Upsilon(\Omega^*(I)) - I \right| \\ & \leq \left| \Upsilon(\Omega^*(I)) - \left(\Omega^{(q)}\right)^{-1}(\Omega^*(I)) \right| + \left| \left(\Omega^{(q)}\right)^{-1}(\Omega^*(I)) - \left(\Omega^{(q)}\right)^{-1}(\Omega^{(q)}(I)) \right| \\ & \leq \left| \Upsilon - \left(\Omega^{(q)}\right)^{-1} \right|_{F^*} + \frac{2L_q}{\mu_q} \left| \Omega^* - \Omega^{(q)} \right|_{G^*}. \end{aligned} \quad (2.36)$$

For the estimate of the second term, we have used the following two facts: on one hand, part (b) of lemma 2.1 gives the bound

$$\left| \frac{\partial \Omega^{(q)}}{\partial I}(I') v \right| \geq \frac{\mu_q}{2L_q} |v| \quad \forall v \in \mathbb{R}^n, \quad \forall I' \in G_q;$$

on the other hand, by (2.34–2.35) the segment joining $\Omega^{(q)}(I)$ and $\Omega^*(I)$ is contained in F_q . Then, since the bound obtained in (2.36) tends to zero for $q \rightarrow \infty$, we deduce that $\Upsilon(\Omega^*(I)) = I$, and therefore Ω^* is one-to-one. A symmetric argument allows to prove that $\Omega^*(\Upsilon(J)) = J$ for every $J \in F^*$. This implies that $\Omega^*(G^*) \supset F^*$. Thus, the map Ω^* is one-to-one and $\Omega^*(G^*) = F^*$.

We also see, from proposition 2.4, that

$$\left| \omega^{(q)} - \omega^{(q-1)} \right|_{G_q, \rho_2^{(q-1)}} \leq \xi_{q-1}, \quad \left| h^{(q)} - h^{(q-1)} \right|_{G_q, \rho_2^{(q-1)}} \leq \eta_{q-1}.$$

This implies that the sequences $\omega^{(q)}$ and $h^{(q)}$ converge to some continuous maps ω^* and h^* , respectively. Note also that, for $I \in G^*$,

$$\Omega^*(I) = \left(\frac{\overline{\omega^*}(I)}{\omega_n^*(I)}, a h^*(I) \right). \quad (2.37)$$

From (2_q) we deduce, for every $q \geq 0$, the following bound to be used later:

$$\left| \omega^* - \omega^{(q)} \right|_{G^*} \leq \sum_{s \geq q} \xi_s \leq \frac{2^7 M K^{\tau+1} \varepsilon}{\nu l \beta \cdot 2^{(\tau+2)q}}. \quad (2.38)$$

D. Convergence of the canonical transformations. Next we estimate how near to the identity map the transformations $\Psi^{(q)}$ are. Applying part (d) of proposition 2.4 and using (1_{q-1}), (2.18) and (2.20), one deduces that, for every $q \geq 1$,

$$\begin{aligned} \left| \Phi^{(q)} - \text{id} \right|_{G_q, \sigma^{(q)}, c_q} &\leq \frac{2A_q K_q^\tau}{l_{q-1} \beta'_{q-1}} \cdot \varepsilon_{q-1} \leq \frac{2^5 K_q^\tau}{\nu l \beta} \cdot \frac{8\varepsilon}{\nu \rho_1 \cdot 2^{(2\tau+2)(q-1)}} \\ &= \frac{2^8 K^\tau \varepsilon}{\nu^2 l \rho_1 \beta \cdot 2^{(\tau+2)(q-1)}} \leq \frac{\delta_2^{(q)}}{8 \cdot 2^{q-1}}, \end{aligned} \quad (2.39)$$

where we write $\sigma^{(q)} = \rho^{(q-1)} - \delta_2^{(q)}/2$. Then, applying property (1.16) of section 1.2.2,

$$\left| D\Phi^{(q)} - \text{Id} \right|_{G_q, \rho^{(q)}, c_q} \leq \frac{2}{\delta_2^{(q)}} \left| \Phi^{(q)} - \text{id} \right|_{G_q, \sigma^{(q)}, c_q} \leq \frac{1}{4 \cdot 2^{q-1}}.$$

Let x, y such that the segment joining them is contained $\mathcal{D}_{\rho^{(q)}}(G_q)$. The mean value theorem gives the bound:

$$\left| \Phi^{(q)}(x) - \Phi^{(q)}(y) \right|_{c_q} \leq \left| D\Phi^{(q)} \right|_{G_q, \rho^{(q)}, c_q} \cdot |x - y|_{c_q}.$$

By (2.39),

$$\left| \Phi^{(q)}(x) - x \right|_{c_q} \leq \delta_2^{(q)}, \quad \left| \Phi^{(q)}(y) - y \right|_{c_q} \leq \delta_2^{(q)}.$$

Then, since $\rho^{(q)} + \delta^{(q)} = \rho^{(q-1)}$, it turns out that the segment joining $\Phi^{(q)}(x)$ and $\Phi^{(q)}(y)$ is contained in $\mathcal{D}_{\rho^{(q-1)}}(G_{q-1})$. Therefore,

$$\begin{aligned} &\left| \Phi^{(q-1)} \left(\Phi^{(q)}(x) \right) - \Phi^{(q-1)} \left(\Phi^{(q)}(y) \right) \right|_{c_{q-1}} \\ &\leq \left| D\Phi^{(q-1)} \right|_{G_{q-1}, \rho^{(q-1)}, c_{q-1}} \cdot \left| \Phi^{(q)}(x) - \Phi^{(q)}(y) \right|_{c_{q-1}} \\ &\leq 2^{\tau+1-\nu} \left| D\Phi^{(q-1)} \right|_{G_{q-1}, \rho^{(q-1)}, c_{q-1}} \cdot \left| \Phi^{(q)}(x) - \Phi^{(q)}(y) \right|_{c_q}, \end{aligned}$$

where we have used that $c_{q-1}/c_q = 2^{\tau+1-\nu}$. Iterating this argument and putting the successive bounds obtained together, we arrive at the estimate

$$\begin{aligned} &\left| \Psi^{(q)}(x) - \Psi^{(q)}(y) \right|_{c_1} \\ &\leq 2^{(\tau+1-\nu)(q-1)} \left| D\Phi^{(1)} \right|_{G_1, \rho^{(1)}, c_1} \cdot \left| D\Phi^{(2)} \right|_{G_2, \rho^{(2)}, c_2} \cdots \left| D\Phi^{(q)} \right|_{G_q, \rho^{(q)}, c_q} \cdot |x - y|_{c_q} \\ &\leq 2^{(\tau+1-\nu)(q-1)} \left(1 + \frac{1}{4} \right) \left(1 + \frac{1}{4 \cdot 2} \right) \cdots \left(1 + \frac{1}{4 \cdot 2^{q-1}} \right) \cdot |x - y|_{c_q} \\ &\leq 2^{(\tau+1-\nu)(q-1)} \cdot e^{1/2} |x - y|_{c_q} \leq 2^{(\tau+1-\nu)(q-1)} \cdot 2 |x - y|_{c_q}, \end{aligned} \quad (2.40)$$

which holds for $q \geq 1$, and for every x, y such that the segment joining them is contained in $\mathcal{D}_{\rho^{(q)}}(G_q)$. Now, given $q \geq 2$ and $x \in \mathcal{D}_{\rho^{(q)}}(G_q)$, we put $y = \Phi^{(q)}(x)$ and apply (2.40) with $q-1$ instead of q . We obtain:

$$\begin{aligned} \left| \Psi^{(q)}(x) - \Psi^{(q-1)}(x) \right|_{c_1} &= \left| \Psi^{(q-1)} \left(\Phi^{(q)}(x) \right) - \Psi^{(q-1)}(x) \right|_{c_1} \\ &\leq 2^{(\tau+1-\nu)(q-2)} \cdot 2 \left| \Phi^{(q)}(x) - x \right|_{c_{q-1}} \\ &\leq 2^{(\tau+1-\nu)(q-1)} \cdot 2 \left| \Phi^{(q)}(x) - x \right|_{c_q} \leq \frac{2^9 K^\tau \varepsilon}{\nu^2 l \rho_1 \beta \cdot 2^{(1+\nu)(q-1)}}, \end{aligned} \quad (2.41)$$

where (2.39) has been used. This estimate holds for $q \geq 2$, but one readily sees from (2.39) that it is also true for $q = 1$ (we put $\Psi^{(0)} = \text{id}$). Clearly, estimate (2.41) implies that the sequence of transformations $\Psi^{(q)}$ converges to a map

$$\Psi^* : \mathcal{D}_{(\frac{\rho_1}{4}, 0)}(G^*) = \mathcal{W}_{\frac{\rho_1}{4}}(\mathbb{T}^n) \times G^* \longrightarrow \mathcal{D}_\rho(G)$$

and we deduce, for every $q \geq 0$, the estimate

$$\left| \Psi^* - \Psi^{(q)} \right|_{G^*, (\frac{\rho_1}{4}, 0), c_1} \leq \frac{2^{10} K^\tau \varepsilon}{\nu^2 l \rho_1 \beta \cdot 2^{(1+\nu)q}}. \quad (2.42)$$

Moreover, by carrying to the limit the equation $H \circ \Psi^{(q)} = h^{(q)} + R^{(q)}$, we see that $H \circ \Psi^* = h^*(I)$ on $\mathcal{D}_{(\frac{\rho_1}{4}, 0)}(G^*)$.

E. Stability estimates. Next we see that, for $q \rightarrow \infty$, the motions associated to the transformed Hamiltonian $H^{(q)} = h^{(q)} + R^{(q)}$ and the quasiperiodic motions of $h^{(q)}$ become closer and closer. Let us denote $x^{(q)}(t) = (\phi^{(q)}(t), I^{(q)}(t))$ the trajectory of $H^{(q)}$ corresponding to a given initial condition $x^{(q)}(0) = x_0^* = (\phi_0^*, I_0^*) \in \mathbb{T}^n \times G_q$, and let $\hat{x}^{(q)}(t) := (\hat{\phi}^{(q)}(t), I_0^*) = (\phi_0^* + \omega^{(q)}(I_0^*)t, I_0^*)$ the corresponding trajectory of the integrable part $h^{(q)}$. It is clear that $\hat{x}^{(q)}(t)$ is defined for all $t \in \mathbb{R}$. Like in lemma 1.5, let us denote

$$T_q := \inf \left\{ t > 0 : \left| I^{(q)}(t) - I_0^* \right| > \delta_2^{(q+1)} \text{ or } \left| \phi^{(q)}(t) - \hat{\phi}^{(q)}(t) \right|_\infty > \delta_1^{(q+1)} \right\}. \quad (2.43)$$

Clearly, $x^{(q)}(t)$ is defined and belongs to $\mathcal{D}_{\rho^{(q)}}(G_q)$ for $0 \leq t \leq T_q$ (we remark that our use of $\delta^{(q+1)}$ instead of $\rho^{(q)}$ is just due to the fact that we shall take some advantage of the “ c_{q+1} -norm”). From the Hamiltonian equations associated to $H^{(q)}$

$$\dot{I}^{(q)}(t) = -\frac{\partial R^{(q)}}{\partial \phi} \left(x^{(q)}(t) \right), \quad \dot{\phi}^{(q)}(t) = \omega^{(q)} \left(I^{(q)}(t) \right) + \frac{\partial R^{(q)}}{\partial I} \left(x^{(q)}(t) \right),$$

we get the bounds:

$$\left| \dot{I}^{(q)}(t) \right| \leq \left\| \frac{\partial R^{(q)}}{\partial \phi} \right\|_{G_q, \rho^{(q)}} \leq \varepsilon_q, \quad (2.44)$$

$$\begin{aligned} \left| \dot{\phi}^{(q)}(t) - \omega^{(q)}(I_0^*) \right|_\infty &\leq M_q \left| I^{(q)}(t) - I_0^* \right| + \left\| \frac{\partial R^{(q)}}{\partial I} \right\|_{G_q, \rho^{(q)}, \infty} \\ &\leq 2M \left| I^{(q)}(t) - I_0^* \right| + \frac{\varepsilon_q}{c_{q+1}} \\ &\leq 2M\delta_2^{(q+1)} + \frac{\varepsilon_q}{c_{q+1}} \leq 3M\delta_2^{(q+1)}. \end{aligned} \quad (2.45)$$

In the second bound, we have used the inequality

$$\frac{\varepsilon_q}{c_{q+1}} \leq M\delta_2^{(q+1)}, \quad (2.46)$$

which comes from the bounds (1_q) and (2.18–2.20). Thus, since one of the inequalities defining (2.43) is an equality for $t = T_q$, we have

$$\delta_2^{(q+1)} = \left| I^{(q)}(T_q) - I_0^* \right| \leq T_q \varepsilon_q$$

or

$$\delta_1^{(q+1)} = \left| \phi^{(q)}(T_q) - \hat{\phi}^{(q)}(T_q) \right|_\infty \leq T_q \cdot 3M\delta_2^{(q+1)}. \quad (2.47)$$

Therefore,

$$T_q \geq \min \left(\frac{\delta_2^{(q+1)}}{\varepsilon_q}, \frac{\delta_1^{(q+1)}}{3M\delta_2^{(q+1)}} \right) \geq T'_q := \frac{1}{3Mc_{q+1}}, \quad (2.48)$$

where the inequality (2.46) has been used again. This implies:

$$\left| x^{(q)}(t) - \hat{x}^{(q)}(t) \right|_{c_{q+1}} \leq \delta_2^{(q+1)} \quad \text{for } |t| \leq T'_q. \quad (2.49)$$

Since $H^{(q)} = H \circ \Psi^{(q)}$ and $\Psi^{(q)}$ is canonical, it turns out that $\Psi^{(q)}(x^{(q)}(t))$ is a trajectory of H , defined for $|t| \leq T'_q$. For large values of q , this trajectory remains near the torus $\Psi^{(q)}(\mathbb{T}^n \times \{I_0^*\})$. Note that T'_q tends to infinity for $q \rightarrow \infty$.

F. Invariant tori. Assume now that $x_0^* \in \mathbb{T}^n \times G^*$, and write $x^*(t) = (\phi_0^* + \omega^*(I_0^*)t, I_0^*)$, $t \in \mathbb{R}$. Note that

$$\left| \hat{x}^{(q)}(t) - x^*(t) \right|_{c_{q+1}} \leq c_{q+1} \left| \omega^{(q)}(I_0^*) - \omega^*(I_0^*) \right|_{\infty} \cdot |t| \leq c_{q+1} \left| \omega^{(q)} - \omega^* \right|_{G^*, \infty} \cdot T'_q \leq \delta_2^{(q+1)}$$

for

$$|t| \leq T''_q := \frac{\delta_1^{(q+1)}}{\left| \omega^{(q)} - \omega^* \right|_{G^*, \infty}},$$

which also tends to infinity, by (2.38). Then,

$$\left| x^{(q)}(t) - x^*(t) \right|_{c_{q+1}} \leq 2\delta_2^{(q+1)} \quad \text{for } |t| \leq T'''_q := \min(T'_q, T''_q).$$

Next, we see that the trajectory $\Psi^{(q)}(x^{(q)}(t))$ is very close to $\Psi^*(x^*(t))$ for large values of q . Indeed, for $|t| \leq T'''_q$,

$$\begin{aligned} & \left| \Psi^{(q)}(x^{(q)}(t)) - \Psi^*(x^*(t)) \right|_{c_1} \\ & \leq \left| \Psi^{(q)}(x^{(q)}(t)) - \Psi^{(q)}(x^*(t)) \right|_{c_1} + \left| \Psi^{(q)}(x^*(t)) - \Psi^*(x^*(t)) \right|_{c_1} \\ & \leq 2^{(\tau+1-\nu)(q-1)} \cdot 4\delta_2^{(q+1)} + \left| \Psi^{(q)} - \Psi^* \right|_{G^*, (\frac{p_1}{4}, 0), c_1} \\ & = 4c_1 \delta_1^{(q+1)} + \left| \Psi^{(q)} - \Psi^* \right|_{G^*, (\frac{p_1}{4}, 0), c_1}, \end{aligned} \quad (2.50)$$

where we have applied (2.40). The bound obtained in (2.50) tends to zero, by (2.42). Then, for every fixed t , we see that $\Psi^{(q)}(x^{(q)}(t))$ exists for q large enough, and its limit is $\Psi^*(x^*(t))$. This fact and the continuity of the flow of H imply that $\Psi^*(x^*(t))$ is also a trajectory of H , which is defined for all $t \in \mathbb{R}$. This holds for every initial condition $x_0^* = (\phi_0^*, I_0^*) \in \mathbb{T}^n \times G^*$. Hence $\Psi^*(\mathbb{T}^n \times \{I_0^*\})$ is an invariant torus of H , with frequency vector $\omega^*(I_0^*)$. Moreover, the energy on the torus is $H(\Psi^*(\phi_0^*, I_0^*)) = h^*(I_0^*)$.

The preserved invariant tori are thus parametrized by the transformed actions $I_0^* \in G^*$. We are now going to parametrize the preserved tori by their original actions. First, let us see that $\Omega(\widehat{G}) \subset F^*$ (the Diophantine set F^* has been introduced in (2.33)). Indeed, using part (b) of lemma 2.1 and the fact that $\beta = \gamma/L$, we see that $\Omega\left(\mathcal{G} - \frac{2\gamma}{\mu}\right) \subset F - \beta$. On the other hand, given $I \in \widehat{G}$, we deduce from the Diophantine condition fulfilled by $\omega(I)$ that

$$\left| \bar{k} \cdot \overline{\Omega}(I) + k_n \right| \geq \frac{\gamma/|\omega_n(I)|}{|k|_1^\tau} \geq \frac{\beta}{|k|_1^\tau}$$

and therefore $\Omega(I) \notin \Delta\left(k, \frac{\beta}{|k|_1^\tau}\right)$ for every $k \neq 0$ (we point out that this estimate motivated our choice $\beta = \gamma/L$). Hence $\Omega(\widehat{G}) \subset F^*$ and, since $\Omega^*: G^* \rightarrow F^*$ is one-to-one, we can take for the set of invariant tori a parameter $I_0 \in \widehat{G}$ (note that some of the invariant tori are thus neglected). We define, for $(\phi_0, I_0) \in \mathcal{W}_{\frac{p_1}{4}}(\mathbb{T}^n) \times \widehat{G}$,

$$\mathcal{T}(\phi_0, I_0) = \Psi^*(\phi_0, I_0^*),$$

where $I_0^* = (\Omega^*)^{-1}(\Omega(I_0)) \in G^*$. One then obtains part (a): the set $\mathcal{T}(\mathbb{T}^n \times \{I_0\})$ is an invariant torus of H , with frequency $\omega^*(I_0^*)$ and energy $h^*(I_0^*)$. Since $\Omega^*(I_0^*) = \Omega(I_0)$, we deduce from (2.37) that $\omega^*(I_0^*)$ is colinear to $\omega(I_0)$ and that $h^*(I_0^*) = h(I_0)$.

For (b), let us write, for $(\phi_0, I_0^*) \in \mathcal{W}_{\frac{\rho_1}{4}}(\mathbb{T}^n) \times G^*$,

$$\Psi^*(\phi_0, I_0^*) = \left(\phi_0 + \Psi_\phi^*(\phi_0, I_0^*), I_0^* + \Psi_I^*(\phi_0, I_0^*) \right).$$

Then, for $(\phi_0, I_0) \in \mathcal{W}_{\frac{\rho_1}{4}}(\mathbb{T}^n) \times \widehat{G}$,

$$\mathcal{T}_\phi(\phi_0, I_0) = \Psi_\phi^*(\phi_0, I_0^*), \quad \mathcal{T}_I(\phi_0, I_0) = \Psi_I^*(\phi_0, I_0^*) + I_0 - I_0^*.$$

Using (2.42) and (2.19), we get the following estimates:

$$\begin{aligned} \left| \Psi_\phi^*(\phi_0, I_0^*) \right|_\infty &\leq \frac{1}{c_1} |\Psi^* - \text{id}|_{G^*, (\frac{\rho_1}{4}, 0), c_1} \leq \frac{2^{14} M K^{2\tau+1} \varepsilon}{\nu^2 l^2 \beta^2}, \\ \left| \Psi_I^*(\phi_0, I_0^*) \right| &\leq |\Psi^* - \text{id}|_{G^*, (\frac{\rho_1}{4}, 0), c_1} \leq \frac{2^{10} K^\tau \varepsilon}{\nu^2 l \rho_1 \beta}. \end{aligned}$$

By (2.34) and (2.25),

$$\begin{aligned} |I_0^* - I_0| &\leq \left| (\Omega^*)^{-1} - \Omega^{-1} \right|_{F^*} \leq \sum_{s \geq 0} \frac{2L_s a \eta'_s}{\mu_s} \leq \frac{8La}{\mu} \sum_{s \geq 0} \eta'_s \\ &\leq \frac{2^7 LM}{l^2 \mu} \cdot \frac{2^7 L K^{\tau+1} \varepsilon}{\nu l \beta} = \frac{2^{14} L^2 M K^{\tau+1} \varepsilon}{\nu l^3 \mu \beta}. \end{aligned}$$

By putting these bounds together, applying the inequalities $\hat{\rho} \leq \nu \rho_1$ and $K \leq 2/\hat{\rho}$ and writing the estimate in terms of γ instead of β , we get part (b).

G. Estimate of the measure. Finally, we carry out the estimate of part (c). Writing $\widehat{G}^* = (\Omega^*)^{-1} \left(\Omega(\widehat{G}) \right)$,

the invariant tori found fill the set $\mathcal{T}(\mathbb{T}^n \times \widehat{G}) = \Psi^*(\mathbb{T}^n \times \widehat{G}^*)$. Since the transformations $\Psi^{(q)}$ are canonical,

$$\text{mes} \left[\Psi^{(q)}(\mathbb{T}^n \times \widehat{G}^*) \right] = \text{mes}(\mathbb{T}^n \times \widehat{G}^*) = (2\pi)^n \cdot \text{mes}(\widehat{G}^*).$$

Using estimate (2.42) and the compacity of $\Psi^*(\mathbb{T}^n \times \widehat{G}^*)$, we get the inequality

$$\text{mes} \left[\Psi^*(\mathbb{T}^n \times \widehat{G}^*) \right] \geq (2\pi)^n \cdot \text{mes}(\widehat{G}^*).$$

Then, to estimate the measure of the complement of the invariant set, it suffices to bound the measure of $\mathcal{G} \setminus \widehat{G}^*$.

First we construct an auxiliary set, included in $\widehat{G}^*$, such that the estimates become easier on it. Let

$$\tilde{\beta} = \frac{64LM\gamma}{l^2\mu}, \quad \tilde{\beta}_q = \left(1 - \frac{1}{2^{\nu q}} \right) \tilde{\beta},$$

for $q \geq 0$, and note that $\tilde{\beta} \geq \beta$. We define the sets

$$\tilde{F}_q = \left(F - \tilde{\beta}_q \right) \setminus \bigcup_{\substack{|k|_1 \leq K_q \\ \bar{k} \neq 0}} \Delta \left(k, \frac{\tilde{\beta}_q}{|k|_1^\tau} \right), \quad \tilde{G}_q = \left(\Omega^{(q)} \right)^{-1} (\tilde{F}_q),$$

and

$$\tilde{F}^* = \bigcap_{q \geq 0} \tilde{F}_q = \left(F - \tilde{\beta} \right) \setminus \bigcup_{\substack{k \in \mathbb{Z}^n \\ \bar{k} \neq 0}} \Delta \left(k, \frac{\tilde{\beta}}{|k|_1^\tau} \right), \quad \tilde{G}^* = \bigcap_{q \geq 0} \tilde{G}_q.$$

From the fact that $\Omega^{(q)}(\tilde{G}_q) = \tilde{F}_q$ for every q , we deduce $\Omega^*(\tilde{G}^*) = \tilde{F}^*$. Let us check that $\Omega(\widehat{G}) \supset \tilde{F}^*$. Indeed, from part (a) of lemma 2.1, we get that $\Omega\left(\mathcal{G} - \frac{2\gamma}{\mu}\right) \supset F - \tilde{\beta}$. Moreover, given $J = \Omega(I) \in \tilde{F}^*$, for every $k \in \mathbb{Z}^n$ with $\bar{k} \neq 0$ we have

$$\left| \bar{k} \cdot \bar{J} + k_n \right| \geq \frac{\tilde{\beta}}{|k|_1^\tau}$$

and hence

$$|k \cdot \omega(I)| \geq \frac{\tilde{\beta} |\omega_n(I)|}{|k|_1^\tau} \geq \frac{l\tilde{\beta}}{|k|_1^\tau} \geq \frac{\gamma}{|k|_1^\tau}.$$

For $\bar{k} = 0$, it is clear that the Diophantine estimate is also fulfilled since $|\omega_n(I)| \geq l \geq \gamma$. Hence $\Omega(\widehat{G}) \supset \tilde{F}^*$ and therefore $\widehat{G}^* \supset \tilde{G}^*$. Then,

$$\text{mes} \left(\mathcal{G} \setminus \widehat{G}^* \right) \leq \sum_{q=1}^{\infty} \text{mes} \left(\tilde{G}_{q-1} \setminus \tilde{G}_q \right).$$

For $q \geq 1$ we have the estimate

$$\text{mes} \left(\tilde{G}_{q-1} \setminus \tilde{G}_q \right) \leq \frac{2^{2n-7} l^2 L^{n-2}}{\mu^{n-1} M} \cdot \text{mes} \left(\tilde{F}_{q-1} \setminus \left(\tilde{F}_q - a\eta'_{q-1} \right) \right).$$

It has been used that $\Omega^{(q-1)}(\tilde{G}_{q-1}) = \tilde{F}_{q-1}$ and that $\Omega^{(q-1)}(\tilde{G}_q) \supset \tilde{F}_q - a\eta'_{q-1}$. This inclusion comes from part (g) of proposition 2.4. Another point we have used is the bound

$$\left| \det \left(\frac{\partial \Omega^{(q-1)}}{\partial I}(I) \right) \right| \geq \frac{\mu_{q-1}^{n-1} a}{L_{q-1}^{n-2}} \geq \frac{\mu^{n-1} M}{2^{2n-7} l^2 L^{n-2}},$$

given by part (c) of lemma 2.1. In accordance to the notation of lemma 2.5, we have

$$\tilde{F}_{q-1} = F \left(\tilde{\beta}_{q-1}, \tilde{\beta}_{q-1}, K_{q-1} \right), \quad \tilde{F}_q = F \left(\tilde{\beta}_q, \tilde{\beta}_q, K_q \right).$$

Applying that lemma,

$$\begin{aligned} \text{mes} \left(\tilde{F}_{q-1} \setminus \tilde{F}_q \right) &\leq D \left(\tilde{\beta}_q - \tilde{\beta}_{q-1} \right) \\ &\quad + 2(\text{diam } F)^{n-1} \left(\sum_{\substack{|k|_1 \leq K_{q-1} \\ \bar{k} \neq 0}} \frac{\tilde{\beta}_q - \tilde{\beta}_{q-1}}{|k|_1^\tau \cdot |\bar{k}|} + \sum_{\substack{K_{q-1} < |k|_1 \leq K_q \\ \bar{k} \neq 0}} \frac{\tilde{\beta}_q}{|k|_1^\tau \cdot |\bar{k}|} \right), \\ \text{mes} \left(\tilde{F}_q \setminus \left(\tilde{F}_q - a\eta'_{q-1} \right) \right) &\leq \left(D + 2^{n+1} (\text{diam } F)^{n-1} K_q^n \right) \cdot a\eta'_{q-1}. \end{aligned}$$

Putting these estimates together, we get

$$\begin{aligned} \text{mes} \left(\mathcal{G} \setminus \widehat{G}^* \right) &\leq \frac{2^{2n-7} l^2 L^{n-2}}{\mu^{n-1} M} \left(D\tilde{\beta} + 2(\text{diam } F)^{n-1} \sum_{\substack{k \in \mathbb{Z}^n \\ \bar{k} \neq 0}} \frac{\tilde{\beta}}{|k|_1^\tau \cdot |\bar{k}|} \right. \\ &\quad \left. + D \sum_{q=1}^{\infty} a\eta'_{q-1} + 2^{n+1} (\text{diam } F)^{n-1} \sum_{q=1}^{\infty} K_q^n a\eta'_{q-1} \right). \end{aligned} \quad (2.51)$$

It is crucial to use the condition $\tau > n - 1$ in checking that the three series taking part in the right hand side of (2.51) are convergent. Indeed, for the first series,

$$\sum_{\substack{k \in \mathbb{Z}^n \\ \bar{k} \neq 0}} \frac{1}{|k|_1^\tau \cdot |\bar{k}|} \leq \sum_{\substack{k \in \mathbb{Z}^{n-1} \\ \bar{k} \neq 0}} \sum_{k_n \in \mathbb{Z}} \frac{\sqrt{n}}{\left(|\bar{k}|_1 + |k_n| \right)^\tau \cdot |\bar{k}|_1} \leq \sqrt{n} 2^{n-1} \sum_{j=1}^{\infty} \sum_{k_n \in \mathbb{Z}} \frac{j^{n-3}}{(j + |k_n|)^\tau},$$

where we have used that the number of vectors $\bar{k} \in \mathbb{Z}^{n-1}$ with $|\bar{k}|_1 = j \geq 1$ can be bounded by $2^{n-1} j^{n-2}$. The series indexed by k_n can be bounded by comparing it with an integral:

$$\sum_{k_n \in \mathbb{Z}} \frac{1}{(j + |k_n|)^\tau} \leq \frac{1}{j^\tau} + 2 \int_0^\infty \frac{dx}{(j+x)^\tau} = \frac{1}{j^\tau} + \frac{2}{(\tau-1)j^{\tau-1}} \leq \frac{\tau+1}{\tau-1} \cdot \frac{1}{j^{\tau-1}}.$$

We have used that $\tau > 1$ since $n \geq 2$. Then,

$$\sum_{\substack{k \in \mathbb{Z}^n \\ k \neq 0}} \frac{1}{|k|_1^\tau \cdot |k|} \leq \frac{\sqrt{n} 2^{n-1} (\tau + 1)}{\tau - 1} \sum_{j=1}^{\infty} \frac{1}{j^{\tau-n+2}},$$

which converges by the condition $\tau > n - 1$. It is easy to check that the second and the third series of (2.51) converge, using the bound

$$a\eta'_{q-1} \leq \frac{\nu l^3 \mu^2}{2^{\tau+20} L^3 M^2 K^{\tau+1} \cdot 2^{(\tau+2)(q-1)}} \cdot \beta,$$

which comes from estimates (2.25) and (2.20). Writing all bounds in terms of γ instead of $\tilde{\beta}$ or β , we get from (2.51) a bound of the type

$$\text{mes} \left(\mathcal{G} \setminus \hat{G}^* \right) \leq C' \gamma,$$

where C' is a constant depending on $n, \tau, \text{diam } F, D, K, M, L, l, \mu$. We then get estimate (c), with $C = (2\pi)^n C'$. This constant may be explicitated if desired. $\square$

Remarks

1. All of the sequences introduced at the beginning of the proof have linear convergence. Of course, alternative choices for those sequences are possible provided the restrictions imposed by proposition 2.4 are fulfilled.
2. The reason of our choice of K_q and $\delta_1^{(q)}$ will be transparent in the next section, where we see that, for a small ν , the remainders decrease in an almost quadratic way.
3. The estimates of part (b) on the deformation of the perturbed invariant tori from the unperturbed ones are essentially the same of [Nei81].

2.1.5 Fast convergence and nearly-invariant tori

We have established in the previous section the linear convergence to zero of the sizes of the successive remainders. This kind of convergence is enough (and very suitable) for the proof of the existence of invariant tori. But in the current section we show that the remainders actually decrease much faster, and we take advantage on this fact. Indeed, by stopping the iterative process at an appropriate step, we deduce that the domain obtained is full of nearly-invariant tori, i.e. Nekhoroshev-like estimates hold for the trajectories starting on these tori.

One may look our theorem 2.2 on effective stability as an attempt to make KAM and Nekhoroshev theorems closer. Indeed, we provide Nekhoroshev-like estimates which are very near, from a quantitative point of view, to KAM theorem. From the practical point of view, this result is more significant than KAM theorem. Indeed, if the coordinates of a given unperturbed invariant torus are known just approximately, up to a precision r , it is not possible to decide whether the frequency associated to this torus is Diophantine or not, and therefore one cannot deduce that this torus survives in the perturbation. In fact, in checking the Diophantine condition it has no sense to go farther than a finite order $K^{(r)}$ (tending to infinity as $r \rightarrow 0$). However, this finite test is enough to ensure that the torus is still included in the domain at an appropriate step of the iterative process and that this torus survives in the perturbation at least in the form of a nearly-invariant torus: a trajectory starting on this torus remains near to it up to a stability time which is exponentially long in $1/r$.

This result is similar to the one of [MG93], which does not however worry about optimal estimates. Moreover, in that paper the stability estimates are expressed in terms of the stability time, previously fixed, instead of r .

Another related result is obtained in [PW94] and [MG95], where it is shown that KAM tori are “sticky”: estimates are given for the time to move away from a fixed KAM torus. The estimates are exponential in [PW94] and “superexponential” (but only for quasiconvex systems) in [MG95]. This result requires the transformation to normal form to hold in a full neighborhood of the given KAM torus, which is achieved in the quoted papers by carrying out the Kolmogorov’s approach to KAM theorem instead

of the Arnold's one. But our result seems in practice more useful since the existence of a KAM torus is not used for the estimates.

We notice that theorem 2.1 gives a large family of invariant tori if γ is small. But for large values of γ one cannot guarantee the preservation of any invariant tori even if (2.17) is satisfied, since the set $\widehat{G}_\gamma$ may be empty. Actually, there is a maximum value γ_0 such that $\widehat{G}_\gamma$ is empty for $\gamma > \gamma_0$ (in the case $n = 2$, the set $\widehat{G}_{\gamma_0}$ corresponds to the noble frequencies). Nevertheless, in theorem 2.2 the nearly-invariant tori are parametrized by a set $G_\gamma^{(r)}$ (defined below) containing $\widehat{G}_\gamma$ properly. Then, for some interval of values $\gamma > \gamma_0$ we may still ensure the existence of nearly-invariant tori.

Theorem 2.2. *Consider notations and hypothesis as in theorem 2.1 and assume also that*

$$\varepsilon \leq \frac{\nu^2 \sigma l^2 \hat{\rho}^{2\tau+2}}{2^{2\tau+17} L^2 M} \cdot \gamma^2, \quad (2.52)$$

where we define $\sigma := \min_{s \geq 0} \frac{e^{(2-2^{1-\nu}) \cdot 2^{(1-\nu)s}}}{2^{(2\tau+1)s}} > 0$. Let

$$0 < r \leq r_0 := \frac{\hat{\rho}^{\tau+1}}{2^{\tau+2} M} \cdot \gamma$$

given, and write

$$\begin{aligned} \widehat{G}^{(r)} &= \widehat{G}_\gamma^{(r)} := \left\{ I \in \mathcal{G} - \frac{2\gamma}{\mu} : |k \cdot \omega(I)| \geq \frac{\gamma}{|k|_1^\tau} \quad \forall k \in \mathbb{Z}^n, 0 < |k|_1 \leq K^{(r)} \right\}, \\ G^{(r)} &= G_\gamma^{(r)} := \mathcal{U}_r \left(\widehat{G}^{(r)} \right), \end{aligned}$$

where

$$K^{(r)} := \frac{2}{\hat{\rho}} \left(\frac{r_0}{r} \right)^{1/(\tau+1+\nu)}.$$

Then, there exist an analytic map $A^{(r)} : G^{(r)} \rightarrow \mathcal{G}$ and a real analytic canonical transformation $\Upsilon^{(r)} : \mathcal{D} \left(\frac{\rho_1}{4}, \frac{\nu l r}{2^{\tau+5} L} \right) \left(A^{(r)} \left(G^{(r)} \right) \right) \rightarrow \mathcal{D}_\rho(\mathcal{G})$ such that, writing $\mathcal{T}^{(r)} = \Upsilon^{(r)} \circ (\text{id} \times A^{(r)})$, any torus $\mathcal{T}^{(r)}(\mathbb{T}^n \times \{I_0\})$, with $I_0 \in G^{(r)}$ has the property that, for every trajectory $(\phi(t), I(t)) = \Upsilon^{(r)}(\hat{\phi}(t), \hat{I}(t))$ of H with $(\phi(0), I(0))$ belonging to this torus, one has:

$$\left| \hat{I}(t) - A^{(r)}(I_0) \right| \leq \sqrt{\frac{2\varepsilon}{M}} \cdot \exp \left\{ -\frac{1}{2} \left(\frac{r_0}{r} \right)^{(1-\nu)/(\tau+1+\nu)} \right\}, \quad (2.53)$$

$$\left| \hat{\phi}(t) - \left(\hat{\phi}(0) + \lambda^{(r)}(I_0)t \right) \right|_\infty \leq \frac{\nu \rho_1}{4} \left(\frac{r}{r_0} \right)^{\nu/(\tau+1+\nu)}, \quad (2.54)$$

for

$$|t| \leq \frac{\nu \rho_1}{51 \sqrt{M} \varepsilon} \left(\frac{r}{r_0} \right)^{\nu/(2\tau+2)} \cdot \exp \left\{ \frac{1}{2} \left(\frac{r_0}{r} \right)^{(1-\nu)/(\tau+1+\nu)} \right\}, \quad (2.55)$$

where the vector $\lambda^{(r)}(I_0)$ is colinear to $\omega(I_0)$. Moreover, if E denotes the energy of the trajectory $(\phi(t), I(t))$,

$$|E - h(I_0)| \leq \frac{2^{2n+1} \varepsilon}{\hat{\rho}} \cdot \exp \left\{ -\left(\frac{r_0}{r} \right)^{(1-\nu)/(\tau+1+\nu)} \right\}.$$

Proof We go again into the iterative process of the proof of theorem 2.1. Improving the argument given there for the linear estimate (1_q), we are going to see that the successive sizes of the remainders admit an almost quadratic estimate. We first notice that, choosing K as in the proof of theorem 2.1, and taking into account the definition $\beta = \gamma/L$ and the inequalities $\hat{\rho} \leq 2/K$ and $\hat{\rho} \leq \nu \rho_1/16$, we deduce from (2.52) the inequality

$$\varepsilon \leq \frac{\nu^3 \sigma l^2 \rho_1 \beta^2}{2^{20} M K^{2\tau+1}}. \quad (2.56)$$

We next prove that, for every $q \geq 0$,

$$\varepsilon_q \leq \frac{32\varepsilon}{\nu\rho_1} \cdot e^{-2(1-\nu)q}. \quad (2.57)$$

Indeed, this is true for $q = 0$ by (2.22). Given $q \geq 1$ and assuming the estimate true for $q - 1$, we are going to establish it for q . From (2.27) and the inequality $K\hat{\rho} \geq 1$, we deduce

$$K_q \delta_1^{(q)} \geq \frac{\nu K \rho_1}{8} \cdot 2^{(1-\nu)(q-1)} \geq \ln 2 + 2^{(1-\nu)(q-1)},$$

and therefore

$$e^{-K_q \delta_1^{(q)}} \leq \frac{1}{2} e^{-2^{(1-\nu)(q-1)}}.$$

Moreover, applying the inequalities (2.18) and (2.56), the definition of σ and the hypothesis that (2.57) holds for ε_{q-1} ,

$$\begin{aligned} \frac{14A_q K_q^\tau}{l_{q-1} \beta'_{q-1} \delta_2^{(q)}} \cdot \varepsilon_{q-1} &\leq \frac{2^8 K_q^\tau}{\nu l \beta} \cdot \frac{64M K_q^{\tau+1}}{\nu l \beta} \cdot \frac{32\varepsilon}{\nu \rho_1} \cdot e^{-2^{(1-\nu)(q-1)}} \\ &\leq \frac{1}{2} e^{-(2^{1-\nu}-1) \cdot 2^{(1-\nu)(q-1)}}. \end{aligned} \quad (2.58)$$

Then, from (2.26) we deduce:

$$\varepsilon_q \leq \left(\frac{1}{2} e^{-2^{(1-\nu)(q-1)}} + \frac{1}{2} e^{-(2^{1-\nu}-1) \cdot 2^{(1-\nu)(q-1)}} \right) \cdot \varepsilon_{q-1} \leq e^{-(2^{1-\nu}-1) \cdot 2^{(1-\nu)(q-1)}} \cdot \varepsilon_{q-1},$$

which gives estimate (2.57) for ε_q .

The stability time in (2.49) can also be improved. Recall that we denote $x^{(q)}(t) = (\phi^{(q)}(t), I^{(q)}(t))$ the trajectory of $H^{(q)}$ such that $x^{(q)}(0) = (\phi_0^*, I_0^*) \in \mathbb{T}^n \times G_q$. We deduce from the inequality (2.44) that, for $0 \leq t \leq T_q$,

$$|I^{(q)}(t) - I_0^*| \leq T_q \varepsilon_q$$

(T_q was introduced in (2.43)). Then, we may replace (2.45) by the next alternative bound:

$$\left| \dot{\phi}^{(q)}(t) - \omega^{(q)}(I_0^*) \right|_\infty \leq 2MT_q \varepsilon_q + \frac{\varepsilon_q}{c_{q+1}} \leq 5MT_q \varepsilon_q,$$

where (2.48) has been used. Then, the inequality (2.47) becomes

$$\delta_1^{(q+1)} \leq T_q^2 \cdot 5M \varepsilon_q,$$

and we obtain:

$$T_q \geq \min \left(\frac{\delta_2^{(q+1)}}{\varepsilon_q}, \sqrt{\frac{\delta_1^{(q+1)}}{5M \varepsilon_q}} \right) = \tilde{T}_q := \sqrt{\frac{\delta_1^{(q+1)}}{5M \varepsilon_q}},$$

where we have used (2.46) to see that the minimum is given by the second term. Hence, for every initial condition $(\phi_0^*, I_0^*) \in \mathbb{T}^n \times G_q$, the corresponding trajectory of $H^{(q)}$ satisfies:

$$\left| I^{(q)}(t) - I_0^* \right| \leq \tilde{T}_q \varepsilon_q = \sqrt{\frac{\delta_1^{(q+1)} \varepsilon_q}{5M}}, \quad \left| \phi^{(q)}(t) - (\phi_0^* + \omega^{(q)}(I_0^*) t) \right|_\infty \leq \delta_1^{(q+1)}, \quad (2.59)$$

for

$$|t| \leq \tilde{T}_q. \quad (2.60)$$

This stability time is much better than the one of (2.49), because of the quadratic behaviour of ε_q . This estimate says that $\mathbb{T}^n \times \{I_0^*\}$ is a nearly-invariant torus of $H^{(q)}$ for every $I_0^* \in G_q$, since every trajectory starting at a point on this torus remains near a quasiperiodic motion with frequency vector $\omega^{(q)}(I_0^*)$ for a long time. Then, the torus $\Psi^{(q)}(\mathbb{T}^n \times \{I_0^*\})$ is also nearly-invariant for the flow of H .

We are now going to choose $q = q(r) \geq 1$, as large as possible, such that $F_q \supset \Omega(G^{(r)})$. Given $I_0 \in G^{(r)}$, there exists $I'_0 \in \widehat{G}^{(r)}$ such that $|I'_0 - I_0| \leq r$. We get $I_0 \in \mathcal{G} - \left(\frac{2\gamma}{\mu} - r\right)$ and hence

$$\Omega(I_0) \in F - \left(\beta - \frac{\mu r}{2L}\right) \quad (2.61)$$

by part (b) of lemma 2.1. On the other hand, for $0 < |k|_1 \leq K^{(r)}$,

$$|k \cdot \omega(I_0)| \geq \frac{\gamma}{|k|_1^\tau} - |k| \cdot Mr$$

and therefore

$$\left| \bar{k} \cdot \bar{\Omega}(I_0) + k_n \right| \geq \frac{1}{|\omega_n(I_0)|} \left(\frac{\gamma}{|k|_1^\tau} - |k| \cdot Mr \right) \geq \frac{\beta}{|k|_1^\tau} - \frac{|k| \cdot Mr}{L}. \quad (2.62)$$

We deduce from (2.61–2.62) that $J_0 \in F_q$ provided the following inequalities are fulfilled:

$$K^{(r)} \geq K_q, \quad r \leq \frac{L}{M} \cdot \frac{\beta - \beta_q}{K_q^{\tau+1}}.$$

Noting that $\beta - \beta_q = \beta/2^{\nu q}$ and reminding that $K \leq 2/\hat{\rho}$, we see that it suffices to choose q such that the inequality

$$2^{(\tau+1+\nu)(q-1)} \leq \frac{r_0}{r} \quad (2.63)$$

holds. Hence, we choose $q \geq 1$ as the maximum integer such that this happens. We then have also

$$2^{(\tau+1+\nu)q} \geq \frac{r_0}{r}. \quad (2.64)$$

With this choice of q , we have $\Omega(G^{(r)}) \subset F_q$. We take $A^{(r)} := \left(\Omega^{(q)}\right)^{-1} \circ \Omega$, and note that $A^{(r)}(G^{(r)}) \subset G_q$. The transformation $\Upsilon^{(r)} := \Psi^{(q)}$ is defined on $\mathcal{D}_{\rho^{(q)}}(G_q)$, and we have the inequalities $\rho_1^{(q)} \geq \rho_1/4$ and

$$\rho_2^{(q)} = \frac{\nu l \beta}{32 M K^{\tau+1} \cdot 2^{(\tau+1)q}} \geq \frac{\nu l \hat{\rho}^{\tau+1} \beta}{2^{\tau+6} M \cdot 2^{(\tau+1)q}} = \frac{\nu l r_0}{2^4 L \cdot 2^{(\tau+1)q}} \geq \frac{\nu l r}{2^{\tau+5} L},$$

where we have used the inequality (2.63). This gives, in function of r , the complex domain where $\Upsilon^{(r)}$ is defined. For $(\phi_0, I_0) \in \mathbb{T}^n \times G^{(r)}$, we put

$$\mathcal{T}^{(r)}(\phi_0, I_0) = \Psi^{(q)}(\phi_0, I_0^*),$$

where $I_0^* = A^{(r)}(I_0) \in G_q$. If $(\phi(t), I(t))$ is a trajectory of H starting on the torus $\mathcal{T}^{(r)}(\mathbb{T}^n \times \{I_0\})$, then $(\hat{\phi}(t), \hat{I}(t))$ is a trajectory of $H^{(q)}$, with $\hat{I}(0) = I_0^*$. We can thus apply the stability estimate of (2.59–2.60). Using the inequalities (2.57), (2.18) and (2.63–2.64), we get the bounds

$$\begin{aligned} \varepsilon_q &\leq \frac{32\varepsilon}{\nu \rho_1} \cdot \exp \left\{ - \left(\frac{r_0}{r} \right)^{(1-\nu)/(\tau+1+\nu)} \right\}, \\ \delta_1^{(q+1)} &\leq \frac{\nu \rho_1}{4 \cdot 2^{\nu q}} \leq \frac{\nu \rho_1}{4} \left(\frac{r}{r_0} \right)^{\nu/(\tau+1+\nu)}, \\ \delta_1^{(q+1)} &\geq \frac{\nu \rho_1}{16 \cdot 2^{\nu(q-1)}} \geq \frac{\nu \rho_1}{16} \left(\frac{r}{r_0} \right)^{\nu/(\tau+1+\nu)}. \end{aligned}$$

Including these bounds in (2.59–2.60), we get (2.53–2.55). Note that we put $\lambda^{(r)}(I_0) = \omega^{(q)}(I_0^*)$, which is colinear to $\omega(I_0)$ since $\Omega^{(q)}(I_0^*) = \Omega(I_0)$. Finally, the energy of the trajectory $(\phi(t), I(t))$ is

$$E = H(\phi(0), I(0)) = H^{(q)}(\hat{\phi}(0), I_0^*) = h(I_0) + R^{(q)}(\hat{\phi}(0), I_0^*)$$

since $h^{(q)}(I_0^*) = h(I_0)$. Then,

$$|E - h(I_0)| \leq \left| R^{(q)}(\hat{\phi}(0), I_0^*) \right| \leq \left| R_0^{(q)} \right|_{G_q} + \left| \frac{\partial R^{(q)}}{\partial \phi} \right|_{G_q} \cdot \pi^n \leq \eta_q + \pi^n \varepsilon_q.$$

To get a quadratic estimate for η_q , we proceed as in (2.29) but we now use (2.58), (2.18) and (2.57):

$$\eta_q \leq \frac{7A_q K_q^\tau}{c_q l_{q-1} \beta'_{q-1}} \cdot \varepsilon_{q-1}^2 \leq \frac{\delta_1^{(q)} \varepsilon_{q-1}}{2} \cdot \frac{1}{2} e^{-(2^{1-\nu}-1) \cdot 2^{(1-\nu)(q-1)}} \leq 2\varepsilon \cdot e^{-2^{(1-\nu)q}}.$$

Then,

$$|E - h(I_0)| \leq \left(2 + \frac{32\pi^n}{\nu \rho_1} \right) \varepsilon \cdot e^{-2^{(1-\nu)q}} \leq \frac{2^{2n+1} \varepsilon}{\hat{\rho}} \cdot \exp \left\{ - \left(\frac{r_0}{r} \right)^{(1-\nu)/(\tau+1+\nu)} \right\}. \quad \square$$

Remarks

1. To give an idea of how this theorem should be applied in practice, assume that I_0 is the action of a given unperturbed torus, for which we just know an approximation I'_0 , with $|I'_0 - I_0| \leq r$. If $I'_0 \in \widehat{G}_\gamma^{(r)}$, i.e. the frequency ratios of $\omega(I'_0)$ satisfy the Diophantine condition (1.2) up to order $K^{(r)}$, then the invariant torus corresponding to the action I_0 survives as a nearly-invariant torus.
2. We have omitted statements like parts (b) and (c) of theorem 2.1 because they would be exactly the same, with $\mathcal{T}^{(r)}$ instead of $\mathcal{T}$.
3. If the size ε of the perturbation is fixed, we could take r small and the stability estimate given in (2.53–2.55) is then much better than the one provided by Nekhoroshev theorem. This is due to the fact that the estimate has been expressed in the transformed coordinates $(\hat{\phi}, \hat{I})$ provided by the canonical transformation $\Upsilon^{(r)}$. These coordinates are better because the nearly-invariant tori are given by equations $\hat{I} = \text{const}$. In Nekhoroshev theorem, the stability estimate includes the coordinate change because it is expressed in the original coordinates.
4. The comparison between the estimates (2.53–2.54) for action and angular variables shows that the separation from a given torus remains much smaller than the separation from a linear flow inside this torus.
5. The stability exponent given in (2.55) is larger (as near to $1/(\tau+1)$ as wanted) if we choose the parameter ν near to zero.
6. Roughly speaking, the set $G_\gamma^{(r)}$ parametrizing the nearly-invariant tori has a very large boundary for r small. However, the “area” of this boundary is finite, which means that the set $G_\gamma^{(r)}$ is not as strange as the Cantorian set $\widehat{G}_\gamma$ provided by KAM theorem. An alternative way to express this fact is used in [MG93]: the set of nearly-invariant tori contains balls of a suitable radius, and hence it contains inner points.

We can also get “superexponential” stability estimates, like in [MG95], by means of an alternative approach. However, we need to assume that the unperturbed Hamiltonian h is quasiconvex. Applying the iterative process of KAM theorem, our starting Hamiltonian H is transformed after q steps into $H^{(q)} = h^{(q)} + R^{(q)}$. If h is m -quasiconvex with $m > 0$ and we assume $\varepsilon = O(m)$, then $h^{(q)}$ is also quasiconvex and Nekhoroshev theorem may be applied to $H^{(q)}$. In this way, we can obtain for every trajectory $(\phi^{(q)}(t), I^{(q)}(t))$ of $H^{(q)}$, with initial condition in $\mathbb{T}^n \times G_q$, a stability estimate of the type

$$|I^{(q)}(t) - I^{(q)}(0)| \leq R \quad \text{for } |t| \leq T,$$

with

$$R \sim \varepsilon_q^{1/2n}, \quad T \sim \exp \left\{ \left(\frac{1}{\varepsilon_q} \right)^{1/2n} \right\}.$$

Choosing $q = q(r)$ as in (2.63–2.64), we get

$$R \sim \left(\varepsilon \cdot \exp \left\{ - \left(\frac{1}{r} \right)^c \right\} \right)^{1/2n}, \quad T \sim \exp \left\{ \left(\frac{1}{\varepsilon} \cdot \exp \left\{ \left(\frac{1}{r} \right)^c \right\} \right)^{1/2n} \right\},$$

where we have put $c = (1 - \nu)/(\tau + 1 + \nu)$. The stability radius R and the stability time T substitute the ones obtained in (2.53) and (2.55), respectively.

2.2 Appendix: proofs of some technical lemmas

Proof of lemma 1.2 Given $(\phi_0, I_0) \in \mathcal{D}_{\rho-t\delta}(G)$, let $(\phi(s), I(s)) = \Phi_s(\phi_0, I_0)$. First, we prove that

$$|\phi(s) - \phi_0|_\infty \leq t \left\| \frac{\partial W}{\partial I} \right\|_{G, \rho, \infty}, \quad |I(s) - I_0| \leq t \left\| \frac{\partial W}{\partial \phi} \right\|_{G, \rho, 1}, \quad (2.65)$$

for $0 \leq s \leq t$. Let s_0 be the supremum of the $s \geq 0$ satisfying both inequalities in (2.65). Clearly $s_0 > 0$, and one of these inequalities is an equality for $s = s_0$. On the other hand, we have $(\phi(s), I(s)) \in \mathcal{D}_\rho(G)$ for $0 \leq s \leq s_0$. From the mean value theorem,

$$|\phi(s_0) - \phi_0|_\infty \leq s_0 \cdot \sup_{0 \leq s \leq s_0} \left\| \frac{\partial W}{\partial I}(\phi(s), I(s)) \right\|_\infty \leq s_0 \left\| \frac{\partial W}{\partial I} \right\|_{G, \rho, \infty}, \quad (2.66)$$

$$|I(s_0) - I_0| \leq s_0 \cdot \sup_{0 \leq s \leq s_0} \left\| \frac{\partial W}{\partial \phi}(\phi(s), I(s)) \right\| \leq s_0 \left\| \frac{\partial W}{\partial \phi} \right\|_{G, \rho} \leq s_0 \left\| \frac{\partial W}{\partial \phi} \right\|_{G, \rho, 1}. \quad (2.67)$$

Thus, $s_0 \geq t$ and (2.65) is true. This implies that Φ_t is defined in $\mathcal{D}_{\rho-t\delta}(G)$ and that the bound (a) holds. We can deduce the inclusion (b) from the fact that Φ_{-t} is the flow at time t of $-W$.

To see (c), note that $f \circ \Phi_t$ is defined in $\mathcal{D}_{\rho-t\delta}(G)$. Since W is analytic, $f \circ \Phi_t$ is also analytic in t , and hence the Lie series expansion (1.5) for $r_m(f, W, t)$ holds. Given $l \geq m + 1$, let $\eta = \delta/(l - m)$. For $j = m + 1, \dots, l$, we have

$$\begin{aligned} \|L_W^j f\|_{G, \rho-(j-m)t\eta} &\leq \frac{2}{c} \left\| D(L_W^{j-1} f) \right\|_{G, \rho-(j-m)t\eta, c} \cdot \|DW\|_{G, \rho, c} \\ &\leq \frac{2}{t\hat{\eta}_c} \left\| L_W^{j-1} f \right\|_{G, \rho-(j-1-m)t\eta} \cdot \|DW\|_{G, \rho, c}. \end{aligned}$$

Thus,

$$\|L_W^l f\|_{G, \rho-t\delta} \leq \left(\frac{2 \|DW\|_{G, \rho, c}}{t\hat{\eta}_c} \right)^{l-m} \cdot \|L_W^m f\|_{G, \rho} \leq (l - m)! \left(\frac{2e \|DW\|_{G, \rho, c}}{t\hat{\delta}_c} \right)^{l-m} \cdot \|L_W^m f\|_{G, \rho},$$

where we have used that $k^k \leq e^k \cdot k!$ for $k \geq 1$. In this way, the bound that we obtain for $\|r_m(f, W, t)\|_{G, \rho-t\delta}$ is

$$\sum_{l=m}^{\infty} \frac{t^l}{l!} \|L_W^l f\|_{G, \rho-t\delta} \leq \left[\sum_{l=m}^{\infty} \frac{(l - m)!}{l!} \cdot \left(\frac{2e \|DW\|_{G, \rho, c}}{\hat{\delta}_c} \right)^{l-m} \right] \cdot t^m \|L_W^m f\|_{G, \rho},$$

this series being convergent for $\|DW\|_{G, \rho, c} < \hat{\delta}_c/2e$. $\square$

Remark The bounds (2.66–2.67) are based on the special structure of Hamiltonian equations. Our choice of the ∞ -norm for the angular variables was motivated by (2.66). Concerning the action variables, the best choice would be, according to (2.67), the 1-norm, but our use of Euclidean geometry in the geometric parts of Nekhoroshev and KAM theorems made us choose the 2-norm.

Proof of lemma 1.5 Assume first $K\rho_1 \geq 1$. Let $\delta = \rho/3$. From (1.19), we see that

$$A = 1 + \frac{2M}{\alpha} \cdot \frac{\rho_2}{\rho_1} \leq 1 + \frac{1}{K\rho_1} \leq 2.$$

Then, theorem 1.2 provides a canonical transformation $\Psi : \mathcal{D}_{\frac{2\rho}{3}}(G) \longrightarrow \mathcal{D}_\rho(G)$ such that $H \circ \Psi = h + Z^* + R^*$, with $Z^* = Z^*(I)$, and

$$\|DR^*\|_{G, \frac{2\rho}{3}, c} \leq 3e^{-\frac{K\rho_1}{6}} \cdot \|DR\|_{G, \rho, c}.$$

Let us denote

$$\eta = \frac{8}{\alpha} \|DR\|_{G, \rho, c}.$$

By estimate (c) of theorem 1.2 and the second condition of (1.24),

$$|\Psi - \text{id}|_{G, \frac{2\rho}{3}, c} \leq \eta \leq \frac{\rho_2}{15K\rho_1} \leq \frac{\rho_2}{15}.$$

Moreover, by the inclusion (d) of theorem 1.2, we have $\Psi(\mathcal{D}_{\frac{2\rho}{3}}(G)) \supset \mathcal{D}_{\frac{\rho}{2}}(G) \supset \mathbb{T}^n \times G$ and therefore we can write $(\phi(0), I(0)) = \Psi(\phi_0^*, I_0^*)$ and, since Ψ preserves real domains, $(\phi_0^*, I_0^*) \in \mathbb{T}^n \times \mathcal{V}_{\frac{\rho_2}{15}}(G)$. Let $(\phi^*(t), I^*(t))$ be the trajectory of $H \circ \Psi$ with $(\phi^*(0), I^*(0)) = (\phi_0^*, I_0^*)$. Let

$$T = \inf \left\{ t > 0 : |I^*(t) - I^*(0)| > \eta \right\}$$

(the procedure for negative times is exactly the same). For $0 \leq t \leq T$, we obtain $(\phi^*(t), I^*(t)) \in \mathcal{D}_{\frac{2\rho}{3}}(G)$. Since Ψ takes the motions of $H \circ \Psi$ into motions of H , we get that $(\phi(t), I(t)) = \Psi(\phi^*(t), I^*(t))$ is also defined for $0 \leq t \leq T$, and obtain the estimate

$$|I(t) - I(0)| \leq |I(t) - I^*(t)| + |I^*(t) - I^*(0)| + |I^*(0) - I(0)| \leq 3\eta.$$

Next, we proceed to obtain a lower bound for T . Let $\Delta I^* = I^*(T) - I^*(0)$. Clearly, $|\Delta I^*| = \eta$. On the other hand, by using the form of the Hamiltonian equations and the fact that the normal form Z^* only depends on the action variables, we obtain

$$|\Delta I^*| \leq T \cdot \left\| \frac{\partial R^*}{\partial \phi} \right\|_{G, \frac{2\rho}{3}} \leq T \cdot \|DR^*\|_{G, \frac{2\rho}{3}, c} \leq T \cdot 3e^{-\frac{K\rho_1}{6}} \cdot \|DR\|_{G, \rho, c},$$

and it follows that

$$T \geq \frac{\eta}{3 \|DR\|_{G, \rho, c}} e^{\frac{K\rho_1}{6}} \geq \frac{2}{\alpha} e^{\frac{K\rho_1}{6}}.$$

For $K\rho_1 < 1$, one obtains, by working in original coordinates,

$$|I(t) - I(0)| \leq \frac{24}{\alpha} \|DR\|_{G, \rho, c} \quad \text{for } |t| \leq \frac{24}{\alpha},$$

and it is then easy to see that this stability time is longer than the one proclaimed in (1.25). $\square$

Proof of lemma 1.6 First we assume $K\rho_1 \geq M/m$. Let $\delta = \rho/3$. Like in the proof of lemma 1.5, we have $A \leq 2$. Note that

$$\|DZ\|_{G, \rho, c} + \|DR\|_{G, \rho, c} \leq \frac{m\rho_2^2}{350\rho_1} \leq \frac{\alpha\rho_2}{122K\rho_1}. \quad (2.68)$$

Then, theorem 1.2 provides a canonical transformation $\Psi : \mathcal{D}_{\frac{2\rho}{3}}(G) \longrightarrow \mathcal{D}_\rho(G)$ such that $H \circ \Psi = h + Z^* + R^*$, with $Z^* \in \mathbf{R}(\mathcal{M}, K)$, and

$$\begin{aligned} \|DZ^*\|_{G, \frac{2\rho}{3}, c} + \|DR^*\|_{G, \frac{2\rho}{3}, c} &\leq \|DZ\|_{G, \rho, c} + 2\|DR\|_{G, \rho, c}, \\ \|DR^*\|_{G, \frac{2\rho}{3}, c} &\leq 3e^{-\frac{K\rho_1}{6}} \cdot \|DR\|_{G, \rho, c}. \end{aligned}$$

Moreover, by estimate (c) of theorem 1.2 and the inequality (2.68),

$$|\Psi - \text{id}|_{G, \frac{2\rho}{3}, c} \leq \frac{8}{\alpha} \|DR\|_{G, \rho, c} \leq \frac{\rho_2}{15K\rho_1} \leq \frac{m\rho_2}{15M}.$$

Like in lemma 1.5, we can write $(\phi(0), I(0)) = \Psi(\phi_0^*, I_0^*)$, with $(\phi_0^*, I_0^*) \in \mathbb{T}^n \times \mathcal{V}_{\frac{m\rho_2}{15M}}(G)$. Let $(\phi^*(t), I^*(t))$ be the trajectory of $H \circ \Psi$ with $(\phi^*(0), I^*(0)) = (\phi_0^*, I_0^*)$. Let

$$T = \inf \left\{ t > 0 : |I^*(t) - I^*(0)| > \frac{\rho_2}{2} \right\}.$$

For $0 \leq t \leq T$, we have $(\phi^*(t), I^*(t)) \in \mathcal{D}_{\frac{2\rho}{3}}(G)$. We then obtain the estimate

$$|I(t) - I(0)| \leq |I(t) - I^*(t)| + |I^*(t) - I^*(0)| + |I^*(0) - I(0)| \leq \frac{m\rho_2}{15M} + \frac{\rho_2}{2} + \frac{m\rho_2}{15M} \leq \rho_2.$$

We introduce the notations

$$\Delta\phi^* = \phi^*(T) - \phi^*(0), \quad \Delta I^* = I^*(T) - I^*(0),$$

and, for a function $f(\phi, I)$,

$$\Delta f = f(\phi^*(T), I^*(T)) - f(\phi^*(0), I^*(0)).$$

The definition of T clearly implies that $|\Delta I^*| = \rho_2/2$.

We notice that, since Z^* is in normal form with respect to $\mathcal{M}$, it does not contribute to ΔI^* in any direction lying in $\mathcal{M}^\perp$. More precisely, let P denote the orthogonal projection onto the one-dimensional space $\langle \Pi_{\mathcal{M}}\omega(I(0)) \rangle$. By the specific form of the Hamiltonian equations, we have

$$P\Delta I^* = - \int_0^T P \left(\frac{\partial R^*}{\partial \phi}(\phi^*(t), I^*(t)) \right) dt$$

and it follows that the $\Pi_{\mathcal{M}}\omega(I(0))$ -component of the vector ΔI^* is small up to an exponentially long time:

$$|P\Delta I^*| \leq T \cdot \left\| \frac{\partial R^*}{\partial \phi} \right\|_{G, \frac{2\rho}{3}} \leq T \cdot \|DR^*\|_{G, \frac{2\rho}{3}, c} \leq T \cdot 3e^{-\frac{K\rho_1}{6}} \cdot \|DR\|_{G, \rho, c}. \quad (2.69)$$

To bound the whole vector ΔI^* we use the quasiconvexity condition on h . By Taylor formula, one has

$$\Delta h = \omega(I_0^*) \cdot \Delta I^* + \int_0^1 (1-s) \frac{\partial^2 h}{\partial I^2}(I_0^* + s\Delta I^*) (\Delta I^*, \Delta I^*) ds. \quad (2.70)$$

We notice that, since Ψ preserves real domains, $I_0^* + s\Delta I^* \in \mathcal{U}_{\rho_2}(G)$ for $0 \leq s \leq 1$. For a fixed s , we write $\Delta I^* = P_s \Delta I^* + Q_s \Delta I^*$, where P_s and Q_s denote the orthogonal projections onto $\langle \omega(I_0^* + s\Delta I^*) \rangle$ and $\langle \omega(I_0^* + s\Delta I^*) \rangle^\perp$, respectively. Thus, applying the quasiconvexity condition at the point $I_0^* + s\Delta I^*$ (and this is the only time that we use it), we obtain

$$\left| \frac{\partial^2 h}{\partial I^2}(I_0^* + s\Delta I^*) (Q_s \Delta I^*, Q_s \Delta I^*) \right| \geq m|Q_s \Delta I^*|^2.$$

We deduce that

$$\begin{aligned} & \left| \frac{\partial^2 h}{\partial I^2}(I_0^* + s\Delta I^*) (\Delta I^*, \Delta I^*) \right| \\ & \geq m|Q_s \Delta I^*|^2 - 2M|P_s \Delta I^*| \cdot |Q_s \Delta I^*| - M|P_s \Delta I^*|^2 \\ & = m|\Delta I^*|^2 - (m|P_s \Delta I^*| + 2M|Q_s \Delta I^*| + M|P_s \Delta I^*|) \cdot |P_s \Delta I^*| \\ & \geq m|\Delta I^*|^2 - 4M|\Delta I^*| \cdot |P_s \Delta I^*|. \end{aligned}$$

From formula (2.70) we obtain

$$\frac{m}{2} |\Delta I^*|^2 \leq |\Delta h| + |\omega(I_0^*) \cdot \Delta I^*| + 4M|\Delta I^*| \int_0^1 (1-s) |P_s \Delta I^*| ds,$$

and hence

$$\frac{m\rho_2^2}{8} \leq |\Delta h| + |\omega(I_0^*) \cdot \Delta I^*| + 2M\rho_2 \int_0^1 (1-s) |P_s \Delta I^*| ds. \quad (2.71)$$

Next we bound the terms appearing in the right hand side of (2.71). To bound $|P_s \Delta I^*|$ we use that the vector $\omega(I_0^* + s\Delta I^*)$ is near to $\Pi_{\mathcal{M}}\omega(I(0))$. More precisely, we apply the following property: given $v, v' \in \mathbb{R}^n$, if $P_{(v)}$ and $P_{(v')}$ denote the orthogonal projections onto the one-dimensional spaces $\langle v \rangle$ and $\langle v' \rangle$, respectively, then for every vector $u \in \mathbb{R}^n$ one has:

$$|P_{(v)}u - P_{(v')}u| \leq \frac{4|v - v'|}{|v|} \cdot |u|.$$

First we notice that, from lemma 1.3 and the fact that $\mathcal{M} \neq \mathbb{Z}^n$ and $K \geq 1$, we deduce $|\omega(I)| \geq \alpha/2$ for $I \in \mathcal{U}_{\rho_2}(G)$. Then, applying the property, one has:

$$\begin{aligned} |P_s \Delta I^* - P \Delta I^*| &\leq \frac{4}{\left| \omega(I_0^* + s\Delta I^*) \right|} \left| \omega(I_0^* + s\Delta I^*) - \Pi_{\mathcal{M}}\omega(I(0)) \right| \cdot |\Delta I^*| \\ &\leq \frac{4\rho_2}{\alpha} \left| \omega(I_0^* + s\Delta I^*) - \Pi_{\mathcal{M}}\omega(I(0)) \right|. \end{aligned}$$

Using that $\omega(G)$ is η -close to $\mathcal{M}$ -resonances, we get

$$\begin{aligned} \left| \omega(I_0^* + s\Delta I^*) - \Pi_{\mathcal{M}}\omega(I(0)) \right| &\leq M |I_0^* + s\Delta I^* - I(0)| + |\omega(I(0)) - \Pi_{\mathcal{M}}\omega(I(0))| \\ &\leq \left(\frac{m}{15} + \frac{sM}{2} \right) \rho_2 + \eta \leq \left(\frac{m}{12} + \frac{sM}{2} \right) \rho_2. \end{aligned} \quad (2.72)$$

Thus,

$$|P_s \Delta I^*| \leq |P \Delta I^*| + |P_s \Delta I^* - P \Delta I^*| \leq |P \Delta I^*| + \frac{4\rho_2^2}{\alpha} \left(\frac{m}{12} + \frac{sM}{2} \right)$$

and we obtain, using the first condition of (1.28),

$$\int_0^1 (1-s) |P_s \Delta I^*| ds \leq \frac{1}{2} |P \Delta I^*| + \frac{4\rho_2^2}{\alpha} \left(\frac{m}{24} + \frac{M}{12} \right) \leq \frac{1}{2} |P \Delta I^*| + \frac{m\rho_2^2}{96M}.$$

To bound $|\omega(I_0^*) \cdot \Delta I^*|$, we put $s = 0$ in (2.72):

$$|\omega(I_0^*) \cdot \Delta I^*| \leq |\Pi_{\mathcal{M}}\omega(I(0))| \cdot |P \Delta I^*| + |\omega(I_0^*) - \Pi_{\mathcal{M}}\omega(I(0))| \cdot |\Delta I^*| \leq L |P \Delta I^*| + \frac{m\rho_2^2}{24}.$$

Finally, by energy conservation,

$$\begin{aligned} \Delta h = -\Delta(Z^* + R^*) &= -\int_0^1 \left(\frac{\partial(Z^* + R^*)}{\partial \phi} (\phi_0^* + s\Delta \phi^*, I_0^* + s\Delta I^*) \cdot \Delta \phi^* \right. \\ &\quad \left. + \frac{\partial(Z^* + R^*)}{\partial I} (\phi_0^* + s\Delta \phi^*, I_0^* + s\Delta I^*) \cdot \Delta I^* \right) ds \end{aligned}$$

and we deduce

$$\begin{aligned} |\Delta h| &\leq \left\| \frac{\partial(Z^* + R^*)}{\partial \phi} \right\|_{G, \frac{2\rho}{3}, 1} \cdot |\Delta \phi^*|_{\infty} + \left\| \frac{\partial(Z^* + R^*)}{\partial I} \right\|_{G, \frac{2\rho}{3}} \cdot |\Delta I^*| \\ &\leq \left(\pi + \frac{\sqrt{n}}{c} \cdot \frac{\rho_2}{2} \right) \cdot \|D(Z^* + R^*)\|_{G, \frac{2\rho}{3}, c} \\ &\leq (2\pi + \sqrt{n}\rho_1) \cdot (\|DZ\|_{G, \rho, c} + \|DR\|_{G, \rho, c}) \\ &\leq \frac{(2\pi + 1)m\rho_2^2}{350} \leq \frac{m\rho_2^2}{48}. \end{aligned}$$

We insert all of these estimates in (2.71) and obtain:

$$\frac{m\rho_2^2}{8} \leq \left(\frac{1}{48} + \frac{1}{24} + \frac{1}{48} \right) m\rho_2^2 + (L + M\rho_2) |P \Delta I^*| \leq \frac{m\rho_2^2}{12} + \frac{49L}{48} |P \Delta I^*|,$$

where we used that $M\rho_2 \leq L/48$ since $\alpha \leq L$. By estimate (2.69), it follows that

$$T \geq \frac{m\rho_2^2}{74L\|DR\|_{G,\rho,c}} e^{\frac{K\rho_1}{6}} \geq \frac{m\rho_2^2}{74L\|DR\|_{G,\rho,c}} e^{\frac{mK\rho_1}{6M}}.$$

For $K\rho_1 < M/m$, one may work in original coordinates. Then, one obtains:

$$|I(t) - I(0)| \leq \rho_2 \quad \text{for } |t| \leq \frac{\rho_2}{\|DR\|_{G,\rho,c}}.$$

It is not hard to check that this stability time is longer than the one proclaimed in (1.29). $\square$

Proof of lemma 2.1 A simple computation gives, for $I \in G$ and $v \in \mathbb{R}^n$,

$$\frac{\partial\Omega}{\partial I}(I)v = \left(\frac{\partial\bar{\Omega}}{\partial I}(I)v, \frac{\partial\Omega_n}{\partial I}(I)v \right) = \left(\frac{1}{\omega_n(I)} \left(\frac{\partial\bar{\omega}}{\partial I}(I)v - \frac{\partial\omega_n}{\partial I}(I)v \frac{\bar{\omega}(I)}{\omega_n(I)} \right), a\omega(I) \cdot v \right).$$

We have the bound

$$\begin{aligned} \left| \frac{\partial\bar{\Omega}}{\partial I}(I)v \right| &\leq \frac{1}{\omega_n(I)^2} \left(\left| \frac{\partial\bar{\omega}}{\partial I}(I)v \right| \cdot |\omega_n(I)| + \left| \frac{\partial\omega_n}{\partial I}(I)v \right| \cdot |\bar{\omega}(I)| \right) \\ &\leq \frac{1}{\omega_n(I)^2} \left| \frac{\partial\omega}{\partial I}(I)v \right| \cdot |\omega(I)| \leq \frac{M|\omega(I)|}{l^2} |v| \end{aligned} \quad (2.73)$$

and we then get estimate (a):

$$\left| \frac{\partial\Omega}{\partial I} \right|_G \leq \sqrt{\left(\frac{ML}{l^2} \right)^2 + (aL)^2} \leq 2La. \quad (2.74)$$

To prove parts (b) and (c) we use the isoenergetic condition. For any $v \in \langle \omega(I) \rangle^\perp$, we have

$$\begin{aligned} \left| \frac{\partial\bar{\Omega}}{\partial I}(I)v \right| &= \left| \frac{1}{\omega_n(I)} \left(\frac{\partial\bar{\omega}}{\partial I}(I)v - \frac{\partial\omega_n}{\partial I}(I)v \frac{\bar{\omega}(I)}{\omega_n(I)} \right) \right| \\ &= \left| \frac{1}{\omega_n(I)} \left(\frac{\partial\omega}{\partial I}(I)v - \frac{\partial\omega_n}{\partial I}(I)v \frac{\omega(I)}{\omega_n(I)} \right) \right| \geq \frac{\mu}{|\omega_n(I)|} |v|, \end{aligned} \quad (2.75)$$

where we have used the fact that the vector

$$\frac{\partial\omega}{\partial I}(I)v - \frac{\partial\omega_n}{\partial I}(I)v \frac{\omega(I)}{\omega_n(I)}$$

has its n -th component vanishing. Moreover, the isoenergetic nondegeneracy has been used to bound the size of this vector from below. Now, consider an orthonormal basis $e_1, \dots, e_n$ of $\mathbb{R}^n$ with the first $n-1$ vectors belonging to $\langle \omega(I) \rangle^\perp$ and the last one belonging to $\langle \omega(I) \rangle$. Let $P = (\bar{P}, P_n)$ be the $(n \times n)$ -matrix having these vectors as columns. Let us write:

$$\frac{\partial\Omega}{\partial I}(I)P = \begin{pmatrix} \frac{\partial\bar{\Omega}}{\partial I}(I)\bar{P} & \frac{\partial\bar{\Omega}}{\partial I}(I)P_n \\ \frac{\partial\Omega_n}{\partial I}(I)\bar{P} & \frac{\partial\Omega_n}{\partial I}(I)P_n \end{pmatrix} = \begin{pmatrix} A & \bar{b} \\ 0 & b_n \end{pmatrix}. \quad (2.76)$$

It follows directly from (2.75) that

$$|A\bar{v}| \geq \frac{\mu}{|\omega_n(I)|} |\bar{v}| \quad \forall \bar{v} \in \mathbb{R}^{n-1}.$$

Note also that $|\bar{b}| \leq M|\omega(I)|/l^2$ by (2.73). Moreover, $b_n = a\omega(I) \cdot e_n$ and hence $|b_n| = a|\omega(I)|$. Then, computing the inverse of the matrix (2.76) and carrying out a rough bound on its norm,

$$\begin{aligned} \left| \left(\frac{\partial \Omega}{\partial I}(I) \right)^{-1} \right| &\leq \left| \begin{pmatrix} A^{-1} & -\frac{1}{b_n} A^{-1} \bar{b} \\ 0 & \frac{1}{b_n} \end{pmatrix} \right| \leq |A^{-1}| + \frac{1}{|b_n|} |A^{-1}| |\bar{b}| + \frac{1}{|b_n|} \\ &\leq \frac{|\omega_n(I)|}{\mu} + \frac{1}{a|\omega(I)|} \cdot \frac{|\omega_n(I)|}{\mu} \cdot \frac{M|\omega(I)|}{l^2} + \frac{1}{a|\omega(I)|} \\ &\leq \frac{L}{\mu} + \frac{LM}{l^2 \mu a} + \frac{1}{al} \leq \frac{L}{\mu} \left(1 + \frac{2M}{l^2 a} \right). \end{aligned} \quad (2.77)$$

This estimate implies (b), by our condition on a . To obtain the lower bound (c) for the determinant, we take into account the expression (2.76) again:

$$\left| \det \left(\frac{\partial \Omega}{\partial I}(I) \right) \right| \geq \left(\frac{\mu}{|\omega_n(I)|} \right)^{n-1} \cdot a|\omega(I)| \geq \frac{\mu^{n-1} a}{L^{n-2}}.$$

Finally, we prove (d). For $I \in G$ and $u, v \in \mathbb{R}^n$,

$$\begin{aligned} \frac{\partial^2 \Omega}{\partial I^2}(I)(u, v) &= \left(\frac{\partial^2 \bar{\Omega}}{\partial I^2}(I)(u, v), \frac{\partial^2 \Omega_n}{\partial I^2}(I)(u, v) \right) \\ &= \left(\frac{\frac{\partial^2 \bar{\Omega}}{\partial I^2}(I)(u, v)}{\omega_n(I)} - \frac{\left(\frac{\partial \omega_n}{\partial I}(I) u \right) \left(\frac{\partial \bar{\Omega}}{\partial I}(I) v \right) + \left(\frac{\partial \omega_n}{\partial I}(I) v \right) \left(\frac{\partial \bar{\Omega}}{\partial I}(I) u \right)}{\omega_n(I)^2} \right. \\ &\quad \left. - \frac{\left(\frac{\partial^2 \omega_n}{\partial I^2}(I)(u, v) \right) \bar{\omega}(I)}{\omega_n(I)^2} + \frac{2 \left(\frac{\partial \omega_n}{\partial I}(I) u \right) \left(\frac{\partial \omega_n}{\partial I}(I) v \right) \bar{\omega}(I)}{\omega_n(I)^3}, a \frac{\partial^2 h}{\partial I^2}(I)(u, v) \right). \end{aligned}$$

We can bound this expression like in (2.73–2.74):

$$\begin{aligned} \left| \frac{\partial^2 \bar{\Omega}}{\partial I^2}(I)(u, v) \right| &\leq \frac{1}{\omega_n(I)^2} \left(\left| \frac{\partial^2 \omega}{\partial I^2}(I)(u, v) \right| \cdot |\omega(I)| + \left| \frac{\partial \omega}{\partial I}(I) u \right| \cdot \left| \frac{\partial \omega}{\partial I}(I) v \right| \right) \\ &\quad + \frac{2}{|\omega_n(I)|^3} \left| \frac{\partial \omega_n}{\partial I}(I) u \right| \cdot \left| \frac{\partial \omega_n}{\partial I}(I) v \right| \cdot |\bar{\omega}(I)| \\ &\leq \left(\frac{M' L}{l^2} + \frac{3M^2 L}{l^3} \right) |u| |v|, \end{aligned}$$

and we deduce estimate (d):

$$\left| \frac{\partial^2 \Omega}{\partial I^2} \right|_G \leq \sqrt{\left(\frac{M' L}{l^2} + \frac{3M^2 L}{l^3} \right)^2 + (aM)^2} \leq \left(\frac{M'}{2M} + \frac{3M}{l} \right) La. \quad \square$$

Remark If the condition $a \geq 2M/l^2$ is removed, then estimate (b) has to be substituted by (2.77), which is actually worse if a is taken too small.

Proof of lemma 2.2 Clearly, it suffices to check the result for the vectors $v \in \langle \tilde{\omega} \rangle^\perp$ such that $|v| = 1$. One has $|\omega \cdot v| \leq \varepsilon$ for these vectors. Writing $v = v_1 + v_2$, with $v_1 \in \langle \omega \rangle^\perp$ and $v_2 \in \langle \omega \rangle$, one deduces that

$$|v_2| \leq \frac{\varepsilon}{|\omega|}, \quad |v_1| \geq 1 - \frac{\varepsilon}{|\omega|}.$$

By the hypothesis,

$$|Av + \lambda\omega| \geq |Av_1 + \lambda\omega| - |Av_2| \geq \mu|v_1| - |A| \cdot |v_2| \geq \mu \left(1 - \frac{\varepsilon}{|\omega|}\right) - |A| \frac{\varepsilon}{|\omega|} \geq \mu - \frac{2|A|\varepsilon}{|\omega|}.$$

Then, if we assume that $|\lambda\tilde{\omega}| \leq 2|\tilde{A}|$, we obtain

$$\begin{aligned} |\tilde{A}v + \lambda\tilde{\omega}| &\geq |Av + \lambda\omega| - \left|(\tilde{A} - A)v\right| - |\lambda(\tilde{\omega} - \omega)| \\ &\geq \mu - \frac{2|A|\varepsilon}{|\omega|} - \varepsilon' - \frac{2|\tilde{A}|}{|\tilde{\omega}|}\varepsilon \geq \mu - \frac{4M\varepsilon}{l} - \varepsilon'. \end{aligned}$$

In the case $|\lambda\tilde{\omega}| > 2|\tilde{A}|$, the proof is much easier:

$$|\tilde{A}v + \lambda\tilde{\omega}| \geq |\lambda\tilde{\omega}| - |\tilde{A}v| \geq |\tilde{A}| \geq |A| - \varepsilon' \geq \mu - \varepsilon'. \quad \square$$

Proof of lemma 2.3 For a fixed $J \in F - \frac{4M\varepsilon}{\tilde{m}}$, we are going to prove that there exists a unique point $I^* \in G$ solving $\tilde{\Omega}(I^*) = J$. This aim is attained with the help of a modified Newton algorithm. Let us consider

$$I^{(0)} = \Omega^{-1}(J) \in G - \frac{4\varepsilon}{\tilde{m}}$$

as a first approximation, and we have to see that the map

$$\Lambda(I) = I - \left(\frac{\partial \tilde{\Omega}}{\partial I} (I^{(0)}) \right)^{-1} (\tilde{\Omega}(I) - J)$$

has a unique fixed point in G . We first compute the derivative of this map:

$$\frac{\partial \Lambda}{\partial I}(I) = \text{Id} - \left(\frac{\partial \tilde{\Omega}}{\partial I} (I^{(0)}) \right)^{-1} \frac{\partial \tilde{\Omega}}{\partial I}(I) = \left(\frac{\partial \tilde{\Omega}}{\partial I} (I^{(0)}) \right)^{-1} \left(\frac{\partial \tilde{\Omega}}{\partial I} (I^{(0)}) - \frac{\partial \tilde{\Omega}}{\partial I}(I) \right),$$

and therefore

$$\left| \frac{\partial \Lambda}{\partial I}(I) \right| \leq \frac{\tilde{M}'}{\tilde{m}} |I - I^{(0)}| \quad \text{if } |I - I^{(0)}| \leq \frac{4\varepsilon}{\tilde{m}}, \quad (2.78)$$

because the segment joining $I^{(0)}$ and I is fully contained in G . Starting at $I^{(0)}$, we consider the sequence defined by $I^{(k)} = \Lambda(I^{(k-1)})$, $k \geq 1$. We check by induction that

$$|I^{(k)} - I^{(k-1)}| \leq \frac{\varepsilon}{2^{k-1}\tilde{m}}$$

and $I^{(k)} \in G$ for every $k \geq 1$. Indeed, this is true for $k = 1$. For $k > 1$, the induction hypothesis implies that the distance from $I^{(0)}$ to $I^{(k-1)}$ or $I^{(k-2)}$ is less than $2\varepsilon/\tilde{m}$. The same holds for every point in the segment joining $I^{(k-1)}$ and $I^{(k-2)}$. Then, using (2.78) and (2.10) we obtain

$$|I^{(k)} - I^{(k-1)}| = \left| \Lambda(I^{(k-1)}) - \Lambda(I^{(k-2)}) \right| \leq \frac{\tilde{M}'}{\tilde{m}} \cdot \frac{2\varepsilon}{\tilde{m}} |I^{(k-1)} - I^{(k-2)}| \leq \frac{1}{2} |I^{(k-1)} - I^{(k-2)}|.$$

Thus, the sequence $I^{(k)}$ converges, for $k \rightarrow \infty$, to a fixed point of Λ which we name I^* . This point satisfies

$$|I^* - I^{(0)}| \leq \frac{2\varepsilon}{\tilde{m}} \quad (2.79)$$

and therefore

$$I^* \in G - \frac{2\varepsilon}{\tilde{m}}. \quad (2.80)$$

Then,

$$\Omega(I^*) \in F - \frac{2\varepsilon m}{\tilde{m}} \subset F - 2\varepsilon. \quad (2.81)$$

The point I^* is the unique fixed point of Λ . Indeed, assuming that there is another fixed point $I^{**} \neq I^*$, we have $\tilde{\Omega}(I^*) = \tilde{\Omega}(I^{**})$ and hence $|\Omega(I^*) - \Omega(I^{**})| \leq 2\varepsilon$. Then, we have $|I^* - I^{**}| \leq 2\varepsilon/m$ because the whole segment joining $\Omega(I^*)$ and $\Omega(I^{**})$ is contained in F , by (2.81). We deduce from (2.79) that the distance from $I^{(0)}$ to every point in the segment joining I^* and I^{**} is less or equal than $\frac{2\varepsilon}{m} + \frac{2\varepsilon}{m} < \frac{4\varepsilon}{m}$. Applying (2.78), we get a contradiction:

$$|I^* - I^{**}| = |\Lambda(I^*) - \Lambda(I^{**})| < \frac{\tilde{M}'}{\tilde{m}} \cdot \frac{4\varepsilon}{\tilde{m}} |I^* - I^{**}| \leq |I^* - I^{**}|.$$

Given a subset $\tilde{F} \subset F - \frac{4M\varepsilon}{\tilde{m}}$, the map $\tilde{\Omega}$ is one-to-one on $\tilde{G} = \left(\tilde{\Omega}\right)^{-1}(\tilde{F})$. Moreover, one has $\tilde{G} \subset G - \frac{2\varepsilon}{\tilde{m}}$ by (2.80). For the proof of the other inclusion, note that $\tilde{\Omega}(G \setminus \tilde{G}) \cap \tilde{F} = \emptyset$. Then, since $|\tilde{\Omega} - \Omega|_G \leq \varepsilon$, we have $\Omega(G \setminus \tilde{G}) \cap (\tilde{F} - \varepsilon) = \emptyset$, and we deduce that $\Omega(\tilde{G}) \supset \tilde{F} - \varepsilon$.

Finally, we check that $\left|(\tilde{\Omega})^{-1} - \Omega^{-1}\right|_{\tilde{F}} \leq \varepsilon/m$. For a fixed $J \in \tilde{F}$, let $I = \Omega^{-1}(J)$, $\tilde{I} = (\tilde{\Omega})^{-1}(J)$. We have

$$\left|\Omega(\tilde{I}) - \Omega(I)\right| = \left|\Omega(\tilde{I}) - \tilde{\Omega}(\tilde{I})\right| \leq \varepsilon,$$

and therefore the segment joining $\Omega(I)$ and $\Omega(\tilde{I})$ is contained in F , since $\Omega(I) \in \tilde{F} \subset F - \varepsilon$. Hence, we obtain $|\tilde{I} - I| \leq \varepsilon/m$. $\square$

Proof of lemma 2.5 The estimate of part (a) comes from the inclusion

$$\begin{aligned} F(d, \beta, K) \setminus F(d', \beta', K') &\subset ((F - d) \setminus (F - d')) \\ &\cup \bigcup_{\substack{|k|_1 \leq K \\ \bar{k} \neq 0}} \left((F - d) \cap \left(\Delta\left(k, \frac{\beta'}{|k|_1^\tau}\right) \setminus \Delta\left(k, \frac{\beta}{|k|_1^\tau}\right) \right) \right) \\ &\cup \bigcup_{\substack{K < |k|_1 \leq K' \\ \bar{k} \neq 0}} \left((F - d) \cap \Delta\left(k, \frac{\beta'}{|k|_1^\tau}\right) \right) \end{aligned}$$

and the fact that, for $0 \leq \alpha \leq \alpha'$ and $\bar{k} \neq 0$,

$$\text{mes} \left[(F - d) \cap \left(\Delta(k, \alpha') \setminus \Delta(k, \alpha) \right) \right] \leq (\text{diam } F)^{n-1} \cdot \frac{2(\alpha' - \alpha)}{|\bar{k}|}. \quad (2.82)$$

Concerning part (b), we first remark that, for $b \geq 0$,

$$F(d, \beta, K) - b \supset (F - (d + b)) \setminus \bigcup_{\substack{|k|_1 \leq K \\ \bar{k} \neq 0}} \Delta\left(k, \frac{\beta}{|k|_1^\tau} + |\bar{k}|b\right).$$

Then, proceeding like in part (a) and applying (2.82) again,

$$\text{mes} [(F(d, \beta, K) \setminus (F(d, \beta, K) - b))] \leq Db + \sum_{\substack{|k|_1 \leq K \\ \bar{k} \neq 0}} (\text{diam } F)^{n-1} \cdot 2b.$$

From the fact that the number of integer vectors $k \in \mathbb{Z}^n \setminus \{0\}$ with $|k|_1 \leq K$ can be estimated by $2^n K^n$, one gets part (b). It is worth noting that this estimate expresses the “growth” of the boundary of the domain when the resonances are removed. $\square$

Chapter 3

Single resonances

Recall that in a *nearly-integrable* Hamiltonian

$$H(\phi, I) = h(I) + \varepsilon f(\phi, I), \quad (3.1)$$

where ε is a small perturbation parameter, KAM theorem fails on resonances, that is, for actions I such that there exists a non-zero integer vector k such that

$$\langle k, \omega(I) \rangle = 0, \quad (3.2)$$

where $\omega = \partial_I h$. For small $|\varepsilon| \neq 0$, under the conditions of Nekhoroshev theorem, the variation of the actions $|I(t) - I(0)|$ can grow slowly but the dynamics can be very complicated: there can exist, in principle, chaotic trajectories or even unstable (in the sense that they can wander very far from their initial conditions). Let us begin with single resonances, that is, the set of resonant actions I such the module of integer vector k satisfying (3.2) is one-dimensional.

3.1 One step of normal form near a single resonance

Near a single resonance, under some generic hypotheses, we are going to carry out *one* step of (resonant) normal form procedure and try to obtain a new “simple” expression of the Hamiltonian. To reach such a *hyperbolic normal form*, we will have to impose some nondegeneracy conditions on the perturbation f , since no hyperbolicity can be obtained from the unperturbed Hamiltonian h . Essentially, we follow [DG01], which also relies on Eliasson [Eli94] and Niederman [Nie97] (see also [RW98, RW00]).

To simplify the notation, the number of degrees of freedom in (3.1) will be, from now on, $n+1$ instead of n . Thus, we write the angle-action variables are $(\phi, I) \in \mathbb{T}^{n+1} \times \mathbb{R}^{n+1}$.

Having selected an action $I^* = 0$, the unperturbed Hamiltonian h in (3.1) can be written (disregarding the additive constant) as:

$$h(I) = \langle \lambda^*, I \rangle + \frac{1}{2} \langle QI, I \rangle + O_3(I).$$

Assume, for the selected action, that the associated frequency vector $\lambda^* = \partial_I h(0) \in \mathbb{R}^{n+1}$ has a *single resonance* ($\langle k^*, \lambda^* \rangle = 0$ for a certain $k^* \in \mathbb{Z}^{n+1} \setminus \{0\}$ and $\langle k, \lambda^* \rangle \neq 0$ for any $k \in \mathbb{Z}^{n+1}$ not co-linear to k^*). By a classical algebraic result, we can assume λ^* of the form

$$\lambda^* = (0, \omega^*),$$

where $\omega^* \in \mathbb{R}^n$ is nonresonant. In fact, we shall assume a Diophantine condition on ω^* like in (1.2).

Rewrite $\phi \in \mathbb{T}^{n+1}$ as $(x, \varphi) \in \mathbb{T} \times \mathbb{T}^n$ and $I \in \mathbb{T}^{n+1}$ as $(y, I) \in \mathbb{R} \times \mathbb{R}^n$, so that $(\phi, I) = (x, y, \varphi, I) \in \mathbb{T} \times \mathbb{R} \times \mathbb{T}^n \times \mathbb{R}^n$, and the matrix $Q = \partial_I^2 h(0)$ as

$$\begin{pmatrix} \beta^2 & q^\top \\ q & Q \end{pmatrix},$$

where we have put $\beta^2 > 0$ in order to fix ideas, $q \in \mathbb{R}^n$, and the new matrix Q is $n \times n$. We will assume $\beta = 1$; this can be achieved replacing y, I by $y/\beta, I/\beta$ (changing in this way the time scale by a factor

β), and rewriting ω^*/β , q/β^2 , Q/β^2 as ω^* , q , Q respectively, and redefining also the function f . Then, we can write our Hamiltonian in the form

$$\begin{aligned} H(x, y, \varphi, I) &= h(y, I) + \varepsilon f(x, y, \varphi, I), \\ h(y, I) &= \langle \omega^*, I \rangle + \frac{y^2}{2} + \langle q, I \rangle y + \frac{1}{2} \langle QI, I \rangle + O_3(y, I). \end{aligned}$$

We now perform *one* step of resonant normal form procedure: following the Lie method as already introduced in section 1.2.1, we seek for functions $W(x, \varphi)$ and $R(x, y, \varphi, I) = O(y, I)$ such that

$$\{W, h\} + V + R = f, \quad (3.3)$$

where $V(x)$ is the periodic function obtained by averaging with respect to the angles φ :

$$V(x) = \overline{f(x, 0, \cdot, 0)} = \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} f(x, 0, \varphi, 0) d\varphi, \quad x \in \mathbb{T}.$$

The construction of W and R is easily carried out: one first solves the equation

$$\langle \omega^*, \partial_\varphi W \rangle + V = f(\cdot, 0, \cdot, 0)$$

with the help of standard small divisors estimates, as the ones used in the proof of KAM theorem, and then one takes R simply by fitting equation (3.3). The time-1 symplectic flow Φ of the generating Hamiltonian εW leads to

$$H \circ \Phi = H + \{H, \varepsilon W\} + O(\varepsilon^2) = h + \varepsilon(V + R) + O(\varepsilon^2) = H_0 + H_1,$$

with

$$\begin{aligned} H_0(x, y, I; \varepsilon) &= \langle \omega^*, I \rangle + \frac{y^2}{2} + \varepsilon V(x) + \langle q, I \rangle y + \frac{1}{2} \langle QI, I \rangle, \\ H_1(x, y, \varphi, I; \varepsilon) &= \varepsilon R(x, y, \varphi, I) + O_3(y, I) + O(\varepsilon^2). \end{aligned}$$

with H_0 (the truncated normal form) playing the rôle of the integrable Hamiltonian, and H_1 being the perturbation of some size $\varepsilon\mu$ where μ is going to be determined in terms of ε .

This expression generalizes an example introduced by Lochak [Loc90a, Loc92] in order to point out the main difficulties concerning the detection of the diffusion. In canonical variables $(x, y, \varphi, I) \in \mathbb{T} \times \mathbb{R} \times \mathbb{T}^n \times \mathbb{R}^n$, *Lochak's example* is:

$$H(x, y, \varphi, I) = \frac{1}{2} (y^2 + \langle I, I \rangle) + \varepsilon(\cos x - 1) + \varepsilon\mu F(x, \varphi), \quad (3.4)$$

where F is an analytic function on a complex neighborhood of $\mathbb{T}^{n+1}$. Indeed, Lochak's example is a generalization of the famous *Arnold's example* proposed in 1964 by Arnold in [Arn64], as a first example of a extremely slow phenomenon of instability, which received the name of *Arnold diffusion*. The Hamiltonian proposed by Arnold is a nonautonomous Hamiltonian, periodic in the time variable t : in canonical variables $(x, y, \varphi_1, I_1) \in \mathbb{T} \times \mathbb{R} \times \mathbb{T} \times \mathbb{R}$,

$$H(x, y, \varphi_1, I_1, t) = \frac{1}{2} (y^2 + I_1^2) + \varepsilon(\cos x - 1) (1 + \mu(\sin \varphi_1 + \cos t)),$$

with ε and μ as two independent parameters.

It can be assumed, except for degenerate cases, that the function $V(x)$ has a unique and nondegenerate maximum x_0 ; we denote $\alpha^2 = -V''(x_0) > 0$. Then, for $\varepsilon > 0$, the 1-degree-of-freedom Hamiltonian

$$P(x, y; \varepsilon) = \frac{y^2}{2} + \varepsilon V(x),$$

has a hyperbolic point in $(x_0, 0)$, with (homoclinic) separatrices. The case $\varepsilon < 0$ is analogous, provided one considers a minimum instead of a maximum. Then, the Hamiltonian H_0 has whiskered tori with coincident whiskers associated to this hyperbolic point. Note that H_0 constitutes a Hamiltonian situated between the unperturbed Hamiltonian h and the perturbed one H , which possesses hyperbolic invariant tori but their whiskers still coincide. Note also that, in general, H_0 is not an uncoupled Hamiltonian

because of the *coupling term* $\langle q, I \rangle y$. This seems an additional complication, but it cannot be avoided if one starts with an arbitrary unperturbed Hamiltonian h .

The Lyapunov exponents of the hyperbolic point of P are $\pm\sqrt{\varepsilon}\alpha$, which tend to zero for $\varepsilon \rightarrow 0^+$. To have fixed Lyapunov exponents, we can perform the following (non-canonical) linear change: we replace y, I by $\sqrt{\varepsilon}y, \sqrt{\varepsilon}I$. The new system is still Hamiltonian if we divide the Hamiltonian by ε (making in this way a change of time scale by a factor $\sqrt{\varepsilon}$). We obtain for $H = H_0 + H_1$ the expressions:

$$H_0 = \langle \omega, I \rangle + \frac{y^2}{2} + V(x) + \langle q, I \rangle y + \frac{1}{2} \langle QI, I \rangle, \quad (3.5)$$

$$H_1 = R(x, \sqrt{\varepsilon}y, \varphi, \sqrt{\varepsilon}I) + \frac{1}{\varepsilon} O_3(\sqrt{\varepsilon}y, \sqrt{\varepsilon}I) + O(\varepsilon) = O(\mu), \quad (3.6)$$

where

$$\omega = \frac{\omega^*}{\sqrt{\varepsilon}}, \quad \mu = \sqrt{\varepsilon}.$$

We close this section by remarking that an essential point in the approach described in this work is to have an integrable H_0 . A similar procedure could have been carried out for double resonances (or higher multiplicity) instead of single ones, but then H_0 would not be, in general, integrable.

3.2 Regular and singular hyperbolic Hamiltonians

For $\varepsilon \rightarrow 0^+$, the study of the Hamiltonian (3.5–3.6) is a singular perturbation problem, due to the *fast frequencies* $\omega = \omega^*/\sqrt{\varepsilon}$ in the unperturbed Hamiltonian H_0 . We are thus confronted with a *singular* system, often referred to as *weakly hyperbolic*, and also called *a-priori stable* according to the terminology introduced in [CG94]. In fact, this case can be referred to as *totally singular*, because *all* the frequencies are fast.

The singular problem can be avoided if one considers independent parameters, namely a *fixed* $\varepsilon > 0$ (that is, a *fixed* ω in (3.5)) and $\mu \rightarrow 0$. In such a case, the system (3.5–3.6) has the property that the hyperbolicity and the homoclinic orbits are present in the unperturbed Hamiltonian ($\mu = 0$), and are simply perturbed for $|\mu|$ small. In this case, we are confronted with a *regular* or *strongly hyperbolic* system, or also *a-priori unstable*.

This strategy of keeping $\varepsilon > 0$ fixed and letting $\mu \rightarrow 0$ (having in this way a regular system) was introduced by Arnold in order to avoid dealing with a singular perturbation problem. As already remarked in section 0.4, the exponentially small splitting of separatrices predicted by the Melnikov integrals could then be justified only for μ exponentially small in ε .

This regular situation ($\varepsilon > 0$ fixed and μ exponentially small in ε) has been considered in some papers through the construction of appropriate Melnikov integrals [Tre94, Moe96], but their applicability to the existence of Arnold diffusion [HM82, Xia93, Xia94] has overlooked the existence of the gaps between the whiskered tori, as well as the transition properties needed for the invariant tori. (This transition property has been studied in [Dum91, Mar96, Cre00, Nie97].) Also inside this regular situation there is an approach [Bes96, Ber96, Bes97], reminiscent of the parallel shooting method in numerical analysis, which is based on looking directly for the connecting paths of diffusion, using variational methods.

Considering it only from the point of view of bifurcation theory, the relation μ exponentially small in ε is anything but a generic relation between these two parameters. Moreover, from the analysis of the previous section, a power-like relation $\mu = \varepsilon^p$, with $p > 0$, is the natural one from the point of view of perturbation theory (the smaller p , the better). In this singular case, the problem of detecting the splitting of separatrices from the Melnikov integrals is much more intricate because of its exponentially small character with respect to ε .

Concerning the singular problem for 2 degrees of freedom ($n = 1$ in section 3.1), or equivalently area preserving maps, the first results [Nei84, Laz03] appeared in 1984, and now it seems fairly well understood (see, for instance, [DS97] for a survey of results).

For more than 2 degrees of freedom, the existence of intersection between the whiskers can be detected by geometrical and topological methods [Eli94, Bol95], but the effective measure of such intersections involve, in general, small divisors into the expressions for the Melnikov integrals, and arithmetic problems take place in giving asymptotics or lower bounds for such integrals.

As a way to avoiding such small divisors, one can consider different time scales in the frequencies, like for instance $\omega = (\omega_1^*, \omega_2^*/\sqrt{\varepsilon})$ in (3.5). These different time scales take place in some problems of celestial mechanics, and were first considered in [CG94], where the splitting was estimated by direct

Lindstedt expansions, and was wrongly stated as some power of ε , due to some mistaken computations in the third order of such expansions. This error was later on corrected in [GGM99] for the case of *one* fast frequency $\omega_2^*/\sqrt{\varepsilon}$ (one ‘singular’ frequency), and an *even* perturbation $F(x, \varphi)$ with only a finite number of harmonics in the angles x, φ . In this case, the splitting of the separatrices turns out to be $O(\exp(-1/\sqrt{\varepsilon}))$, as in the Arnold’s example, and no problems related with small divisors appear in the exponent of this expression.

The difficult “totally singular” case has been lately receiving special attention. The first formal discussion about the relation between the size of the splitting and the speed of diffusion can be found in [Loc92]. Upper bounds appear in [Gal94], and the first explicit computations showing the arithmetic problems for a concrete frequency were carried out in [Sim94] for fast quasiperiodically forced Hamiltonians (“isochronous systems”).

The paradigmatic example of a pendulum under fast quasiperiodic forcing (the Hamiltonian (3.5–3.6) for $q = 0$, $Q = 0$, $V(x) = \cos x - 1$, and $H_1 = \varepsilon^p m(\varphi) \cos x$, $p > 3$) was studied in [DGJS97] for the case of a nonresonant two-dimensional external frequency $\omega^* = (1, (\sqrt{5} + 1)/2)$, and an asymptotic behavior for the splitting of the type $\Delta \sim \varepsilon^{p/2-1} \exp(-c(\log \varepsilon)/\varepsilon^{1/4})$ was proved, where $c(u)$ is a positive periodic function of u that depends on the arithmetic properties of ω^* and the analyticity properties of $m(\varphi)$.

Lower bounds for the anisochronous Lochak’s example (3.4) with the *same* exponents as in the Nekhoroshev theorem were also stated in [RW98, RW00] for $\mu = \varepsilon^p$ and $p > 0$ big enough, assuming an *even* perturbation $F(x, \varphi)$ (ensuring in this way the existence of a homoclinic orbit), but with a proof containing essential errors.

For the obtainment of asymptotic or lower bounds for the splitting of separatrices, the perturbations H_1 and F are assumed in [DGJS97, RW98, RW00] to possess arbitrarily high harmonics in the angles φ , to ensure that the estimated dominant Fourier mode of the Melnikov integral is not zero. When the perturbation has only a finite number of harmonics (for instance, in the Arnold’s example [Arn64]), the Poincaré–Melnikov theory applied to the original system cannot give the correct asymptotics, since the phenomenon of small divisors does not show up in the Melnikov function. In this case, before applying the results of [DGJS97, RW98, RW00], at least one step of averaging is required to produce a new unperturbed Hamiltonian and a new perturbation with arbitrarily high harmonics (see [Sim94] for an explicit example).

Finally, let us point out that an *essential* assumption in [Gal94, RW98, RW00, GGM99] is the reversibility of the perturbation. This hypothesis is required to ensure the existence of a perturbed homoclinic orbit, to begin the iterative approximation of the whiskers through the study of variational-like equations. This assumption is not required in [DGJS97], where instead an invariant splitting function is defined in some flow-box coordinates provided by a normal form, convergent in a full neighborhood of the whiskered torus, which is constructed with a precise statement of the loss of complex domain in the variable φ . For a recent account of the available results on exponentially small splitting of separatrices with two or even three frequencies, one can look at [DGS04, DG04, DGG14b, DGG14c, DGG14a].

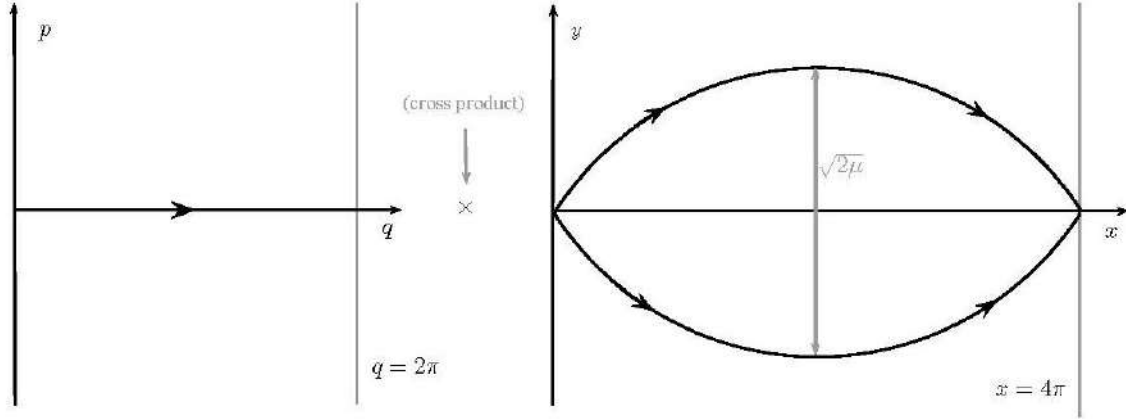
We stop here this account of results, and refer to Lochak [Loc98] for a better organized compendium of results concerning Arnold diffusion.

3.3 The origin of the homoclinic orbits

Homoclinic orbits (doubly asymptotic orbits) go back to Poincaré in 1889 and 1890 ([Poi90a, Poi90b, Poi87]), after a famous error.

In 1885, a Prize in mathematics of H.M. the King Oscar II of Sweden was officially announced. This Prize was promoted by G. Mittag-Leffler, chief-editor of the recently initiated Acta Mathematica (1882-), to celebrate the King Oscar’s 60th anniversary. There appeared several questions to solve, and the first one concerned the stability of the n -body problem.

On January 21, 1889 (King Oscar’s 60th anniversary) the Prize was given to Henry Poincaré for his memoir entitled “On the three body problem and the equations of dynamics”. Although Poincaré did not solve the general problem of stability, he invented the theory of invariant integrals, which gave rise to his famous recurrence theorem, introduced the Poincaré map for general systems as well as the theory of characteristic exponents for periodic orbits. He considered in detail only the restricted three body problem (R3BP), where he found several families of periodic orbits (p.o.), proved the non-existence of first integrals uniform in the mass parameter μ , and introduced the asymptotic surfaces to saddle p.o. and use them to prove the stability of the R3BP.

Figure 3.1: Phase portrait for Hamiltonian (3.3) for $\varepsilon = 0$

Indeed, on page 143, he introduced a simple model of Hamiltonian to study the motions close to the saddle p.o., which were the unstable p.o. which could break the global stability of the R3BP:

$$H(x, q; y, p) = p + y^2 - 2\mu \sin^2 \frac{x}{2} - \mu\varepsilon \cos q \sin x.$$

Hamiltonian (3.3) is 2π -periodic in q and 4π -periodic in x and has the equations:

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial y} = 2y, & \dot{y} &= -\frac{\partial H}{\partial x} = \mu \sin x + \mu\varepsilon \cos q \cos x, \\ \dot{q} &= \frac{\partial H}{\partial p} = 1, & \dot{p} &= -\frac{\partial H}{\partial q} = -\mu\varepsilon \sin q \sin x. \end{aligned}$$

For $\varepsilon = 0$, $H_0(x, q; y, p) = p + y^2 - 2\mu \sin^2 \frac{x}{2}$ has a 2π -periodic solution $x = 0$, $q = t$, $y = 0$, $p = 0$ on the level of energy $H_0 = 0$ which is of saddle type. Poincaré looked for the asymptotic solutions to this p.o. as Lagrangian submanifolds taking the form $y = \frac{\partial S_0}{\partial x}$, $p = \frac{\partial S_0}{\partial q}$ solving the Hamilton-Jacobi eq.

$$H_0 \left(x, q; \frac{\partial S_0}{\partial x}, \frac{\partial S_0}{\partial q} \right) = 0$$

obtaining $S_0 = S_0(x, q) = \mp 2\sqrt{2\mu} \cos \frac{x}{2}$, i.e. $y = \pm \sqrt{2\mu} \sin \frac{x}{2}$, $p = 0$.

The asymptotic surfaces $y = \pm \sqrt{2\mu} \sin \frac{x}{2}$, $p = 0$ are closed surfaces, called also *separatrices*. They are filled with asymptotic solutions to the p.o. (Figure 3.1).

For $0 < |\varepsilon| \ll 1$, he thought that the closed asymptotic surfaces

$$y = \frac{\partial S_0}{\partial x} + \varepsilon \frac{\partial S_1}{\partial x} + o(\varepsilon^2), \quad p = \varepsilon \frac{\partial S_1}{\partial q} + o(\varepsilon^2)$$

persisted and therefore there was stability of the R3BP. To visualize better the result, he introduced the Poincaré map on the section $q = 0 \pmod{2\pi}$:

$$(x(0), q(0) = 0, y(0), p(0)) \mapsto (x(2\pi), q(2\pi) = 2\pi \equiv 0, y(2\pi), p(2\pi)).$$

Restricting it to the level set $H = 0$ ($p = -y^2 + 2\mu \sin^2 \frac{x}{2} + \mu\varepsilon \cos q \sin x$):

$$(x_0, y_0) = (x(0), y(0)) \mapsto (x(2\pi), y(2\pi)) = (x_1, y_1),$$

where the asymptotic surfaces are simply curves $\mathcal{C}$ (Figure 3.2).

Poincaré sent his memoir to be published, and during July 1889, Phragmén, one of the editors of *Acta Mathematica* asked Poincaré for more details about the arguments, since he was not able to understand them. On December 1, 1889, Poincaré sent a letter to Mittag-Leffler saying that he had found an important error, and that the asymptotic surfaces were not necessarily closed: there were two different asymptotic surfaces, which gave rise to two *different* asymptotic curves $\mathcal{C}^s, \mathcal{C}^u$, with different expansions, and he was able to measure the angle between them in a coincident point, which was $\varepsilon\mathcal{J} + o(\varepsilon^2)$, with

$$\mathcal{J} = \frac{2\pi}{\cosh \frac{\pi}{2\sqrt{2\mu}}} \sim 4\pi \exp \left(-\frac{\pi}{2\sqrt{2\mu}} \right).$$

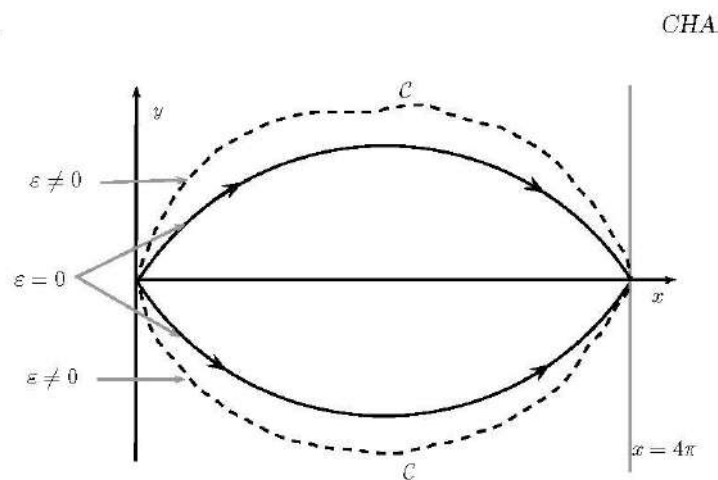


Figure 3.2: Phase portrait for Hamiltonian (3.3) according to Poincaré's first memoir

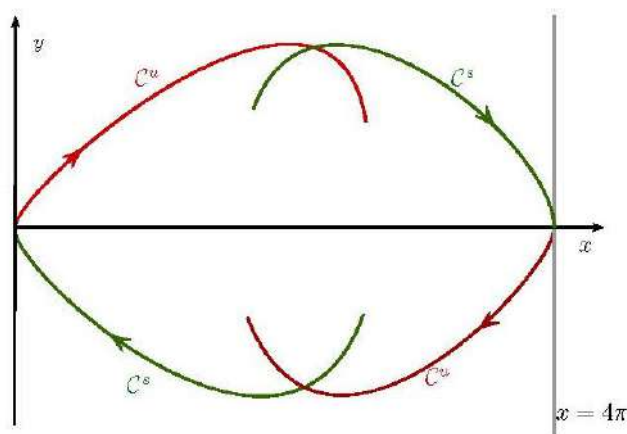


Figure 3.3: Actual splitting of the separatrices

Although the first version of his memoir had already been published, Mittag-Leffler was able to recover all the volumes and destroy them (except two of them, one of which was found by McGehee in the Mittag-Leffler institute), and Poincaré published the new version in 1890, the one we know (he agreed to pay the new edition, spending more money than what he won with the Prize).

Poincaré also noticed that the separation between both asymptotic surfaces was smaller than any power of μ , and asserted that indeed they intersected infinitely many times but that the figure was so complicated that he did not try to draw it.

According to some authors [DH96] this is the first description of chaos. More information can be found in [DH96, BG97]. No more chaos was mentioned until Lorenz in 1963, and Smale in 1965. No more detection of homoclinic orbits was computed until 1963 (Melnikov and Arnold), when the Melnikov method was introduced.

Remark 3.1. Since the R3BP is a 2 degree of freedom Hamiltonian, by KAM theorem (1954-1962), there is stability. [Arn64] is the paper where Arnold conjectures instability for Hamiltonians with more than 2 d.o.f.

Chapter 4

Global instability

4.1 Introduction

The goal of this chapter is to present a generalization of the geometric mechanism for global instability (popularly known as Arnold diffusion) in a priori unstable Hamiltonian systems introduced in [DLS06a]. That paper developed an argument to prove the existence of global instability in a priori unstable nearly integrable Hamiltonian systems (the unperturbed Hamiltonian presents hyperbolicity, so that it can not be expressed globally in action-angle variables) and applied it to a model which presented the so called *large gap problem*. However, in that case, the perturbation was assumed to be a trigonometric polynomial in the angular variables. In the paper [DH09] an accurate process of truncation of the Fourier series of the perturbation is performed and a deeper study of the *geography of resonances* is presented. Using this, some of the results in [DLS06a] are extended, simplified and applied to an a priori unstable Hamiltonian system with a generic perturbation.

The phenomenon of global instability in Hamiltonian systems has attracted the attention of both mathematicians and physicists in the last years due to its remarkable importance for the applications. It deals, essentially, with the question of what is the effect on the dynamics when an autonomous mechanical system is submitted to a small periodic perturbation. More precisely, whether these perturbations accumulate over time giving rise to a long term effect or whether these effects average out.

The instability problem was formulated first by Arnold in 1964. In his celebrated paper [Arn64], Arnold constructed an example for which he proved the existence of trajectories that avoided the obstacles of KAM tori and performed long excursions. The mechanism is based on the existence of transition chains of *transition whiskered tori*, that is, sequences of tori with transitive dynamics given by a quasi-periodic flow, such that the unstable manifold (whisker) of one of these tori intersects transversally the stable manifold (whisker) of the next one. By an obstruction argument, there is an orbit that follows this transition chain, giving rise to an unstable orbit.

The example proposed in [Arn64] turns out to be rather artificial because the perturbation was chosen in such a way that it preserved exactly the complete foliation of invariant tori existing in the unperturbed system. However, a generic perturbation of size ε creates gaps at most of size $\sqrt{\varepsilon}$ in the foliation of persisting KAM tori, whereas it moves the whiskers only by an amount ε . These KAM tori, which are just a continuation of the ones that existed for the integrable system ($\varepsilon = 0$) are commonly known as *primary tori*. The gaps in the foliation of primary tori are centered around resonances, that is, resonant tori that are destroyed by the perturbation. This is what is known in the literature as the *large gap problem* (see, for instance, [Moe96] for a discussion about the large gap problem and, indeed, of the problem of diffusion).

In the last years there has been a notable progress in the comprehension of the mechanisms that give rise to the phenomenon of instability and a variety of methods has been suggested. As an example of this, we will mention that the *large gap problem* has been solved simultaneously by a variety of techniques: different geometrical methods [DLS00, DLS06a, DLS06b] (scattering map) and [Tre04, PT07] (separatrix map); topological methods [GL06] and variational methods [CY04, CY09]. For more information regarding the problem of Arnold diffusion in the absence of gaps as well as time estimates, the reader is referred to [DGLS08].

Of particular interest for the present chapter are [DLS00, DLS06a, DLS06b]. The strategy in the mentioned papers is based on incorporating in the transition chain new invariant objects, created by the resonances, like *secondary tori*, which are invariant KAM tori contractible to a periodic orbit, as well

as the stable and unstable manifolds of lower dimensional tori. The scattering map, introduced by the same authors (see [DLS08] for a geometric study) is the essential tool for the heteroclinic connections between invariant objects of different topology.

In the paper [DH09] the geometric mechanism introduced in the mentioned papers was extended to a wider class of model systems for which the perturbation does not need to have a finite number of harmonics in the angular variables. In particular, the Hamiltonian studied in this chapter has the following form

$$H_\varepsilon(p, q, I, \varphi, t) = \pm \left(\frac{1}{2} p^2 + V(q) \right) + \frac{1}{2} I^2 + \varepsilon h(p, q, I, \varphi, t; \varepsilon), \quad (4.1)$$

where $p \in (-p_0, p_0) \subset \mathbf{R}$, $I \in (I_-, I_+) \subset \mathbf{R}$ and $(q, \varphi, t) \in \mathbb{T}^3$.

The main result of the paper [DH09] introduced concrete hypotheses for global instability of Hamiltonian (4.1), from which the following short version follows:

Theorem 4.1. *Consider the Hamiltonian (4.1) and assume that V and h are C^{r+2} functions which are C^2 generic, with $r > r_0$, large enough. Then there is $\varepsilon^* > 0$ such that for $0 < |\varepsilon| < \varepsilon^*$ and for any interval $[I_-^*, I_+^*] \subset (I_-, I_+)$, there exists a trajectory $\tilde{x}(t)$ of the system with Hamiltonian (4.1) such that for some $T > 0$*

$$I(\tilde{x}(0)) \leq I_-^*; \quad I(\tilde{x}(T)) \geq I_+^*.$$

Remark 4.1. A value of r_0 which follows from the argument in [DH09] is $r_0 = 242$.

The strategy for the proof follows the geometric mechanism proposed in [DLS06a]. Indeed, in order to organize the different invariant objects that are used to construct a transition chain, one first identifies the *normally hyperbolic invariant manifold* (NHIM) present in the system. This NHIM will have associated stable and unstable invariant manifolds that, generically, intersect transversally. Therefore, one can associate to this object two types of dynamics: the *inner* and the *outer*. The outer dynamics takes into account the asymptotic motions to the NHIM and is described by the scattering map. The inner dynamics is the one restricted to the NHIM and contains Cantor families of primary and secondary KAM tori. Since generically these families of KAM tori, invariant for the inner dynamics, are not invariant for the outer dynamics, the combination of both dynamics allows us to construct a transition chain.

The results in [DLS06a] can be applied straightforwardly for the persistence of the NHIM and the transversality of its associated stable and unstable manifolds. The arguments presented in [DH09] focus on the inner dynamics and the study of the invariant objects present in the NHIM.

For Hamiltonian (4.1), resonances correspond to the places where the frequency $I = -l/k$ for $(k, l) \in \mathbb{Z}^2$ is rational and the associated Fourier coefficient $h_{k,l}$ of the perturbation h is nonzero. On these resonances, the foliation of KAM tori in the NHIM is destroyed and gaps between the Cantor family of invariant tori in the NHIM of size $\mathcal{O}(\varepsilon^{1/2} |h_{k_0, l_0}|^{1/2})$ are created, for (k_0, l_0) such that $l/k = l_0/k_0$ and $\gcd(k_0, l_0) = 1$. For a perturbation h which is a C^{r+2} function and C^2 generic, when we restrict it to the NHIM and we write it in adequate coordinates we are left with a C^r perturbation (see the subsection “restriction to NHIM” in [DH09]), so that $|h_{k,l}| \sim |(k, l)|^{-r}$, and therefore the above gaps are of size $\mathcal{O}(\varepsilon^{1/2} |(k_0, l_0)|^{-r/2})$. Moreover, other invariant objects, like secondary tori and lower dimensional tori, are created inside the gap. They correspond to invariant objects of different topology that were not present in the unperturbed system but are generated by the resonances.

In order to study their existence and give an approximate expression for them one combines m steps of averaging plus a KAM Theorem. Notice that in our case, since the perturbation is generic, there will be an infinite number of resonances. The approach in [DH09] for this study is to consider an adequate truncation up to some order M , depending on ε , of the Fourier series of the perturbation h in such a way that we deal only with a finite number of harmonics $|(k, l)| \leq M$ and therefore of resonances.

Another remarkable difference with respect to the results obtained in [DLS06a] is that in that case the size of the gaps created in the foliation of invariant tori was uniform, whereas in this case, since the size is $\mathcal{O}(\varepsilon^{1/2} |(k_0, l_0)|^{-r/2})$, there is a heterogeneous sea of gaps of different sizes. Among them, one distinguishes between *small gaps* and *big gaps*, which are strongly related to the mentioned large gap problem. Indeed, big gaps are those of size bigger or equal than ε and therefore they are generated by resonances $-l_0/k_0$ of order one, such that $|(k_0, l_0)| < \varepsilon^{-1/r}$ or, equivalently, $|(k_0, l_0)|^{-r/2} \geq \varepsilon^{1/2}$ (again, see the paper [DH09] for precise results).

From a more technical point of view, we would like to remark that the main difficulties arise from the fact that in order to perform a resonant averaging procedure, one needs to isolate resonances corresponding to $|(k, l)| \leq M$, for M depending on ε . Consequently, the width L of the resonant domain can not be chosen independently of ε , as it was the case in [DLS06a]. Moreover, along the averaging

procedure one needs to keep track of the $\mathcal{C}^\ell$ norms of the averaged terms and the remainders, and these blow up as a negative power of L . Hence, a good choice for L around a resonance $I = -l/k$ turns out to be $L = L_k \sim \varepsilon^{1/n}/|k|$, where n is the required regularity to apply KAM Theorem after the averaging procedure. Notice that L is not uniform along the resonances but depends on the value $|k|$ of the resonance.

Finally, after m steps of averaging, one can show that the remainder tail, that is, the Fourier coefficients $h_{k,l}$ such that $|(k,l)| > M$ can be neglected. This can be ensured by a fast enough decreasing rate of the coefficients and therefore a large enough regularity r of the perturbation. Thus, the required regularity r will be determined according to the number m of steps of averaging performed, as well as the needed regularity n to apply KAM Theorem after the averaging procedure.

The standard KAM theorem requires to have the Hamiltonian system written in action angle variables. Since near the resonances the system is approximated by one which is close to a pendulum, the action variable becomes singular on the separatrix. This fact, together with the requirement to have the invariant objects close enough (at a distance smaller than ε) implies that the perturbation of the averaged Hamiltonian has to be extremely small in the resonant regions. The immediate consequence of this fact is that, in the case we are considering, it turns out that one has to perform at least $m = 10$ steps of averaging. The needed regularity n to apply KAM Theorem after m averaging steps is $n = 2m + 6$ (see [DH09]). Since the regularity r required to ensure that the remainder tail is smaller than the averaging remainder turns out to be $r > (n - 2)m + 2$, one has to impose $r > r_0 = 242$.

This regularity does not seem to be optimal. Actually, another version of the KAM theorem without the change into action-angle variables like [LGJV05, FLS09] could improve the results in terms of the needed regularity (see also [HLS12] for a numerical implementation). However, it is worth mentioning that less steps of averaging in the resonant domains are required in [DH09] with respect to the results in [DLS06a]. Since in the resonances the behavior of KAM tori is different depending on how close they are to the separatrix (tori are flatter as they are further from the separatrix), different regions are considered where different scalings are performed. This strategy, which was already introduced in [DLS06a], was also improved in [DH09] introducing a new sequence of domains. When applied to the case with a finite number of resonances as in [DLS06a], it turns out that $m = 9$ steps of averaging and $r \geq 26$ are enough. This clearly improves the needed regularity r which was $r \geq 60$ in [DLS06a] because m was chosen $m = 26$.

A quantitative description of the *geography of resonances* and a detailed study of the invariant objects generated by the resonances can be found in [DH09]. The effect of the resonances in a system constitutes a fundamental problem not only for diffusion but also for many other physical applications and it has been an important object of study in the physical literature, see for instance [Chi79, Ten82]. The study performed in [DH09] contributes to understand better the different types of resonances and the geometric objects that one can find therein under an arbitrarily small value of the perturbation parameter ε . Therefore, this study can be very helpful in many physical problems, although in concrete problems, the size of ε is not necessary very small, and other diffusion mechanisms, like Chirikov's overlapping of resonances [Chi79].

We would like to emphasize that for Hamiltonian (4.1), and this is different from the results in [DLS06a], only the resonances of order 1, that is, the ones that appear at the first step of averaging, create big gaps; whereas in [DLS06a], both resonances of order 1 and 2 could generate big gaps. This is because we are dealing with a perturbation that generically will have all the harmonics different from zero. This means that the effect of the resonances associated to the biggest Fourier coefficients (low frequencies) will be detected at the first step of averaging. Since the size of the gap depends on both the order of the resonance and the size of the Fourier coefficient associated to that resonance, the ones that appear at the second step of averaging already correspond to small Fourier coefficients and the size of their gap will be smaller than ε . The immediate consequence of this fact is that one can give all conditions *explicitly* in terms of the original perturbation h .

Following a similar strategy, global instability has been also proven [DLS16] in multidimensional models given by Hamiltonians of the form

$$H(I, \varphi, p, q, t; \varepsilon) = h(I) + \sum_{j=1}^n \pm \left(\frac{1}{2} p_j^2 + V_j(q_j) \right) + \varepsilon Q(I, \varphi, p, q, t; \varepsilon) \quad (4.2)$$

where $I \in \mathcal{I} \subset \mathbb{R}^d$, $\varphi \in \mathbb{T}^d$, $p, q \in \mathbb{R}^n$, $t \in \mathbb{T}^1$. In [DLS16] it is shown that, for $0 < \varepsilon \ll 1$, under regularity and explicit non-degeneracy conditions on the model, there are orbits whose action variables I perform rather arbitrary excursions in a domain of size $O(1)$. This domain includes resonance lines and, hence, large gaps among d -dimensional KAM tori.

Let us mention that results in Arnold diffusion in Hamiltonians with $2 + 1/2$ degrees of freedom which do not present the big gap problem have already been established in [BT99, DLS00, Mat04, Kal03, GT08, Pif06a] and several applications to models coming from Celestial Mechanics with three or more degrees of freedom can be found in [Moe96, Zhe09, CZ11, Xue14, FGKR16, DKRS19].

Of course, we are far from believing that the mechanism discussed in these notes is the only one to produce changes of order one in the actions. In [Tre04, Tre02] the author defines the so-called separatrix map near the normally hyperbolic invariant manifold $\tilde{\Lambda}_\varepsilon$ to obtain results for the a priori unstable case in lower dimensions. Combinations of variational and geometric methods have been recently applied in a-priori unstable Hamiltonians with $2 + 1/2$ degrees of freedom [CY09, Zha11, KZ15, Ber10, Mar13, MS14a, BCV01] which require the Hamiltonian to be positive definite, which is a non-generically (albeit open) property.

For a-priori stable Hamiltonians, where the unperturbed system only depends on the actions and has no hyperbolic structure, variational methods have given results for positive definite Hamiltonians in some cusp-residual sets, see [KZ15, BKZ16].

The case of a-priori unstable systems like (4.2) with $d \geq 2$ presents a difficulty that was not present in the case $d = 1$, namely, that there are points in the normally hyperbolic invariant manifold $\tilde{\Lambda}_\varepsilon$ where the resonances have higher multiplicity (the multiplicity of a resonance is the dimension of its resonance module, see [DLS16]).

The technique used in [DLS03, DLS06a] was to take advantage of the fact that, in the neighborhood of simple resonances, that is, resonances of multiplicity 1, it is possible to introduce a normal form which is integrable, and can be analyzed with great accuracy. Unfortunately, it is well known that multiple resonances, that is, resonances of multiplicity greater or equal than 2, lead to normal forms that are not integrable and need other techniques to be analyzed (see [AKN06, Hal99]). Recent progress in the analysis of double resonances for a-priori stable systems can be found in [Mar13, KZ15, Che19]. We also note that [Tre12] establishes diffusion far from *strong resonances* for the case $n = 1$, $d \geq 2$, using the method of the separatrix map.

4.2 Introduction to the scattering map

Based on [DLS06a, DLS08, DH11], we are going to consider an a priori unstable Hamiltonian systems with $2 + 1/2$ degrees of freedom:

$$\begin{aligned} H_\varepsilon(p, q, I, \varphi, s) &= H_0(p, q, I) + \varepsilon h(p, q, I, \varphi, s; \varepsilon) \\ &= P(p, q) + \frac{I^2}{2} + \varepsilon h(p, q, I, \varphi, s; \varepsilon), \end{aligned} \quad (4.3)$$

where $p, I \in \mathbb{R}$, $q, \varphi, s \in \mathbb{T}$ and $P(p, q)$ is a *pendulum*: $P_\pm(p, q) = P(p, q) = \pm \left(\frac{p^2}{2} + V(q) \right)$ with $V(q)$

2π -periodic with a unique non-degenerate maximum, say at $q = 0$, and take, for instance, $V(0) = 0$. The origin ($p = q = 0$) is thus a saddle equilibrium with associated separatrices included in $P^{-1}(0)$, and one of them, for instance, for $p > 0$, will be written as $\{(p_0(t), q_0(t)), t \in \mathbb{R}\} =: \Gamma$.

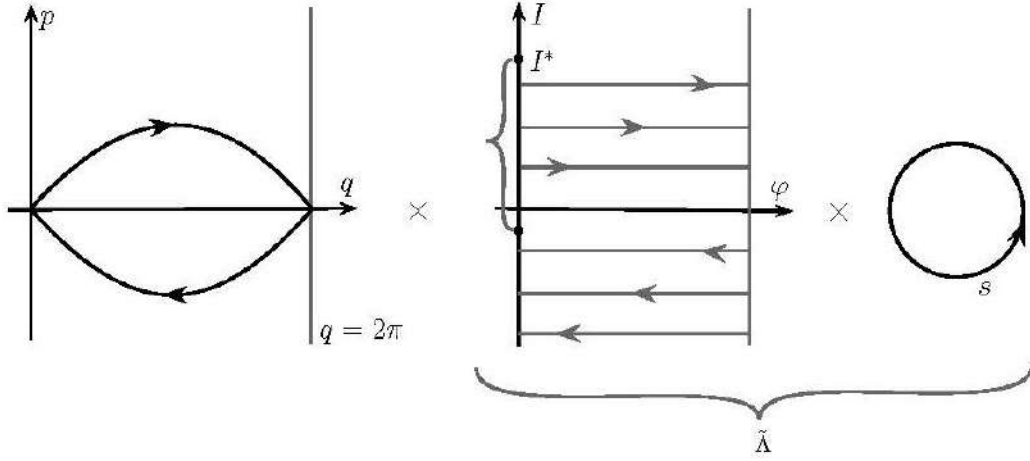
Remark 4.2. The $\pm$ sign in front of P is to emphasize that the Hamiltonian H_0 does not need to be positive definite in the momenta p, I .

Remark 4.3. The Hamiltonian $H_0(p, q, I)$ could have a coupling term between p and I as in (3.5-3.6), but in that case the forthcoming Melnikov potential (4.8) is not so simple.

On the other hand the term $I^2/2$ is usually called a “rotor”. The Hamiltonian H_0 is integrable, but the variables (p, q) are not written in action-angle coordinates, since there is a saddle equilibrium (therefore unstable) at $p = q = 0$. The phase space for $\varepsilon = 0$, i.e., for Hamiltonian H_0 is displayed in Figure 4.1.

The equations associated to H_0 are:

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\partial H_0}{\partial q} = \mp V'(q) & \frac{dI}{dt} &= -\frac{\partial H_0}{\partial \varphi} = 0 & \frac{ds}{dt} &= 1 \\ \frac{dq}{dt} &= \frac{\partial H_0}{\partial p} = \pm p & \frac{d\varphi}{dt} &= \frac{\partial H_0}{\partial I} = I \end{aligned} \quad (4.4)$$

Figure 4.1: Phase portrait for the unperturbed Hamiltonian H_0 .

The pendulum $P(p, q)$ and the rotor I functions are first integrals, i.e., they are constants of motion. We will concentrate ourselves close to the separatrix of the pendulum ($P \simeq 0$). For any interval $[-\frac{1}{2}, I_+^*] \subset \mathbb{R}$

$$\tilde{\Lambda} = \left\{ \left(p = 0, q = 0, I \in \left[-\frac{1}{2}, I_+^* \right], \varphi \in \mathbb{T}, s \in \mathbb{T} \right) \right\}$$

is a 3D *normally hyperbolic invariant manifold* (NHIM)) with inner motion

$$\dot{I} = 0, \quad \dot{\varphi} = I, \quad \dot{s} = 1$$

or, equivalently, trajectories

$$t \mapsto (0, 0, I, \varphi + It, s + t)$$

and coincident 4D stable and unstable invariant manifolds, of equation $P = 0$, from which we consider a piece, a separatrix

$$\tilde{\gamma} := W^0 \tilde{\Lambda} = \left\{ (p_0(\tau), q_0(\tau), I, \varphi, s), \tau \in \mathbb{R}, I \in \left[-\frac{1}{2}, I_+^* \right], (\varphi, s) \in \mathbb{T}^2 \right\} \quad (4.5)$$

with inner motion

$$\dot{\tau} = 1, \quad \dot{I} = 0, \quad \dot{\varphi} = I, \quad \dot{s} = 1$$

or, equivalently, trajectories

$$t \mapsto (p_0(\tau + t), q_0(\tau + t), I, \varphi + tI, s + t).$$

For every I , the unperturbed Hamiltonian H_0 possesses 2D “whiskered tori”

$$\mathcal{T}_I^0 = \{(0, 0, I, \varphi, s), (\varphi, s) \in \mathbb{T}^2\}$$

with frequency $(I, 1)$ and 3D whiskers

$$W^0 \mathcal{T}_I^0 = \{(p_0(\tau), q_0(\tau), I, \varphi, s), \tau \in \mathbb{R}, (\varphi, s) \in \mathbb{T}^2\}.$$

The *scattering map* on $\tilde{\Lambda}$ is the map

$$\begin{aligned} S: \quad \tilde{\Lambda} &\mapsto \tilde{\Lambda} \\ \tilde{x}_- &\mapsto \tilde{x}_+ = S(\tilde{x}_-) \end{aligned}$$

where $\tilde{x}_+ = S(\tilde{x}_-)$ if and only if there exists $\tilde{z} \in W^u(\tilde{\Lambda}) \cap W^s(\tilde{\Lambda})$ such that $\Phi_t(\tilde{x}_\pm) - \Phi_t(\tilde{z}) \rightarrow 0$ when $t \rightarrow \pm\infty$, where Φ_t is the flow associated to the unperturbed Hamiltonian H_0 .

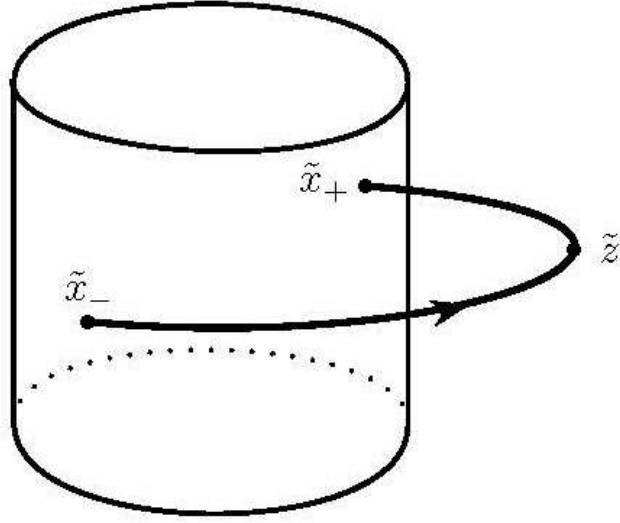


Figure 4.2: The scattering map.

In other words, $\tilde{x}_+ = S(\tilde{x}_-)$ if there exists a “heteroclinic” trajectory between $\tilde{x}_-$ and $\tilde{x}_+$ (but this trajectory is indeed a “homoclinic” trajectory with respect to $\tilde{\Lambda}$). In our case, introducing the parametrizations

$$\begin{aligned}\tilde{x}_0 &= \tilde{x}_0(I, \varphi, s) = (0, 0, I, \varphi, s) \in \tilde{\Lambda} \\ \tilde{z}_0 &= \tilde{z}_0(\tau, I, \varphi, s) = (p_0(\tau), q_0(\tau), I, \varphi, s) \in W^0(\tilde{\Lambda})\end{aligned}\quad (4.6)$$

the flow acts as

$$\begin{aligned}\Phi_{t,0}(\tilde{x}_0) &= (0, 0, I, \varphi + It, s + t) = \tilde{x}_0(I, \varphi + It, s + t) \\ \Phi_{t,0}(\tilde{z}_0) &= (\underbrace{p_0(\tau + t), q_0(\tau + t)}_{\substack{\downarrow t \rightarrow \pm\infty \\ 0}}, I, \varphi + It, s + t) = \tilde{z}_0(\tau + t, I, \varphi + It, s + t)\end{aligned}\quad (4.7)$$

and it is therefore clear that

$$\forall \tilde{x}_0 \in \tilde{\Lambda} \quad \Phi_{t,0}(\tilde{z}_0) - \Phi_{t,0}(\tilde{x}_0) \xrightarrow[t \rightarrow \infty]{} 0,$$

that is, every point $\tilde{x}_0 \in \tilde{\Lambda}$ has a continuum of homoclinic points $\tilde{z}_0 \in W^s(\tilde{\Lambda}) \cap W^u(\tilde{\Lambda}) = W^0(\tilde{\Lambda})$ to itself parameterized by τ : $S_0(\tilde{x}_0) = \tilde{x}_0$, that is, S_0 is the identity on $\tilde{\Lambda}$.

For general (non-integrable) cases, we will see that different homoclinic points $\tilde{z}$ give rise to different scattering maps, or multivalued scattering maps, so one has to restrict the domain of $\tilde{x}_- \in \tilde{\Lambda}$, and of $\tilde{z} \in W^s(\tilde{\Lambda}) \cap W^u(\tilde{\Lambda})$ to have well defined scattering maps, and one has to require that $\tilde{z} \in W^s(\tilde{\Lambda}) \cap W^u(\tilde{\Lambda})$.

Remark 4.4. The homoclinic convergence is indeed exponential:

$$|\Phi_t(\tilde{z}) - \Phi_t(\tilde{x}_\pm)| \leq C e^{-\mu|t|}$$

for $t \rightarrow \pm\infty$, for some $\mu > 0$.

Remark 4.5. The time it takes to connect with “infinite precision”, $\tilde{x}_-$ and $\tilde{x}_+$ along a heteroclinic trajectory is ∞ , but to arrive at neighborhoods of size $\delta > 0$, i.e., “to connect $\tilde{x}_-$ and $\tilde{x}_+$ with precision δ ”, it only takes $t \sim \frac{1}{\mu} \ln \frac{1}{\delta}$.

As it has already been said, $\tilde{\Lambda}$ has an inner dynamics

$$\Phi_{t,0}(\tilde{x}_0) = (0, 0, I, \varphi + It, s + t).$$

If we fix the time $t = 2\pi$, we have the *inner map*:

$$\tilde{x}_0 = (0, 0, I, \varphi, s) \xrightarrow{F} (0, 0, I, \varphi + 2\pi I, s).$$

That is, $\tilde{\Lambda}$ has two dynamics, an inner one F (inner map) and another outer one S (scattering map). The idea is to combine both to design trajectories near $\tilde{\Lambda}$. For this integrable Hamiltonian H_0 , we can combine very few things, since S is trivial and F is almost trivial, since it preserves the action I (see Figure 4.3).

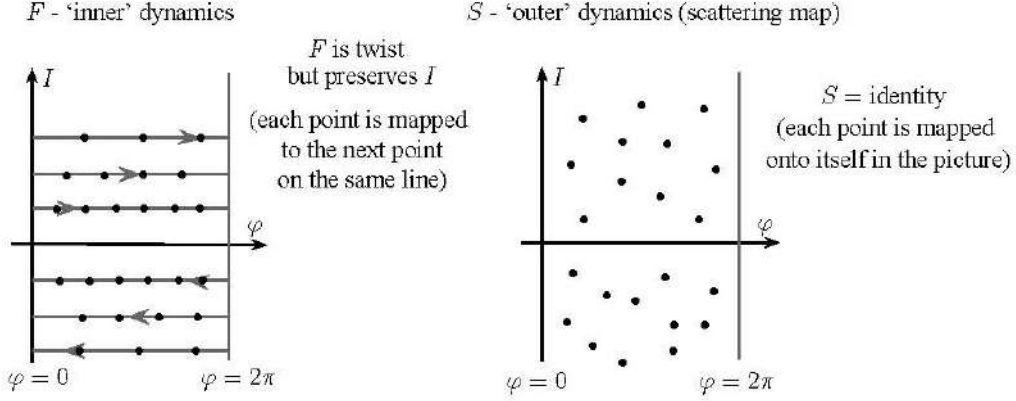


Figure 4.3: Inner and outer dynamics for the unperturbed Hamiltonian

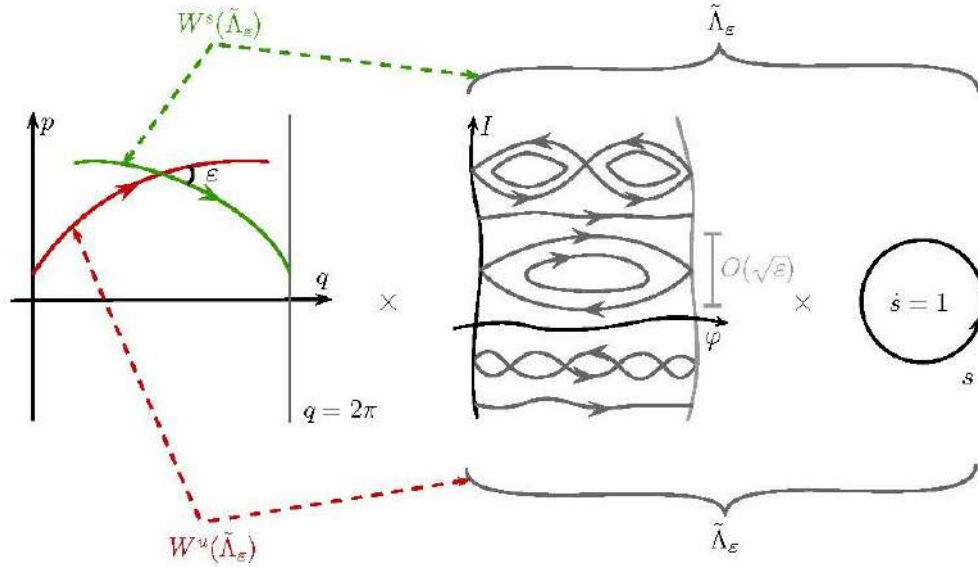


Figure 4.4: Phase portrait for the perturbed Hamiltonian

Being S the identity, it does not alter the trajectories of F :

$$S \circ F^{n_1} \circ S \circ F^{n_2} \circ S \circ F^{n_3} \circ S = F^{n_1+n_2+n_3}.$$

We are now going to consider the case $0 < |\varepsilon| \ll 1$, hoping that the perturbed dynamics of F and S will be different, *without common invariant sets*.

Figure 4.4 is a 5D cartoon describing what will happen for $0 < |\varepsilon| \ll 1$ (except that One needs to imagine 5D and the scattering map is not in the picture).

By the theory of NHIM, if h is C^{r+1} , there exist $\tilde{\Lambda}_\varepsilon$, $W_{loc}^s(\tilde{\Lambda}_\varepsilon)$, $W_{loc}^u(\tilde{\Lambda}_\varepsilon)$ C^r and $\varepsilon - C^r$ -close to $\tilde{\Lambda}$, $W^s(\tilde{\Lambda}) = W^u(\tilde{\Lambda}) = W^0(\tilde{\Lambda}_\varepsilon)$, respectively. Moreover the invariant manifolds of the NHIM are foliated by

asynchrones associated to points on the NHIM:

$$W_{loc}^{s,u}(\tilde{\Lambda}_\varepsilon) = \bigcup_{\tilde{x} \in \tilde{\Lambda}_\varepsilon} W_{loc}^{s,u}(\tilde{x})$$

and one can define the $\mathcal{C}^r$ wave map

$$\tilde{z}^s \in W_{loc}^s(\tilde{\Lambda}_\varepsilon) \xrightarrow{\Omega_\varepsilon^+} \tilde{x}_+ = \Omega_\varepsilon^+(\tilde{z}^s) \in \tilde{\Lambda}_\varepsilon, \text{ for } \tilde{z}^s \in W_{loc}^s(\tilde{x}).$$

The same for Ω_ε^- . For a survey on the theory of NHIM adopted to this problem, one can look at the last section of this chapter, or also at Appendix B of [DLS06b].

The local manifolds can be globalized to

$$W^{s,u}(\tilde{\Lambda}_\varepsilon) = \bigcup_{+, -t < 0} \Phi_{t,\varepsilon} \left(W_{loc}^{s,u}(\tilde{\Lambda}_\varepsilon) \right).$$

If $\tilde{z}^s \in W^s(\tilde{\Lambda}_\varepsilon)$, there exists a unique $\tilde{x}_+ \in \tilde{\Lambda}_\varepsilon$ such that $\tilde{z}^s \in W^s(\tilde{x})$, i.e., $\Phi_{t,\varepsilon}(\tilde{z}^s) - \Phi_{t,\varepsilon}(\tilde{x}) \xrightarrow[t \rightarrow \infty]{} 0$. The convergence is indeed exponential: $|\Phi_{t,\varepsilon}(\tilde{z}^s) - \Phi_{t,\varepsilon}(\tilde{x})| \leq C e^{-\mu t/2}$, $t \rightarrow \infty$. Analogously for $\tilde{z}^u$, $\tilde{x}_-$, $t < 0$. In general, $W^s(\tilde{\Lambda}_\varepsilon) \neq W^u(\tilde{\Lambda}_\varepsilon)$. We look for the points $\tilde{z} \in W^s(\tilde{\Lambda}_\varepsilon) \cap W^u(\tilde{\Lambda}_\varepsilon)$.

The following Proposition 4.2 establishes the existence of transverse intersections for $W^s(\tilde{\Lambda}_\varepsilon)$ and $W^u(\tilde{\Lambda}_\varepsilon)$ along a manifold $\tilde{\gamma}_\varepsilon$ and will provide perturbative formulas for the scattering map associated to these intersections. It relies on a non-degeneracy condition of the Poincaré function, also called *Melnikov potential*, associated to h (and to the homoclinic orbit of the pendulum $\Gamma = (q_0, p_0)$):

$$\begin{aligned} \mathcal{L}(I, \varphi, s) = & - \int_{-\infty}^{+\infty} \left(h(p_0(\sigma), q_0(\sigma), I, \varphi + I\sigma, s + \sigma; 0) \right. \\ & \left. - h(0, 0, I, \varphi + I\sigma, s + \sigma; 0) \right) d\sigma. \end{aligned} \quad (4.8)$$

Proposition 4.2. *Given $(I, \varphi, s) \in [I_-, I_+] \times \mathbb{T} \times \mathbb{T}$, assume that the function $\tau \in \mathbb{R} \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau)$ has a non-degenerate critical point at $\tau = \tau^*(I, \varphi, s)$. (By the implicit function theorem, the function τ^* is smooth).*

Then, for ε small enough, there exists a locally unique point $\tilde{z}$ of the form

$$\tilde{z}(I, \varphi, s; \varepsilon) = \tilde{z}(\tau^*(I, \varphi, s), I, \varphi, s; \varepsilon) = (p_0(\tau) + O(\varepsilon), q_0(\tau) + O(\varepsilon), I, \varphi, s), \quad (4.9)$$

such that $W^s(\tilde{\Lambda}_\varepsilon) \cap W^u(\tilde{\Lambda}_\varepsilon)$ at $\tilde{z}$, that is,

$$\tilde{z} \in W^s(\tilde{\Lambda}_\varepsilon) \cap W^u(\tilde{\Lambda}_\varepsilon) \text{ and } T_{\tilde{z}}W^s(\tilde{\Lambda}_\varepsilon) + T_{\tilde{z}}W^u(\tilde{\Lambda}_\varepsilon) = T_{\tilde{z}}\mathcal{M},$$

where $\mathcal{M} = \mathbb{R} \times \mathbb{T} \times [I_-, I_+] \times \mathbb{T} \times \mathbb{T}$.

In particular, there exist unique points

$$\tilde{x}_\pm = \tilde{x}_\pm(I, \varphi, s; \varepsilon) = (0, 0, I, \varphi, s) + O_{\mathbb{C}^1}(\varepsilon) \in \tilde{\Lambda}_\varepsilon$$

such that

$$|\Phi_{t,\varepsilon}(\tilde{z}) - \Phi_{t,\varepsilon}(\tilde{x}_\pm)| \leq \text{cte.} e^{-\mu|t|/2} \text{ for } t \rightarrow \pm\infty. \quad (4.10)$$

Moreover, expressing the points $\tilde{x}_\pm = \tilde{F}(I_\pm, \varphi_\pm, s_\pm; \varepsilon)$ in terms of the parameterization (4.13) of $\tilde{\Lambda}_\varepsilon$ given in Theorem Appendix 4.4, the following formulas hold:

$$I(\tilde{x}_\pm) = I + O_{\mathbb{C}^1}(\varepsilon), \quad \varphi(\tilde{x}_\pm) = \varphi + O_{\mathbb{C}^1}(\varepsilon), \quad s(\tilde{x}_\pm) = s,$$

and

$$I(\tilde{x}_+) - I(\tilde{x}_-) = \varepsilon \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi - I\tau, s - \tau) + O_{\mathbb{C}^1}(\varepsilon^{1+\varrho}),$$

where τ is given again by $\tau = \tau^(I, \varphi, s)$, and $\varrho > 0$.*

Remark 4.6. The Melnikov potential $\mathcal{L} = \mathcal{L}(I, \varphi, s)$ was introduced in [DG00]. Notice that to look for critical points of $\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau)$ is analytically equivalent to solve the equation

$$I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi - I\tau, s - \tau) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi - I\tau, s - \tau) = 0$$

and geometrically equivalent to look for extrema of $\mathcal{L}$ on the straight line $\{(I, \varphi - I\tau, s - \tau)\}, \tau \in \mathbb{R}$, all this for fixed (I, φ, s) , that is to look for the extrema of $\mathcal{L}$ along trajectories along unperturbed NHIM $\tilde{\Lambda}$.

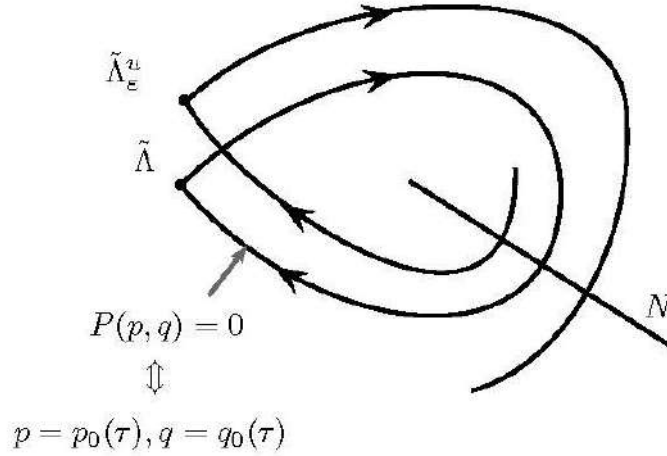


Figure 4.5: Proof of Proposition (4.2)

Proof. The basic idea of the proof of Proposition 4.2 is very standard in Melnikov theory. We start by observing that in the unperturbed case, the stable and unstable manifolds are characterized as the set $\{P = 0\}$ where P is the pendulum part of the unperturbed Hamiltonian. Hence, outside of the critical points of P , we can construct a system of coordinates given by a point in the homoclinic intersection and a value for P . On the other hand, we observe that since P is a conserved quantity in the unperturbed system, $\frac{d}{dt}P$ is small and can be computed perturbatively. Hence, the equation of an invariant manifold can be solved perturbatively and the first term is an integral over the perturbed quantities. Under assumptions of non-degeneracy, this first order calculation is enough to conclude the desired results of existence of transverse intersections (using the implicit function theorem). Similar procedures have been implemented in [DG00]. See also [Tre94]. A different method to prove persistence of intersections—not necessarily transversal—is in [Eli94].

We proceed to give details of the calculation. Recall the parameterizations (4.6) of $\tilde{\Lambda}, W^0(\tilde{\Lambda})$

$$\tilde{x}_0 = \tilde{x}_0(I, \varphi, s) = (0, 0, I, \varphi, s), \quad \tilde{z}_0 = \tilde{z}_0(\tau, I, \varphi, s) = (p_0(\tau), q_0(\tau), I, \varphi, s).$$

From any $\tilde{z}_0 \in W^0(\tilde{\Lambda})$ we throw a straight line N transversal to $W^0(\tilde{\Lambda})$, for instance

$$N = N(\tilde{z}_0) = \tilde{z}_0 + \langle \nabla P(p_0(\tau), q_0(\tau)) \rangle$$

the normal bundle to $W^0(\tilde{\Lambda})$, where $\nabla P = \left(\frac{\partial P}{\partial p}, \frac{\partial P}{\partial q}, 0, 0, 0 \right)$. We note that

$$\tilde{z} \in W^0(\tilde{\Lambda}) \iff P(\tilde{z}) = 0,$$

where $P(\tilde{z})$ means $P(p, q)$ if $\tilde{z} = (p, q, I, \varphi, s)$. Since $W^{s,u}(\tilde{\Lambda}_\varepsilon) = W^0(\tilde{\Lambda}) + O_{C^r}(\varepsilon)$, they intersect N in unique points $\tilde{z}^u, \tilde{z}^s$, which take the form

$$\tilde{z}^{s,u} = \left(p_0(\tau) + \lambda^{s,u} \frac{\partial P}{\partial p}(p_0(\tau), q_0(\tau)), q_0(\tau) + \lambda^{s,u} \frac{\partial P}{\partial q}(p_0(\tau), q_0(\tau)), I, \varphi, s \right),$$

where $\lambda^{s,u} = \lambda^{s,u}(\tau, s; \varepsilon) = O_{C^r}(\varepsilon)$. The key point is that $\tilde{z}^s = \tilde{z}^u$ if and only if $P(\tilde{z}^s) = P(\tilde{z}^u)$, which is the equation to solve.

We will apply the fundamental theorem of calculus to $t \mapsto P(\Phi_{t,\varepsilon}(\tilde{z}))$. Differentiating,

$$\frac{d}{dt} (P(\Phi_{t,\varepsilon}(\tilde{z}))) = \{P, H_\varepsilon\}(\Phi_{t,\varepsilon}(\tilde{z})) = \varepsilon \{P, h\}(\Phi_{t,\varepsilon}(\tilde{z})),$$

where $\{P, h\} = \frac{\partial P}{\partial q} \frac{\partial h}{\partial p} - \frac{\partial P}{\partial p} \frac{\partial h}{\partial q}$ is the Poisson bracket of P and h (recall that P only depends on the variables p, q). Therefore

$$P(\Phi_{t_2,\varepsilon}(\tilde{z})) = P(\Phi_{t_1,\varepsilon}(\tilde{z})) + \varepsilon \int_{t_1}^{t_2} \{P, h\}(\Phi_{\sigma,\varepsilon}(\tilde{z})) d\sigma.$$

For $\tilde{z} = \tilde{z}^{s,u}$, there exist unique $\tilde{x}_\pm \in \tilde{\Lambda}_\varepsilon$ such that

$$|\Phi_{t,\varepsilon}(\tilde{z}^{s,u}) - \Phi_{t,\varepsilon}(\tilde{x}_\pm)| \leq Ce^{-\mu|t|/2} \quad \text{for } \pm t \in [0, \infty).$$

We note that $\tilde{x}_\pm = \tilde{x}_0 + O_{C^r}(\varepsilon)$, so that $P(x_\pm) = P(\varepsilon p_\pm, \varepsilon q_\pm) = O(\varepsilon^2)$, because $P(0, 0) = 0, \nabla P(0, 0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. Also, by Gronwall,

$$\begin{aligned} \Phi_{t,\varepsilon}(\tilde{z}^{s,u}) - \Phi_{t,0}(\tilde{z}^0) &= O_{C^r}(\varepsilon), \pm t \geq 0, \\ |\Phi_{t,\varepsilon}(\tilde{x}_\pm) - \Phi_{t,0}(\tilde{x}_0)|_{C^r} &\leq C_1 |\tilde{x}_\pm - \tilde{x}_0| e^{K\varepsilon|t|} \leq C_2 \varepsilon e^{K\varepsilon|t|}, \end{aligned}$$

where this last bound only takes into account that $\tilde{x}_\pm$ belongs to the NHIM $\tilde{\Lambda}_\varepsilon$. Taking $|t| \leq C_3 \ln \frac{1}{\varepsilon}$, $\Phi_{t,\varepsilon}(\tilde{x}_\pm) - \Phi_{t,0}(\tilde{x}_0) = O_{C^r}(\varepsilon^{\rho_1})$, $0 < \rho_1 < 1$ (indeed $0 \ll \rho_1 \lesssim 1$).

We now apply the integral formula above for $\tilde{z} = \tilde{z}^s, \tilde{x}_+, t_1 = \infty, t_2 = 0$

$$\begin{aligned} P(\tilde{z}^s) - P(\tilde{x}_+) &= -\varepsilon \int_0^\infty (\{P, h\}(\Phi_{\sigma,\varepsilon}(\tilde{z}^s)) - \{P, h\}(\Phi_{\sigma,\varepsilon}(\tilde{x}_+))) d\sigma \\ &= -\varepsilon \left(\int_0^{C_3 \ln \frac{1}{\varepsilon}} \dots + \int_{C_3 \ln \frac{1}{\varepsilon}}^\infty \dots \right) \\ &= -\varepsilon \int_0^{C_3 \ln \frac{1}{\varepsilon}} \dots + O_{C^r}(\varepsilon^{1+\rho_2}), \quad \rho_2 > 0 \end{aligned}$$

since

$$\left| \int_{C_3 \ln \frac{1}{\varepsilon}}^\infty \dots \right| \leq C_4 \int_{C_3 \ln \frac{1}{\varepsilon}}^\infty e^{-\frac{\mu\sigma}{2}} d\sigma = \frac{2C_4}{\mu} e^{-\frac{\mu C_3}{2} \ln \frac{1}{\varepsilon}} = \frac{2C_4}{\mu} \varepsilon^{\frac{\mu C_3}{2}} = O_{C^r}(\varepsilon^{\rho_2}).$$

Thus

$$\begin{aligned} P(\tilde{z}^s) &= -\varepsilon \int_0^{C_3 \ln \frac{1}{\varepsilon}} (\{P, h\}(\Phi_{\sigma,\varepsilon}(\tilde{z}^s)) - \{P, h\}(\Phi_{\sigma,\varepsilon}(\tilde{x}_\pm))) d\sigma + O_{C^r}(\varepsilon^{1+\rho_2}) \\ &= -\varepsilon \int_0^{C_3 \ln \frac{1}{\varepsilon}} \left(\{P, h\}(\Phi_{\sigma,0}(\tilde{z}^0)) - \underbrace{\{P, h\}(\Phi_{\sigma,0}(\tilde{x}_0))}_{P(\tilde{x}_0)=0} \right) d\sigma + O_{C^r}(\varepsilon^{1+\rho_1}) \\ &\quad + O_{C^r}(\varepsilon^{1+\rho_2}) \\ &= -\varepsilon \int_0^\infty \{P, h\}(\Phi_{\sigma,0}(\tilde{z}^0)) d\sigma + O_{C^r}(\varepsilon^{1+\rho}), \quad \rho > 0. \end{aligned}$$

Analogously for $P(\tilde{z}^u)$, substituting $-\varepsilon \int_0^\infty \dots$ by $\varepsilon \int_{-\infty}^0 \dots$. Subtracting,

$$\begin{aligned} P(\tilde{z}^u) - P(\tilde{z}^s) &= \underbrace{\varepsilon \int_{-\infty}^\infty \{P, h\}(p_0(\tau + \sigma), q_0(\tau + \sigma), s + \sigma) d\sigma}_{\frac{\partial L}{\partial \tau}(\tau, I, \varphi, s)} + O_{C^r}(\varepsilon^{1+\rho}) \\ &= \varepsilon \frac{\partial L}{\partial \tau}(\tau, I, \varphi, s) + O_{C^r}(\varepsilon^{1+\rho}), \quad \rho > 0. \end{aligned}$$

where $L(\tau, I, \varphi, s)$ is given by

$$\begin{aligned} L(\tau, I, \varphi, s) &= - \int_{-\infty}^{+\infty} \left(h(p_0(\tau + \sigma), q_0(\tau + \sigma), I, \varphi + I\sigma, s + \sigma) \right. \\ &\quad \left. - h(0, 0, I, \varphi + I\sigma, s + \sigma) \right) d\sigma. \end{aligned} \tag{4.11}$$

From the expression of $L(\tau, I, \varphi, s)$, it is immediate to check that

$$L(\tau + t, I, \varphi + It, s + t) = L(\tau, I, \varphi, s) \text{ for any } t \in \mathbb{R}.$$

Therefore, writing $t = -\tau$, we arrive at

$$L(\tau, I, \varphi, s) = L(0, I, \varphi - I\tau, s - \tau) = \mathcal{L}(I, \varphi - I\tau, s - \tau),$$

where $\mathcal{L}$ is the Melnikov potential defined in (4.8). Then, $P(\tilde{z}^u) = P(\tilde{z}^s)$ is equivalent to

$$\varepsilon \frac{\partial}{\partial \tau} \{ \mathcal{L}(I, \varphi - I\tau, s - \tau) \} + O_{\mathbb{C}^1}(\varepsilon^{1+\rho}) = 0.$$

By the implicit function Theorem, non-degenerate critical points τ of the function $\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau)$ give rise, for ε small enough, to transverse intersections of the stable and unstable manifolds of $\tilde{\Lambda}_\varepsilon$ along points $\tilde{z} = \tilde{z}(\tau, I, \varphi, s; \varepsilon)$ of the form (4.9).

By the implicit function theorem, we can find a function τ^* defined in an open set where $\tau^*(I; \varphi, s)$ is a critical point of $\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau)$.

To finish the proof of Proposition 4.2, we consider the expression of the points $\tilde{x}_\pm = \tilde{\mathcal{F}}(I_\pm, \varphi_\pm, s_\pm; \varepsilon)$ in terms of the parameterization (4.13) of $\tilde{\Lambda}_\varepsilon$ given in Theorem Appendix 4.4. Since we already know the existence of $\tilde{z}$ given in (4.9) such that (4.10) holds, it is clear that

$$I(\tilde{x}_\pm) = I + O_{\mathbb{C}^1}(\varepsilon), \quad \varphi(\tilde{x}_\pm) = \varphi + O_{\mathbb{C}^1}(\varepsilon), \quad s(\tilde{x}_\pm) = s,$$

and to finish the proof of Proposition 4.2 it only remains to obtain the formula for $I(\tilde{x}_+) - I(\tilde{x}_-)$.

We apply now the Fundamental Theorem of Calculus to

$$t \mapsto I(\Phi_{t,\varepsilon}(\tilde{x}_\pm)) - I(\Phi_{t,\varepsilon}(\tilde{z})),$$

to get

$$I(\tilde{x}_\pm) - I(\tilde{z}) = \varepsilon \int_{\pm\infty}^0 \left(\{I, h\}(\Phi_{\sigma,\varepsilon}(\tilde{x}_\pm)) - \{I, h\}(\Phi_{\sigma,\varepsilon}(\tilde{z})) \right) d\sigma,$$

where $\{I, h\} = \partial_\varphi I \partial_I h - \partial_I I \partial_\varphi h = -\partial_\varphi h$ is the Poisson bracket of the functions I and h . Subtracting the expressions above, we get

$$\begin{aligned} I(\tilde{x}_+) - I(\tilde{x}_-) &= \varepsilon \int_0^{+\infty} \frac{\partial h}{\partial \varphi}(\Phi_{\sigma,\varepsilon}(\tilde{z})) - \frac{\partial h}{\partial \varphi}(\Phi_{\sigma,\varepsilon}(\tilde{x}_+)) d\sigma \\ &\quad + \varepsilon \int_{-\infty}^0 \frac{\partial h}{\partial \varphi}(\Phi_{\sigma,\varepsilon}(\tilde{z})) - \frac{\partial h}{\partial \varphi}(\Phi_{\sigma,\varepsilon}(\tilde{x}_-)) d\sigma. \end{aligned}$$

We already know that

$$\Phi_{t,\varepsilon}(\tilde{z}) = \Phi_{t,0}(\tilde{z}_0) + O_{\mathbb{C}^1}(\varepsilon), \quad \forall t \in \mathbb{R}.$$

Taking c_2 sufficiently small (but independent of ε) and using Gronwall inequality we have, for $-c_2 |\log \varepsilon| \leq t \leq c_2 |\log \varepsilon|$

$$\Phi_{t,\varepsilon}(\tilde{x}_\pm) = \Phi_{t,0}(\tilde{x}_0) + O_{\mathbb{C}^1}(\varepsilon^{\varrho_1}),$$

for some $\varrho_1 > 0$.

From equation (4.10), we deduce that there exists a constant $c_1 > 0$ such that

$$\left| \int_{\pm c_2 |\log \varepsilon|}^{\pm\infty} \left(\frac{\partial h}{\partial \varphi}(\Phi_{\sigma,\varepsilon}(z)) - \frac{\partial h}{\partial \varphi}(\Phi_{\sigma,\varepsilon}(x_\pm)) \right) d\sigma \right| \leq c_1 e^{-\mu c_2 |\log \varepsilon|/2} = O_{\mathbb{C}^1}(\varepsilon^{\varrho_2}),$$

and, since for the unperturbed system we have the same kind of behavior, we can conclude finally that,

for some $\varrho > 0$

$$\begin{aligned}
& I(\tilde{x}_+) - I(\tilde{x}_-) \\
&= -\varepsilon \int_{-c_2|\log \varepsilon|}^{+c_2|\log \varepsilon|} \left(\frac{\partial h}{\partial \varphi}(q_0(\tau + \sigma), p_0(\tau + \sigma), I, \varphi + I\sigma, s + \sigma) \right. \\
&\quad \left. - \frac{\partial h}{\partial \varphi}(0, 0, I, \varphi + I\sigma, s + \sigma) \right) d\sigma + O_{\mathbb{C}^1}(\varepsilon^{1+\varrho}) \\
&= -\varepsilon \int_{-\infty}^{+\infty} \left(\frac{\partial h}{\partial \varphi}(q_0(\tau + \sigma), p_0(\tau + \sigma), I, \varphi + I\sigma, s + \sigma) \right. \\
&\quad \left. - \frac{\partial h}{\partial \varphi}(0, 0, I, \varphi + I\sigma, s + \sigma) \right) d\sigma + O_{\mathbb{C}^1}(\varepsilon^{1+\varrho}) \\
&= -\varepsilon \int_{-\infty}^{+\infty} \left(\frac{\partial h}{\partial \varphi}(q_0(r), p_0(r), I, \varphi + Ir - I\tau, s + r - \tau) \right. \\
&\quad \left. - \frac{\partial h}{\partial \varphi}(0, 0, I, \varphi + Ir - I\tau, s + r - \tau) \right) dr + O_{\mathbb{C}^1}(\varepsilon^{1+\varrho}) \\
&= -\varepsilon \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi - I\tau, s - \tau) + O_{\mathbb{C}^1}(\varepsilon^{1+\varrho}).
\end{aligned}$$

□

Remark 4.7. Observe that, by the definition of $\tau^*(I, \varphi, s)$, the function $\mathcal{L}(I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s))$ is a solution of the equation

$$I\partial_\varphi f(I, \varphi, s) + \partial_s f(I, \varphi, s) = 0,$$

or, equivalently, there exists a function $\mathcal{L}^*(I, \theta)$, that we will call the *reduced Poincaré function*, defined by

$$\mathcal{L}(I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s)) =: \mathcal{L}^*(I, \varphi - Is). \quad (4.12)$$

Under the assumptions of Proposition 4.2, again by the definition of τ^* , the function $\mathcal{L}^*$ verifies

$$\frac{\partial \mathcal{L}}{\partial x}(I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s)) = \frac{\partial \mathcal{L}^*}{\partial x}(I, \varphi - Is),$$

for $x = I, \varphi, s$.

We can now define the *scattering map* for the perturbed Hamiltonian. Let W be an open set in $[-\frac{1}{2}, I_+^*] \times \mathbb{T}^2$ such that for all $(I, \varphi, s) \in W$ there exists a unique critical point $\tau^* = \tau^*(I, \varphi, s)$ of

$$\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau)$$

in such a way that $(I, \varphi, s) \in W \mapsto \tau^*(I, \varphi, s) \in \mathbb{R}$ is $\mathcal{C}^r$, and therefore

$$\tilde{z} = \tilde{z}(I, \varphi, s; \varepsilon) = (p_0(\tau^*) + O_{\mathcal{C}^r}(\varepsilon), q_0(\tau^*) + O_{\mathcal{C}^r}(\varepsilon), I, \varphi, s) \in W^s(\tilde{\Lambda}_\varepsilon) \cap W^u(\tilde{\Lambda}_\varepsilon).$$

Let $\tilde{\gamma} = \{\tilde{z}(I, \varphi, s; \varepsilon), (I, \varphi, s) \in W\}$. For any $\tilde{z} \in \tilde{\gamma}$ there exist unique $\tilde{x}_\pm \in \tilde{\Lambda}_\varepsilon$ such that $\Phi_{t, \varepsilon}(\tilde{z}) - \Phi_{t, \varepsilon}(\tilde{x}) \xrightarrow[t \pm \infty]{} 0$. Let

$$H_\pm = \bigcup \{\tilde{x}_\pm\} = \bigcup \{\tilde{x}_\pm(I, \varphi, s; \varepsilon), (I, \varphi, s) \in W\}.$$

Then the scattering map associated to the homoclinic manifold $\tilde{\gamma}$ is $S : H_- \mapsto H_+$ such that $S(\tilde{x}_-) = \tilde{x}_+$. By the previous formula applied to $\tilde{z}^u = \tilde{z}^s = \tilde{z} = \tilde{z}(I, \varphi, s; \varepsilon) \in \tilde{\gamma}$,

$$I_+ - I_- := I(\tilde{x}_+) - I(\tilde{x}_-) = \varepsilon \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi - I\tau^*, s - \tau^*) + O_{\mathcal{C}^r}(\varepsilon^{1+\rho}),$$

where $\tau^* = \tau^*(I, \varphi, s)$. Calling, provisionally,

$$L^*(I, \varphi, s) = \mathcal{L}(I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s))$$

we have that

$$I_+ = I_- + \varepsilon \frac{\partial L^*}{\partial \varphi}(I, \varphi, s) + O_{\mathcal{C}^r}(\varepsilon^{1+\rho}).$$

(Notice that $I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi - I\tau^*, s - \tau^*) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi - I\tau^*, s - \tau^*) = 0$.) It is easy to check that if τ^* is a critical point of

$$\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau),$$

then $\tau^* - \sigma$ is a critical point of

$$\tau \mapsto \mathcal{L}(I, \varphi - I\tau - I\sigma, s - \tau - \sigma) = \mathcal{L}(I, \varphi - I(\tau + \sigma), s - (\tau + \sigma))$$

and by uniqueness of $\tau^*(I, \varphi, s)$ in W

$$\tau^*(I, \varphi - I\sigma - I\tau, s - \sigma) = \tau^*(I, \varphi, s) - \sigma$$

and as consequence

$$L^*(I, \varphi - I\sigma, s - \sigma) = L^*(I, \varphi, s) \quad \forall \sigma.$$

In particular, taking $s = \sigma$,

$$L^*(I, \varphi, s) = L^*(I, \varphi - Is, 0) =: \mathcal{L}^*(I, \underbrace{\varphi - Is}_{\theta})$$

so that $L^*(I, \varphi, s)$ depends essentially on two variables: I and $\theta := \varphi - Is$. Therefore, defining the *Poincaré reduced function*

$$\mathcal{L}^* : \left[-\frac{1}{2}, I_+^*\right] \times \mathbb{T} \mapsto \mathbb{R}$$

as

$$\mathcal{L}^*(I, \theta) = L^*(I, \theta, 0) = \mathcal{L}(I, \theta - I\tau^*(I, \theta, 0), -\tau^*(I, \theta, 0))$$

we can write

$$I_+ = I_- + \varepsilon \frac{\partial}{\partial \varphi} \{ \mathcal{L}^*(I, \theta) \} + O(\varepsilon^{1+\rho}),$$

where $\theta = \varphi - Is$. By the form of the Hamiltonian equations: $\dot{s} = 1$, it is clear that $s_+ = s_- = s$. Finally, by the geometric properties of the scattering map described in the next chapter based on [DLS08], S turns out to be an (exact) symplectic map and therefore it satisfies:

$$S(I, \varphi, s) = \left(I + \varepsilon \frac{\partial}{\partial \varphi} \{ \mathcal{L}^*(I, \theta) \} + O_{\mathcal{C}^r}(\varepsilon^{1+\rho}), \varphi - \varepsilon \frac{\partial}{\partial I} \{ \mathcal{L}^*(I, \theta) \} + O_{\mathcal{C}^r}(\varepsilon^{1+\rho}), s \right),$$

where $\theta = \varphi - Is$, that is, except for an $O_{\mathcal{C}^r}(\varepsilon^{1+\rho})$ error, S is the ε -time map of the Hamiltonian- $\mathcal{L}^*(I, \theta)$, where $\theta = \varphi - Is$, and is therefore $\varepsilon - \mathcal{C}^r$ -close to the identity. Note that s is “frozen”, that is, is constant under the scattering map S .

In coordinates $I, \theta = \varphi - Is$, it is to check that the scattering map is

$$S(I, \theta) = \left(I + \varepsilon \frac{\partial \mathcal{L}^*}{\partial \varphi}(I, \theta) + O_{\mathcal{C}^r}(\varepsilon^{1+\rho}), \varphi - \varepsilon \frac{\partial \mathcal{L}^*}{\partial I}(I, \theta) + O_{\mathcal{C}^r}(\varepsilon^{1+\rho}) \right),$$

where it is more apparent the autonomous character of the Hamiltonian - $\mathcal{L}^*(I, \theta)$ and that the iterates under S , up to terms of $O(\varepsilon^{1+\rho})$, satisfy $\mathcal{L}^*(I, \theta) := \text{const.}$; $\mathcal{L}^*(S(I, \theta, s)) = \mathcal{L}^*(I, \theta, s) + O(\varepsilon^2)$.

4.3 Concrete computations for an example

Consider an example taken from [DH11], with $V(q) = \cos q - 1$, the classical pendulum, where

$$p_0(s) = \frac{2}{\cosh s}, \quad q_0(s) = 4 \arctan e^{\pm s}$$

and a perturbation h of the form $h(p, q, I, \varphi, s; \varepsilon) = f(q)g(\varphi, s)$ to make easier the computation of the Melnikov potential. We have the Hamiltonian:

$$H_\varepsilon(p, q, I, \varphi, s) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{I^2}{2} + \varepsilon f(q)g(\varphi, s) \quad (\mathbf{E1})$$

with associated equations:

$$\begin{aligned} \dot{p} &= -\frac{\partial H_\varepsilon}{\partial q} = \pm \sin q - \varepsilon f'(q)g(\varphi, s) & \dot{I} &= -\frac{\partial H_\varepsilon}{\partial \varphi} = -\varepsilon f(q)\frac{\partial g}{\partial \varphi}(\varphi, s) \\ \dot{q} &= \frac{\partial H_\varepsilon}{\partial p} = \pm p & \dot{\varphi} &= \frac{\partial H_\varepsilon}{\partial I} = I & \dot{s} &= 1 \end{aligned}$$

If we choose $f(q)$ such that $f(0) = f'(0) = 0$ (for instance, $f(q) = \cos q - 1$) [Arn64] $\tilde{\Lambda}$ is preserved invariant for all ε ($p = q = 0 \Rightarrow \dot{p} = \dot{q} = 0$) but also $\dot{I} = 0$ on $\tilde{\Lambda}$, i.e., the dynamics inside $\tilde{\Lambda}$ is also preserved $\forall \varepsilon$ (there are no “gaps” in the tori inside $\tilde{\Lambda}$ for rational I) and this is *not* general. We will choose:

$$f(q) = \cos q \quad (\mathbf{E2})$$

because, although $\tilde{\Lambda}$ is preserved $\forall \varepsilon$ ($f'(0) = 0$), its inner dynamics changes ($f(0) = 1 \neq 0$). On the other hand, we will consider a general g given by its Fourier expansion:

$$g(\varphi, s) = \sum_{(k,l) \in \mathbb{N}^2} a_{kl} \cos(k\varphi - ls - \sigma_{kl}) \quad (\mathbf{E3})$$

assumed to be analytic, but with *all the harmonics*:

$$\hat{\alpha} \rho^{\beta k} r^{\beta l} \leq |a_{kl}| \leq \alpha \rho^k r^l, \text{ where } 1 \leq \beta \leq 2, \quad 0 < \hat{\alpha} < \alpha. \quad (\mathbf{E4})$$

The upper bound on $|a_{kl}|$ only expresses the analyticity of g . The lower bound, more artificial and less general, will make appear *all the resonant tori in first order in ε* . We will also assume that $0 < \rho, r < 1$ are small enough to ensure that the harmonics of order 1 in g are dominant:

$$g = \sum_{k+l \leq 1} + \sum_{k+l \geq 2} = \underbrace{g^{[\leq 1]}}_{O_1(\rho, r)} + \underbrace{g^{[\geq 2]}}_{O_2(\rho, r)}$$

and the same will happen in the Melnikov potential $\mathcal{L}$.

Theorem 4.3. *Under conditions (E1) -(E4), assume that*

$$\lambda := \left| \frac{a_{10}}{a_{01}} \right| < \frac{1}{1.6} \text{ or } \lambda > 1.6$$

and that $0 < \rho \leq \rho^$ and $0 < r \leq r^*$ with $\rho^* = \rho^*(\lambda, \alpha, \hat{\alpha}, \beta)$, $r^* = r^*(\lambda, \alpha, \hat{\alpha}, \beta)$ are small enough, then for all $I_+^* > 0$, $\exists \varepsilon = \varepsilon^*(I_+^*) > 0$ such that for any $-\frac{1}{2} < I_- < I_+ \leq I_+^*$ and $0 < \varepsilon < \varepsilon^*$, there exists a trajectory $(p(t), q(t), I(t), \varphi(t))$ of the Hamiltonian H_ε in (E1) such that for some $T > 0$*

$$I(0) \leq I_-, \quad I(T) \geq I_+.$$

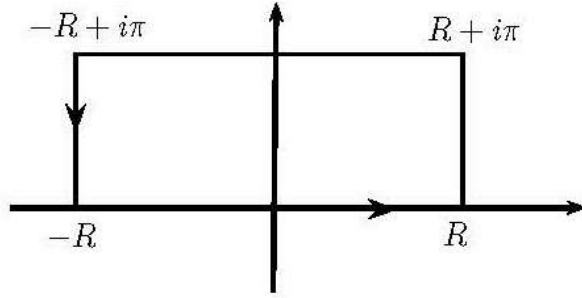
Remark 4.8. Not just any function g in (E3) gives rise to instability. For instance, if $g(\varphi, s) = G(s)$, $\dot{I} = 0$ and therefore $I = \text{const.}$ If $g(\varphi, s) = G(\varphi)$, the Hamiltonian H_ε is autonomous and therefore a first integral. The 2D KAM tori separate the 3D hypersurface $H_\varepsilon = \text{const.}$ and instability is not possible. If $g(\varphi, s) = G(\psi)$, and $\psi = k_0\varphi + l_0t$, a linear combination of φ, t with integer coefficients, a suitable change of coordinates transforms this case to the autonomous case. In all these three cases, $g(\varphi, s)$ has an infinite number of vanishing harmonics.

Computation of the Melnikov potential

Using $\frac{p_0^2}{2} + \cos q_0 - 1 = 0$, $p_0(s) = \frac{2}{\cosh s}$

$$\begin{aligned}
\mathcal{L}(I, \varphi, s) &= - \int_{-\infty}^{\infty} (h(p_0(\sigma), q_0(\sigma), I, \varphi + I\sigma, s + \sigma; 0) - h(0, 0, I, \varphi + I\sigma, s + \sigma; 0)) d\sigma = \\
&= - \int_{-\infty}^{\infty} (\cos q_0(\sigma) - 1) g(\varphi + I\sigma, s + \sigma) d\sigma = \\
&= \frac{1}{2} \int_{-\infty}^{\infty} p_0^2(\sigma) g(\varphi + I\sigma, s + \sigma) d\sigma = \\
&= 2 \sum_{k, l \in \mathbb{N}} a_{kl} \int_{-\infty}^{\infty} \frac{\cos(k\varphi - ls - \sigma_{kl} + (kI - l)\sigma)}{\cosh^2 \sigma} d\sigma = \\
&= \sum_{k, l \in \mathbb{N}} \underbrace{\left(2 \int_{-\infty}^{\infty} \frac{\cos(kI - l)\sigma}{\cosh^2 \sigma} d\sigma a_{kl} \right)}_{A_{kl}(I)} \cos(k\varphi - ls - \sigma_{kl}).
\end{aligned}$$

It is not difficult to compute the integral $J(b) := \int_{-\infty}^{\infty} \frac{\cos b\sigma}{\cosh^2 \sigma} d\sigma = \frac{\pi b}{\sinh \frac{\pi b}{2}}$. Indeed, one can use residues theorem for $\oint_{C_R} \frac{e^{ibz}}{\cosh^2 z} dz$ and the contour of Figure 4.6.

Figure 4.6: Integration contour for $J(b)$

Using the value of the integral above, $A_{kl} = \frac{2\pi(kI - l)}{\sinh(\frac{\pi}{2}(kI - l))} a_{kl}$, and therefore the Melnikov potential has exactly the same non-zero harmonics A_{kl} as the ones a_{kl} of g , modulated by the function $2J(kI - l)$.

To find homoclinic points to the NHIM $\tilde{\Lambda}$, we need to look for the critical points of:

$$\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau) = \sum_{(k, l) \in \mathbb{N}^2} A_{kl}(I) \cos(k\varphi - ls - \tau(kI - l))$$

that is, for any (I, φ, s) , the critical points of $\mathcal{L}$ on the straight line:

$$R(I, \varphi, s) = \{(I, \varphi - I\tau, s - \tau), \tau \in \mathbb{R}\} \text{ with slope } (I, 1) \text{ in } \mathbb{T}^2 = \{(\varphi, s)\},$$

which is simply an unperturbed trajectory in $\tilde{\Lambda}$. To do concrete computations, we write $\mathcal{L} = \mathcal{L}^{[\leq 1]} + \mathcal{L}^{[\geq 2]}$ and we concentrate ourselves on

$\mathcal{L}^{[\geq 2]}$ and we concentrate ourselves on

$$\mathcal{L}^{[\leq 1]}(I, \varphi, s) = A_{00} + A_{10}(I) \cos \varphi + A_{01} \cos s$$

with $A_{00} = 4a_{00}$, $A_{10}(I) = \frac{2\pi I}{\sinh \frac{\pi I}{2}} a_{10}$, $A_{01} = \frac{2\pi}{\sinh \frac{\pi}{2}} a_{01}$, where we have performed a shift in the variables (φ, s) to have $\sigma_{10} = \sigma_{01} = 0$.

If $0 < \rho, r \ll 1$, the computations for $\mathcal{L}^{[\leq 1]}$ will be valid for $\mathcal{L}$.

We recall that

$$\frac{\partial}{\partial \tau} (\mathcal{L}(I, \varphi - I\tau, s - \tau)) = - \left(I \frac{\partial \mathcal{L}}{\partial \varphi} + \frac{\partial \mathcal{L}}{\partial s} \right) (I, \varphi - I\tau, s - \tau).$$

Fixing first I , the points $(\varphi, s) \in \mathbb{T}^2$ for which $\tau^*(I, \varphi, s) = 0$ satisfy

$$I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi, s) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi, s) = 0$$

and form curves in the torus $\{(\varphi, s)\}$ which pass through the extrema of $\mathcal{L}$, which will be called “crests” or “ridges” of equation:

$$IA_{10} \sin \varphi + A_{01} \sin s + O_2(\rho, r) = 0$$

or equivalently :

$$\sin s = -\alpha(I) \sin \varphi + O_2(\rho, r), \text{ with } \alpha(I) = \frac{IA_{10}(I)}{A_{01}} = \frac{I^2 \sinh \frac{\pi}{2} a_{10}}{\sinh \frac{\pi I}{2} a_{01}}.$$

By hypothesis (E4), $a_{10}a_{01} \neq 0$ and therefore $A_{01}A_{10}(I) \neq 0$ for any I . Consequently, for every fixed I , the first order trigonometric polynomial

$$(\varphi, s) \mapsto \mathcal{L}^{[\leq 1]}(I, \varphi, s)$$

possesses in $\mathbb{T}^2$ four non-degenerate critical points at $(0, 0)$, $(0, \pi)$, $(\pi, 0)$ and (π, π) (mod 2π): a maximum, a minimum and two saddle points. Without loss of generality and for illustration purposes we will assume from now on that $a_{10} > 0$ and $a_{01} > 0$, so that $A_{10}(I) > 0$ and $A_{01} > 0$ for any I . In this way the maximum of $\mathcal{L}^{[\leq 1]}(I, \cdot, \cdot)$ is attained at $(0, 0) =: M$, the minimum at $(\pi, \pi) =: m$ and the two saddles at $(\pi, 0) =: s_1$ and $(0, \pi) =: s_2$, all mod 2π (Figure 4.7).

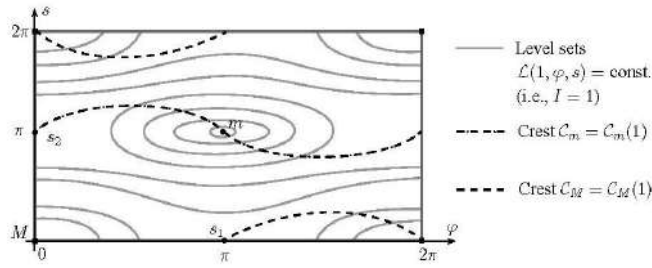


Figure 4.7: Level sets and crests of $\mathcal{L}(1, \cdot, \cdot)$

It is not difficult to check that

$$1.03 \left| \frac{a_{10}}{a_{01}} \right| < 1 \implies |\alpha(I)| < 1 \quad \forall I.$$

$$1.6 \left| \frac{a_{10}}{a_{01}} \right| < 1 \implies \alpha(I)I < 1 \quad \forall I.$$

Therefore, assuming $1.03 \frac{a_{10}}{a_{01}} < 1$ and for ρ, r small enough, there are exactly two crests $\mathcal{C}_M = \mathcal{C}_M(I)$, $\mathcal{C}_m = \mathcal{C}_m(I)$, which are closed curves passing through the maximum $M = (0, 0)$ and the saddle $s_1 = (\pi, 0)$, and the minimum $m = (\pi, \pi)$ and the saddle $s_2 = (0, \pi)$, respectively, and are given by

$$\begin{aligned} \mathcal{C}_M = \mathcal{C}_M(I) : S &= \xi_M(\varphi, I) \pmod{2\pi}, & \xi_M(\varphi, I) &= -\arcsin(\alpha(I) \sin \varphi) + O_2(\rho, r), \\ \mathcal{C}_m = \mathcal{C}_m(I) : S &= \xi_m(\varphi, I) \pmod{2\pi}, & \xi_m(\varphi, I) &= -\arcsin(\alpha(I) \sin \varphi) + \pi + O_2(\rho, r). \end{aligned}$$

Remark 4.9. The case $|\alpha(I)| > 1$ is totally analogous to $|\alpha(I)| < 1$, but exchanging the roles of φ and s .

Fixed $I \in [-\frac{1}{2}, I_+^*]$, the points $(\varphi, s) \in \mathcal{C}_M(I) \cup \mathcal{C}_m(I)$ are the ones which satisfy the equation

$$I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi, s) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi, s) = 0$$

so for them $\tau^*(I, \varphi, s) = 0$ is a critical point of

$$\tau \mapsto \frac{\partial}{\partial \tau} (\mathcal{L}(I, \varphi - I\tau, s - \tau)).$$

For any other point (φ, s) out of the crests $\mathcal{C}_M(I)$, $\mathcal{C}_m(I)$, we want to find critical points $\tau^* = \tau^*(I, \varphi, s)$ of the function above, or equivalently, find a solution τ^* of

$$I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi - I\tau^*, s - \tau^*) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi - I\tau^*, s - \tau^*) = 0$$

which is equivalent to “throw” the straight line $R(I, \varphi, s)$ hoping that it cuts, better transversally, to $\mathcal{C}_M(I)$ or $\mathcal{C}_m(I)$ (Figure 4.8).

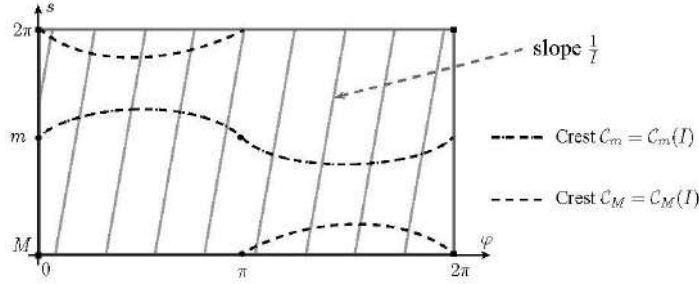


Figure 4.8: Intersection of the lines $R(I, \varphi, s)$ with the crests $\mathcal{C}_M(I)$ and $\mathcal{C}_m(I)$

From now on, we choose only one of these cuts, the “first one” with the crest $\mathcal{C}_M$. The intersection will be transversal if

$$\frac{\partial \xi_M}{\partial \varphi}(\varphi, I) < \frac{1}{I}, \quad \forall \varphi \in \mathbb{T},$$

which is equivalent to $\alpha(I)I < 1$ and is implied by $1.6 \left| \frac{a_{10}}{a_{01}} \right| < 1$. We state this in the following proposition.

Proposition 4.1. *For all $(I, \varphi, s) \in [-\frac{1}{2}, I_+^*] \times \mathbb{T}^2$ the values τ^* for which $\tau \mapsto \mathcal{L}(I, \varphi - I\tau, s - \tau)$ has critical points, are attained at the intersections of the straight line $R(I, \varphi, s)$ with the crests $\mathcal{C}_M(I)$ or $\mathcal{C}_m(I)$, and are non-degenerate if $1.6 \left| \frac{a_{10}}{a_{01}} \right| < 1$ or $1.6 \left| \frac{a_{10}}{a_{01}} \right| > 1$.*

Under this condition, a maximal domain of definition $H = H_M$ containing the crest $\mathcal{C}_M(I)$, where τ^* is continuous, consists of excluding the other crest $\mathcal{C}_m(I)$:

$$H = \left\{ (I, \varphi, s) \in \left[-\frac{1}{2}, I_+^* \right] \times \mathbb{T}^2 : (\varphi, s) \notin \mathcal{C}_m(I) \right\}.$$

The associated scattering map $S : H_\varepsilon \subset H \subset \tilde{\Lambda} \mapsto \tilde{\Lambda}$ is:

$$\tilde{x}_- \mapsto \tilde{x}_+$$

$$S(I, \varphi, s) = \left(I + \varepsilon \frac{\partial}{\partial \varphi}(\mathcal{L}^*(I, \varphi - Is)) + O_{C^r}(\varepsilon^2), \varphi - \varepsilon \frac{\partial}{\partial \varphi}(\mathcal{L}^*(I, \varphi - Is)) + O_{C^r}(\varepsilon^2), s \right)$$

where $\mathcal{L}^*(I, \varphi - Is) = \mathcal{L}^*(I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s))$ or in coordinates $I, \theta = \varphi - Is$,

$$S(I, \theta, s) = \left(I + \varepsilon \frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) + O_{C^r}(\varepsilon^2), \varphi - \varepsilon \frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) + O_{C^r}(\varepsilon^2), s \right)$$

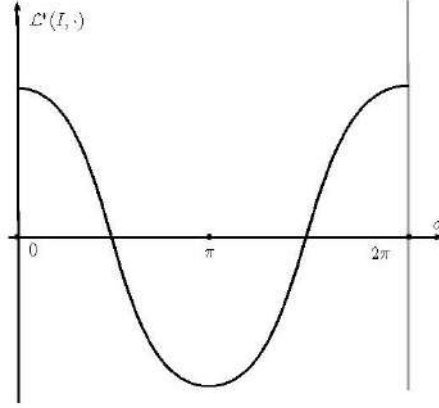
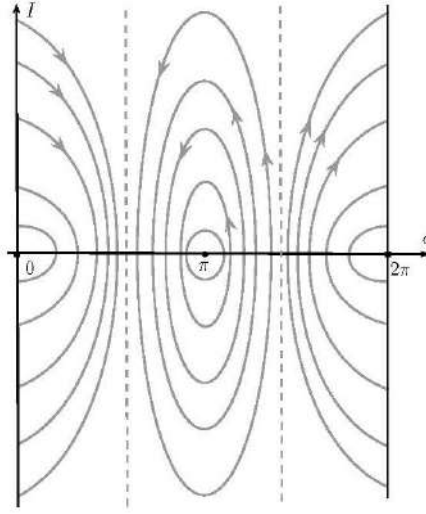
where $\mathcal{L}^*(I, \theta) = \mathcal{L}(I, \theta - I\tau^*(I, \theta, 0), -\tau^*(I, \theta, 0))$. For $I = 0$ ($\varphi = \theta$), $\xi_M(0, \varphi) = 0$ and $\mathcal{L}^*(0, \theta) = A_{00} + A_{10}(0) \cos \theta + A_{01} + O_2(\rho, r)$.

For any $I \in [-\frac{1}{2}, I_+^*]$, one can check that the function $\theta \mapsto \mathcal{L}^*(I, \theta)$ is “cosine-like”: it has a non-degenerate maximum (minimum) close to $\theta = 0 \pmod{2\pi}$ ($\theta = \pi \pmod{2\pi}$), respectively, and is strictly monotone in all the others points θ (Figure 4.9).

A representation of the level curves of $\mathcal{L}^*(I, \theta)$ (for $a_{10} = \frac{1}{4}$ and $a_{01} = \frac{1}{2}$) is Figure 4.10:

The scattering map S , up to order ε^2 , is the ε -time map of the Hamiltonian $-\mathcal{L}^*(I, \theta)$, so the iterates under S satisfy $\mathcal{L}^*(I, \theta) = \text{const.} + O(\varepsilon^2)$.

It has to be noticed that these level sets are very different from the ones corresponding to a family of curves $I = I_0 + O(\varepsilon)$ or even $I = I_0 + O(\sqrt{\varepsilon})$ which are the ones coming from the inner dynamics on $\tilde{\Lambda}$, so there will be transversality between both families, and the diffusion will take place.

Figure 4.9: cosine-like form of $\mathcal{L}^*(I, \cdot)$.Figure 4.10: Level sets of $\mathcal{L}^*$.

4.4 Persistence of the normally hyperbolic invariant manifold and its stable and unstable manifolds

Since the manifold $\tilde{\Lambda}$ is normally hyperbolic, and is locally invariant for the flow (4.4) for $\varepsilon = 0$, by the theory of normally hyperbolic manifolds we have that the manifold persists under small perturbations. Moreover, if the system depends smoothly on parameters, the manifolds—they may be non unique—may be chosen to depend smoothly on parameters.

A formulation of the results of [Fen72, Fen74, Fen77] in the way that we will use them (very similar to the statement of Theorem 4.2 of [DLS00]. See also appendix B of [DLS06b], which contains a detailed proof of an slightly more general result) is:

Theorem 4.4. *Consider a Hamiltonian as in (4.3). Assume that H_ε is uniformly C^r , $r \geq 2$ in all its variables, including ε , in a neighborhood of $\tilde{\Lambda}$ and $\tilde{\gamma}$.*

Then, there exists $\varepsilon^ > 0$ such that for $|\varepsilon| < \varepsilon^*$, there is a C^{r-1} function*

$$\tilde{\mathcal{F}} : \tilde{\Lambda} \times (-\varepsilon^*, \varepsilon^*) \longrightarrow (\mathbb{R} \times \mathbb{T})^2 \times \mathbb{T}$$

such that

$$\tilde{\Lambda}_\varepsilon := \tilde{\mathcal{F}}(\tilde{\Lambda} \times \{\varepsilon\}) \tag{4.13}$$

is locally invariant for the flow (4.4) generated by the vector field $\mathcal{H}_\varepsilon$.

In particular, $\tilde{\Lambda}_\varepsilon$ is ε -close to $\tilde{\Lambda}_0 = \tilde{\Lambda}$ in the C^{r-2} sense.

Moreover, $\tilde{\Lambda}_\varepsilon$ and the vector field $\mathcal{H}_\varepsilon$ can be extended so that it is a normally hyperbolic invariant manifold for the flow (4.4) generated by $\mathcal{H}_\varepsilon$. In particular, it is possible to define local stable and unstable manifolds. That is, we can find a C^{r-1} function $\tilde{\mathcal{F}}^s$ such that the (local) stable manifold of $\tilde{\Lambda}_\varepsilon$ takes the form

$$W_{\tilde{\Lambda}_\varepsilon}^{s,\text{loc}} = \tilde{\mathcal{F}}^s \left(\tilde{\Lambda} \times (0, +\infty) \times \{\varepsilon\} \right). \quad (4.14)$$

If $\tilde{x} = \tilde{\mathcal{F}}(I, \varphi, s; \varepsilon) \in \tilde{\Lambda}_\varepsilon$, then $W_{\tilde{x}}^{s,\text{loc}} = \tilde{\mathcal{F}}^s(\{I\} \times \{\varphi\} \times \{s\} \times (0, \infty) \times \{\varepsilon\})$.

In particular, $W_{\tilde{\Lambda}_\varepsilon}^{s,\text{loc}}$ is ε -close to $W_{\tilde{\Lambda}}^{s,\text{loc}}$ in the C^{r-2} sense.

Analogous results hold for the (local) unstable manifold $W_{\tilde{\Lambda}_\varepsilon}^{u,\text{loc}}$.

The proof of Theorem 4.4 is quite standard in the theory of normally hyperbolic invariant manifolds. It is a straightforward application of the theorems in [Fen74, Fen77, HPS77]. A modern proof is in [Lla00]. A detailed proof tailored for the models considered here is in Appendix B of [DLS06b].

A useful observation is that there is an easy way to obtain smooth dependence on parameters from the standard results on persistence. It suffices to consider the system obtained by taking the product of the original system and the identity in the direction of parameters. The fact that the invariant manifolds for the extended system are regular, gives the fact that the manifolds of the original system depend regularly on parameters.

Note that the coordinates along the unperturbed manifold $\tilde{\Lambda}$ under the unperturbed evolution just rotate or remain invariant. Since $|D\Phi_{t,0}|_{\tilde{\Lambda}}| \leq C|t|$ (see (4.7)), we have that for every $\delta > 0$,

$$|\Phi_{t,0}|_{\tilde{\Lambda}}| \leq C_\delta e^{\delta|t|}.$$

This shows that the tangential exponents along the manifold can be taken as small as we want.

On the other hand, because of assumption **H2**, the point $(p, q) = (0, 0)$ is a hyperbolic point for the pendulum. Since the system (4.4) for $\varepsilon = 0$ is a direct product of rotators—along $\tilde{\Lambda}$ —and a pendulum, the hyperbolic directions of the pendulum become the stable/unstable bundles of the manifold $\tilde{\Lambda}$.

The fact that the tangential exponents are arbitrarily small allows us to conclude that the manifold is as regular as the flow when measured on the C^{r-1} classes, $r \in \mathbb{N}$. (If there was a non-trivial expansion exponent, then the regularity claimed for the manifold would be the infimum of $r - 1$ and a limiting regularity determined by the rates of expansion along the manifold and along the stable/unstable bundles.)

Remark 4.10. In the general theory of the persistence of overflowing locally invariant manifolds, the manifold obtained need not be unique since, in principle, it could depend on some of the choices made in the proof. Nevertheless, when the manifold $\tilde{\Lambda}_\varepsilon$ is invariant and not just locally invariant, it is unique. We will show later that in the manifold $\tilde{\Lambda}_\varepsilon$ there are codimension 1 KAM tori. Therefore we conclude that the portion of $\tilde{\Lambda}_\varepsilon$ between the KAM tori is actually invariant. Hence, for our case, the manifolds will turn out to be unique. Nevertheless, we will not take advantage of this fact since it does not simplify appreciably the proofs and it can fail in more complicated models that can be analyzed by the methods presented here.

Remark 4.11. Note that, as we discuss after Theorem 4.4, the parameterization $\tilde{\mathcal{F}}$ is not uniquely defined even after the locally invariant manifold has been fixed. Indeed, if we compose $\tilde{\mathcal{F}}$ with any diffeomorphism of $\tilde{\Lambda}$ on the right we obtain a different parameterization.

We can make the parameterization unique by imposing that $\tilde{\mathcal{F}}$ does not change the (I, φ, s) coordinates:

$$\Pi_I \tilde{\mathcal{F}}(I, \varphi, s; \varepsilon) = I, \quad \Pi_\varphi \tilde{\mathcal{F}}(I, \varphi, s; \varepsilon) = \varphi, \quad \Pi_s \tilde{\mathcal{F}}(I, \varphi, s; \varepsilon) = s. \quad (4.15)$$

This can be expressed as saying that we write $\tilde{\Lambda}_\varepsilon$ as the graph of a function from $\tilde{\Lambda}$ into the (p, q) plane.

This normalization will be important for us when we compute the map $\tilde{\mathcal{F}}$ in coordinates.

Remark 4.12. We recall that the precise definition of the stable manifolds in normal hyperbolicity theory is that they consist on the points that, under the evolution of the extended system, converge to the invariant manifold with an exponential rate close to that of the original system. It follows from the exponential convergence that $W_{\tilde{\Lambda}_\varepsilon}^s = \bigcup_{\tilde{x} \in \tilde{\Lambda}_\varepsilon} W_{\tilde{x}}^s$ where

$$W_{\tilde{x}}^s = \{\tilde{y} : \text{dist}(\Phi_{t,\varepsilon}(\tilde{x}), \Phi_{t,\varepsilon}(\tilde{y})) \leq C e^{-\tilde{\mu}t}, t > 0\},$$

where $\tilde{\mu} = \mu + O(\varepsilon)$. Moreover $W_{\tilde{x}}^s \cap W_{\tilde{y}}^s = \emptyset$ when $\tilde{x} \neq \tilde{y}$, $\tilde{x}, \tilde{y} \in \tilde{\Lambda}_\varepsilon$. The stable manifolds of the points are as smooth as the flow (when smoothness is measured in the class of C^r spaces $r \in \mathbb{N} \cup \{\infty, \omega\}$).

Nevertheless, the map $\tilde{x} \mapsto W_{\tilde{x}}^s$ could be less regular than the flow, and therefore, the total manifold $W_{\tilde{\Lambda}_\varepsilon}^s = \cup_{\tilde{x} \in \tilde{\Lambda}_\varepsilon} W_{\tilde{x}}^s$ could, in general, be less smooth than the flow. In our case, however, since the tangent exponents are arbitrarily small, if the flow is C^{r-1} , $r-1 \in \mathbb{N}$, then the resulting $W_{\tilde{\Lambda}_\varepsilon}^s$ will be C^{r-1} for small ε .

Analogous results hold for the unstable manifold.

Note that the definition of the (un)stable manifolds for locally invariant manifolds can only be made in an extended system constructed in the proof for which the dynamics is defined for all times. In general, these (un)stable manifolds depend on the extended flow used.

One consequence of that is that $\tilde{\Lambda}_\varepsilon$, $W_{\tilde{\Lambda}_\varepsilon}^s$ may fail to be C^∞ even if the flow is analytic. Nevertheless, when the manifolds are invariant, the stable and unstable manifolds are uniquely defined. In our case, as stated in Remark 4.10, the KAM tori will produce invariant boundaries for $\tilde{\Lambda}_\varepsilon$, hence stable and unstable manifolds will be uniquely defined. The proofs we present, however, do not take advantage of this fact.

4.5 Explicit calculations of the perturbed invariant manifold

In the rest of this section, we will compute rather explicitly the expansions in ε of the map $\tilde{\mathcal{F}}$ for the Hamiltonian (4.3).

We note that the equation that $\tilde{\mathcal{F}}$ has to satisfy so that its range is invariant by the vector field $\mathcal{H}_\varepsilon$ given in (4.4) is

$$\mathcal{H}_\varepsilon \circ \tilde{\mathcal{F}} = D\tilde{\mathcal{F}} \mathbb{R} \quad (4.16)$$

where $\mathbb{R}$ is a vector field in $\tilde{\Lambda}_\varepsilon$. Note that (4.16) expresses that the vector field $\mathcal{H}_\varepsilon$ at a point in the range is tangent to the range of $\tilde{\mathcal{F}}$.

Using equation (4.16) one can find an expansion of the function $\tilde{\mathcal{F}}$.

Proposition 4.5. *The family of mappings $\tilde{\mathcal{F}}$ specified in Theorem 4.4 with the normalization (4.15) admits an expansion*

$$\tilde{\mathcal{F}} = \tilde{\mathcal{F}}_0 + \varepsilon \tilde{\mathcal{F}}_1 + \cdots + \varepsilon^m \tilde{\mathcal{F}}_m + O_{C^{r-m-2}}(\varepsilon^{m+1}),$$

where $\tilde{\mathcal{F}}_0(I, \varphi, s) = (0, 0, I, \varphi, s)$.

In the case that the flow satisfies assumptions **H1–H3**, then the functions $\tilde{\mathcal{F}}_1, \dots, \tilde{\mathcal{F}}_m$ are trigonometric polynomials in φ, s , and $\tilde{\mathcal{F}}_i$ are of class C^{r-1-i} . Moreover, in such a case, $\mathbb{N}(\tilde{\mathcal{F}}_1) \subset \mathbb{N}(h_1)$, $\mathbb{N}(\tilde{\mathcal{F}}_2) \subset (\mathbb{N}(h_1) + \mathbb{N}(h_1)) \cup \mathbb{N}(h_2)$.

Proof. Once we impose normalization (4.15) to $\tilde{\mathcal{F}}$, we can compute $\tilde{\mathcal{F}}_i$ by matching powers of ε in the equation (4.16). We know by Theorem 4.4 that the expansion exists.

Equating terms in the expansion on ε of the equation for invariance (4.16) we obtain, up to order two:

$$\begin{aligned} \mathcal{H}_0 \circ \tilde{\mathcal{F}}_0 &= D\tilde{\mathcal{F}}_0 \mathbb{R}_0 \\ (D\mathcal{H}_0 \circ \tilde{\mathcal{F}}_0) \tilde{\mathcal{F}}_1 + \mathcal{H}_1 \circ \tilde{\mathcal{F}}_0 &= D\tilde{\mathcal{F}}_0 \mathbb{R}_1 + D\tilde{\mathcal{F}}_1 \mathbb{R}_0 \\ (D\mathcal{H}_0 \circ \tilde{\mathcal{F}}_0) \tilde{\mathcal{F}}_2 + \frac{1}{2} (D^2 \mathcal{H}_0 \circ \tilde{\mathcal{F}}_0) \tilde{\mathcal{F}}_1^{\otimes 2} + (D\mathcal{H}_1 \circ \tilde{\mathcal{F}}_0) \tilde{\mathcal{F}}_1 + \mathcal{H}_2 \circ \tilde{\mathcal{F}}_0 &= D\tilde{\mathcal{F}}_0 \mathbb{R}_2 + D\tilde{\mathcal{F}}_1 \mathbb{R}_1 + D\tilde{\mathcal{F}}_2 \mathbb{R}_0. \end{aligned} \quad (4.17)$$

In general, the equation obtained after matching the coefficients of ε^n on both sides of (4.16), is of the form:

$$(D\mathcal{H}_0 \circ \tilde{\mathcal{F}}_0) \tilde{\mathcal{F}}_n - D\tilde{\mathcal{F}}_n \mathbb{R}_0 - D\tilde{\mathcal{F}}_0 \mathbb{R}_n = -\mathcal{H}_n \circ \tilde{\mathcal{F}}_0 + \mathcal{S}_n \quad (4.18)$$

where $\mathcal{S}_n$ is polynomial in $\mathcal{H}_0, \dots, \mathcal{H}_{n-1}$, their derivatives, $\tilde{\mathcal{F}}_0, \dots, \tilde{\mathcal{F}}_{n-1}$, and $\mathbb{R}_0, \dots, \mathbb{R}_{n-1}$.

Clearly, the first equation in (4.17) has as solution $\tilde{\mathcal{F}}_0 = (0, 0, I, \varphi, s)$, and $\mathbb{R}_0 = (0, I, 1)$. Therefore, if one can develop a method to solve equations for $\tilde{\mathcal{F}}_n, \mathbb{R}_n$ of the form of the linear Hamiltonian System (4.18) equal to a preassigned right hand side, we can keep on solving the hierarchy of equations (4.18) to any order.

In our case, since the unperturbed motion due to $\mathbb{R}_0$ is quasi-periodic, the equations of the form (4.18) can be solved quite explicitly using Fourier coefficients. (There are more general theories [Lla00] that allow to solve equations of the form (4.18) even if the motion on the base is not quasi-periodic.)

The theory of the equations that we need is summarized in the following Lemma 4.6. Clearly, applying it recursively, we obtain a proof of Proposition 4.5. $\square$

Lemma 4.6. *Let $\tilde{\mathcal{F}}_0, \mathcal{H}_0, \mathbb{R}_0$ be as in Proposition 4.5. Given a C^s function, $s \geq 1$, $\eta : \tilde{\Lambda} \rightarrow \mathbb{R}^5$, we can find unique C^1 functions $\xi, \rho : \tilde{\Lambda} \rightarrow \mathbb{R}^5$ such that*

$$(D\mathcal{H}_0 \circ \tilde{\mathcal{F}}_0)\xi - D\xi\mathbb{R}_0 - D\tilde{\mathcal{F}}_0\rho = \eta \quad (4.19)$$

and

$$\Pi_I \xi = 0, \quad \Pi_\varphi \xi = 0, \quad \Pi_s \xi = 0. \quad (4.20)$$

Furthermore, ξ, ρ are of class C^s and we have, for a constant C that depends only on $\mathcal{H}_0, \mathbb{R}_0$,

$$\begin{aligned} |\xi|_{C^s} &\leq C |\eta|_{C^s} \\ |\rho|_{C^s} &\leq C |\eta|_{C^s}. \end{aligned}$$

Moreover, if η is a trigonometric polynomial, so are ξ and ρ , and we have $\mathbb{N}(\xi) \subset \mathbb{N}(\eta)$, $\mathbb{N}(\rho) \subset \mathbb{N}(\eta)$.

Proof. Note that the unperturbed flow and its differential at $\tilde{\Lambda}$ preserve the I, φ, s directions. The plane p, q is invariant.

Moreover, $D\tilde{\mathcal{F}}_0$ in the coordinates we are using is a 5×3 matrix. It consists of a 3×3 identity along the I, φ, s directions and 0 along the other directions (p, q) .

The two observations above, immediately give us that we can satisfy the normalization (4.20) in a unique way by setting:

$$\rho = \Pi_{I, \varphi, s} \eta \quad (4.21)$$

from which the regularity claims about ρ follow.

Using again the invariance of the (p, q) plane it suffices to study the equation

$$(D\mathcal{H}_0 \circ \tilde{\mathcal{F}}_0)|_{p, q} \Pi_{p, q} \xi - D\Pi_{p, q} \xi \mathbb{R}_0 = \Pi_{p, q} \eta \quad (4.22)$$

This equation (4.22) can be further reduced by noticing that $D\mathcal{H}_0$ preserves the two eigendirections of the equilibrium point of the pendulum. Hence, if we denote by Π^s, Π^u , the projections along the stable and the unstable components and by μ the eigenvalue, we obtain that (4.22) is equivalent to:

$$\begin{aligned} \mu \Pi^u \xi - D\Pi^u \xi \mathbb{R}_0 &= \Pi^u \eta \\ -\mu \Pi^s \xi - D\Pi^s \xi \mathbb{R}_0 &= \Pi^s \eta \end{aligned} \quad (4.23)$$

The equations (4.23) can be studied easily. For example, they can be studied noting that the operator on the linear Hamiltonian system of (4.23) is diagonal on Fourier series. Hence, if

$$\Pi^s \eta(I, \varphi, s) = \sum_{(k, l) \in \mathbb{N}(\eta)} \hat{\eta}_{k, l}(I) e^{i(k\varphi + ls)},$$

the solution of (4.23) is:

$$\Pi^s \xi(I, \varphi, s) = \sum_{(k, l) \in \mathbb{N}(\eta)} \hat{\eta}_{k, l}(I) [-\mu + i(kI + l)]^{-1} e^{i(k\varphi + ls)} \quad (4.24)$$

and analogously (with $+\mu$ in place of $-\mu$) for $\Pi^u \xi$.

Note that, since $\pm\mu \neq 0$, there are no small denominators in the finite sum (4.24). Then, one can bound the norm of ξ by the norm of η . This finishes the proof of Lemma 4.6. $\square$

Remark 4.13. Even if for us, the solution (4.24) is useful because it gives the Fourier coefficients that will later be the base of the study of resonances, we note that, in geometric perturbation theory, it is common to represent the solution as integral formulas.

For example, in our case, we have:

$$\Pi^s \xi(I, \varphi, s) = \int_0^\infty \eta(I, \varphi - It, s - t) e^{-\mu t} dt$$

Out of the preceding formula, it is easy to read off the regularity properties even in the case that η is not a polynomial.

Chapter 5

Geometric properties of the Scattering map

5.1 Introduction

As we have seen in the previous chapters, a remarkable tool introduced in [DLS00] to study the problem of Arnold diffusion was the scattering map of a normally hyperbolic invariant manifold with intersecting stable and unstable invariant manifolds along a homoclinic manifold. (The paper [Gar00] introduced the *homoclinic map* to a center manifold.)

The use of the scattering map was crucial for the applications in [DLS03, DLS06a, GL06]. In those papers, it was shown that the perturbative computations of the scattering map are a convenient improvement of the Melnikov method since they are geometrically natural. In this chapter, we aim to present a much more systematic development of the perturbative formulas. We note that:

- The perturbative formulas are given by improper integrals which converge uniformly (indeed exponentially fast).
- Most of the calculations are done in a geometrically natural form. Hence, there is no need of assuming that our objects admit a good coordinate system and one can use the method to discuss the existence of heteroclinic intersections among objects of different topological types. This advantage was crucial for [DLS03, DLS06a].
- As we will detail, it is possible to compute the perturbative expansions of the effect of the intersections on some fast variables.

The scattering map relates the past asymptotic trajectory of any orbit in the homoclinic manifold to its future asymptotic behavior. Related ingredients like the phase shift and the scattering phase shift already appear in [CG94, pp. 17, 68] and related ideas in [MP94]. The scattering map is extremely similar to the scattering matrix in quantum mechanics [New02, RS79]. Indeed, we have followed a notation that matches the definitions in quantum mechanics. For a comparison with the quantum mechanics scattering theory see Appendix 5.7.

The first goal of this chapter is to provide a more global definition of the scattering map (in [DLS00, DLS03, DLS08] it was only defined perturbatively) that applies to normally hyperbolic invariant manifolds for which appropriate transversality conditions are met.

More importantly, we will show that, under very general circumstances, the scattering map of a normally hyperbolic invariant manifold inherits the geometric properties of the dynamical system. That is, under transversality properties, if the map is (exact) symplectic then the scattering map is (exact) symplectic. (See Theorem 5.4 for a precise formulation.) These geometric properties allow us to obtain very compact perturbative formulas and several global topological consequences.

The more general definition of the scattering map as well as some elementary properties is considered in Section 5.2. First we introduce the wave operators

$$\begin{aligned}\Omega_{\pm} : W_{\Lambda}^{s,u} &\longrightarrow \Lambda \\ x &\mapsto x_{\pm}\end{aligned}$$

which assign to each point x in the stable (or unstable) manifold, the unique point x_+ (or x_-) in Λ with the same asymptotic trajectory in the future (or in the past).

In the case that the invariant manifolds $W_\Lambda^{s,u}$ intersect transversally and that the intersection is transversal to the unstable foliation, one can choose an “homoclinic channel” Γ where both wave operators are well defined diffeomorphisms with their images (see Definition 5.2).

For such homoclinic channel Γ the scattering map is defined as

$$\sigma = \sigma^\Gamma = \Omega_+ \circ (\Omega_-^\Gamma)^{-1} : \Omega_-(\Gamma) \longrightarrow \Omega_+(\Gamma).$$

The goal of this chapter is to describe the geometric and regularity properties of this map. This will lead to very efficient perturbation theories. Notice that the scattering map as well as the inverse of the wave operators depend on the homoclinic channel Γ chosen. The same happens with its domain and image that, in general, are strict subsets of Λ . Nevertheless we will suppress Γ from the notation unless it causes confusion. The end of Section 5.2 is devoted to adapt the definitions of scattering map to autonomous and non-autonomous flows. Particular attention will be paid to non-autonomous perturbations of autonomous flows.

In Section 5.3 we prove that the scattering map is (exact) symplectic provided that the map f and the normally hyperbolic invariant manifold Λ are (exact) symplectic. Some of these results were also established in [Gar00] by other methods.

The main tool for the proof of the symplectic properties is a result about the geometric properties of holonomy maps on stable manifolds (see Lemma 5.5) which may be of independent interest. For simplicity of presentation, we will just discuss the case of maps. Analogous formulations for flows of the results can be obtained by considering time one-maps.

In the case that the map is exact, in Section 5.3.4 we show that there is a very compact formula (5.28) for the *primitive function* of the scattering map. The formula (5.28) gives the primitive function of the scattering map as a uniformly (indeed exponentially) convergent sum along the connecting orbits. The proof is coordinate independent.

The goal of sections 5.4 and 5.5 is to develop perturbative formulas for the scattering map. In Section 5.4 the general set up for deformation theory of symplectic families of maps is introduced. A perturbation theory for normally hyperbolic invariant manifolds of these families is also presented.

With all these ingredients, Section 5.5 is devoted to obtaining perturbative formulas for the Hamiltonian generating the deformation of the scattering map for a family of symplectic maps. An analogous formula is obtained for Hamiltonian flows.

We note that the perturbative formulas obtained are given in terms of absolutely (indeed exponentially) convergent integrals and that they have a geometric character. We will show that these perturbative formulas can be used to establish the existence of heteroclinic intersections between invariant objects. The fact that they are geometrically natural allows to establish the existence and compute intersections for objects that have different topological types and hence, cannot be fit into a common system of coordinates. These perturbative formulas generalize and unify many of the calculations that are usually done using Melnikov theory.

Finally, in Section 5.6, we apply the perturbative formula of the scattering map in the case of quasiperiodically perturbed geodesic flows already considered in [DLS06b]. In particular, we show that for geodesic flows the scattering map is globally defined in Λ , nevertheless, for the perturbations, there are considerations of domains and monodromy. Even if these considerations were already presented in [DLS00], the global theory of this chapter allows to discuss them more fully. We show that the calculations obtained by the formalism in this chapter agree with the calculations in [DLS00, DLS06a]. The calculations in [DLS00, DLS06a] were done using the fact that some of the variables are slow and that there is a standard perturbation theory for systems with fast-slow variables. The fast-slow methods obtain information on the slow variables components of the scattering map, but are unable to obtain any information on the fast variables components on the scattering map. The geometric methods presented in this chapter, obtain at the same time information of the scattering map both for fast and for slow variables.

5.2 General theory of the scattering map

We will start by recalling some definitions and results from the theory of normally hyperbolic invariant manifolds. The definition of the scattering map of a normally hyperbolic invariant manifold will be introduced in Section 5.2.2. We will show that, as a consequence of the standard theory of normally hyperbolic invariant manifolds, the scattering map is smooth and depends smoothly on parameters.

5.2.1 Notation and known results from the theory of normally hyperbolic invariant manifolds

Standard references on the theory of normally hyperbolic invariant manifolds are [HP70, HPS77, Fen72, Fen74, Pes04, Wig94]. The proofs of all the facts mentioned in this section can be found in these references. Hence, the purpose of this section is just easy reference and setting notation.

Let M be a smooth m -dimensional manifold, $f : M \rightarrow M$ a C^r diffeomorphism, $r \geq 1$.

Definition 5.1. Let $\Lambda \subset M$ be a submanifold invariant under f , $f(\Lambda) = \Lambda$. We say that Λ is a normally hyperbolic invariant manifold if there exist a constant $C > 0$, rates $0 < \lambda < \mu^{-1} < 1$ and a splitting for every $x \in \Lambda$

$$T_x M = E_x^s \oplus E_x^u \oplus T_x \Lambda$$

in such a way that

$$\begin{aligned} v \in E_x^s &\Leftrightarrow |Df^n(x)v| \leq C\lambda^n |v| & n \geq 0 \\ v \in E_x^u &\Leftrightarrow |Df^n(x)v| \leq C\lambda^{|n|} |v| & n \leq 0 \\ v \in T_x \Lambda &\Leftrightarrow |Df^n(x)v| \leq C\mu^{|n|} |v| & n \in \mathbb{Z} \end{aligned} \quad (5.1)$$

We will assume that Λ is compact or that f is uniformly C^r in a neighborhood of Λ . We will also assume without loss of generality that Λ is connected. In the case that Λ is not compact, one has to pay attention to the properties of the map f in a neighborhood of Λ and work out issues such as regularity of extensions, etc.

It follows from (5.1) that E_x^s, E_x^u depend continuously on x . In particular, the dimension of E_x^s, E_x^u is independent of x . In fact, these splittings are $C^{\ell-1}$ with ℓ being any number such that

$$\ell < \min \left(r, \frac{|\log \lambda|}{\log \mu} \right). \quad (5.2)$$

We recall that it is possible to introduce a smooth metric (the adapted metric) in M in such a way that $C = 1$ in (5.1) at the only price of redefining slightly λ, μ .

Given a normally hyperbolic invariant manifold Λ we define

$$\begin{aligned} W_\Lambda^s &= \{y \in M \mid d(f^n(y), \Lambda) \leq C_y \lambda^n, n \geq 0\} \\ W_\Lambda^u &= \{y \in M \mid d(f^n(y), \Lambda) \leq C_y \lambda^{|n|}, n \leq 0\} \end{aligned}$$

Furthermore, for each $x \in \Lambda$, we define

$$\begin{aligned} W_x^s &= \{y \in M \mid d(f^n(x), f^n(y)) \leq C_{x,y} \lambda^n, n \geq 0\} \\ W_x^u &= \{y \in M \mid d(f^n(x), f^n(y)) \leq C_{x,y} \lambda^{|n|}, n \leq 0\} \end{aligned}$$

and we note that $E_x^s = T_x W_x^s$ and $E_x^u = T_x W_x^u$. It is a fact that

$$\begin{aligned} W_\Lambda^s &= \bigcup_{x \in \Lambda} W_x^s \\ W_\Lambda^u &= \bigcup_{x \in \Lambda} W_x^u \end{aligned} \quad (5.3)$$

Moreover, $x \neq \tilde{x} \Rightarrow W_x^s \cap W_{\tilde{x}}^s = \emptyset, W_x^u \cap W_{\tilde{x}}^u = \emptyset$.

The decomposition (5.3) can be expressed as saying that $\{W_x^s\}_{x \in \Lambda}, \{W_x^u\}_{x \in \Lambda}$ give a foliation of W_Λ^s, W_Λ^u , respectively.

We recall that in these circumstances we have that

1. Λ is a C^ℓ manifold with ℓ given in (5.2).
2. W_Λ^s, W_Λ^u are $C^{\ell-1}$ manifolds
3. W_x^s, W_x^u are C^r manifolds
4. The maps $x \mapsto W_x^s, W_x^u$ are $C^{\ell-1-j}$, when W_x^s, W_x^u are given the C^j topologies.

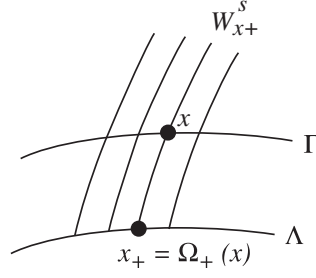


Figure 5.1

Note, in particular, that there are limitations for the regularity of the manifolds besides the regularity of the map which depend on the ratios of the exponents $|\log \lambda|$ and $\log \mu$. These obstructions are sharp in the sense that, for typical maps, the foliations W_Λ^s, W_Λ^u do not have any more regularity than that claimed above.

Note that the leaves of the foliation $\{W_x^s\}_{x \in \Lambda}$ of W_Λ^s are as smooth as the map. Nevertheless, the dependence of these leaves on the point x can be considerably less smooth than the map. This is the reason why the regularity of W_Λ^s is limited by ratios of exponents.

Note that the definition of normal hyperbolicity implies that $\ell \geq 1$, but in this chapter we assume $\ell \geq 2$ in order to have W_Λ^s, W_Λ^u C^1 manifolds. This is important because we will use the implicit function theorem for $C^{\ell-1}$ regular objects.

For a point $x \in W_\Lambda^s$ (resp. $x \in W_\Lambda^u$), we denote by x_+ (resp. x_-) the point in Λ which satisfies $x \in W_{x_+}^s$ (resp. $x \in W_{x_-}^u$).

Note that given a point x , the points x_+, x_- are uniquely defined. Moreover, denoting

$$\begin{aligned} \Omega_\pm : W_\Lambda^{s,u} &\longrightarrow \Lambda \\ x &\mapsto x_\pm, \end{aligned} \quad (5.4)$$

these maps, that we call *wave operators*, are well defined and of class C^ℓ . We note that, with the standing assumptions of this chapter, these maps are always C^1 .

5.2.2 Scattering map of a normally hyperbolic invariant manifold

Now, we turn to the task of defining a scattering map associated to a transversal intersection of W_Λ^s, W_Λ^u .

More precisely, we will assume that there is a normally hyperbolic invariant manifold Λ and a homoclinic manifold $\Gamma \subset W_\Lambda^s \cap W_\Lambda^u$ such that $\forall x \in \Gamma$:

$$\begin{aligned} T_x M &= T_x W_\Lambda^s + T_x W_\Lambda^u \\ T_x W_\Lambda^s \cap T_x W_\Lambda^u &= T_x \Gamma \end{aligned} \quad (5.5)$$

We will refer to (5.5) by saying that the intersection of W_Λ^s and W_Λ^u is transversal along Γ .

If M is m -dimensional, Λ is c -dimensional and the dimensions of E_x^s, E_x^u are d_s, d_u then W_x^s, W_x^u are d_s, d_u -dimensional, W_Λ^s, W_Λ^u are $d_s + c, d_u + c$ -dimensional, respectively. Because of Definition 5.1, we have that $m = c + d_s + d_u$ and therefore, by (5.5), the dimension of Γ has to be $(c + d_s + c + d_u) - m = c$.

The definition of the scattering map requires that the intersection Γ satisfying (5.5) satisfies also that for every point $x \in \Gamma$ we have

$$\begin{aligned} T_x \Gamma \oplus T_x W_{x_+}^s &= T_x W_\Lambda^s \\ T_x \Gamma \oplus T_x W_{x_-}^u &= T_x W_\Lambda^u \end{aligned} \quad (5.6)$$

We will refer to (5.6) by saying that Γ is transversal to the W_x^s, W_x^u foliation. Note that to define (5.6) we assume (5.5). We also call attention that (5.6) is used to define the scattering map locally. This local definition could have some monodromy if extended to domains with non-contractible loops. In Section 5.6.1, we will discuss these phenomenon of monodromy making more geometric the discussion in [DLS00].

Because of the persistence under perturbations of normally hyperbolic invariant manifolds and their stable/unstable manifolds and the transversal intersections between them, we note that if the assumption

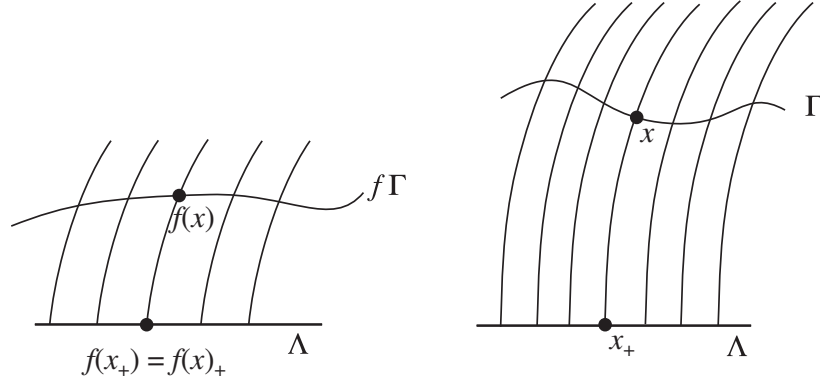


Figure 5.2

(5.5) is satisfied for a map f and manifolds Λ , Γ , then it is also satisfied for any map $\tilde{f}$ in a C^1 neighborhood and for some manifolds $\tilde{\Lambda}$, $\tilde{\Gamma}$. Similarly, we note that the condition $\ell > 2$ holds in some C^1 open sets of maps. For these maps, we can apply the implicit function theorem to conclude that (5.6) holds in C^1 open sets.

Remark 5.1. By the implicit function theorem, if for some $x^* \in W_\Lambda^s \cap W_\Lambda^u$ it is verified that $T_{x^*} W_\Lambda^s \cap T_{x^*} W_\Lambda^u$ is c -dimensional, we can find a locally unique manifold Γ such that

$$T_{x^*} \Gamma = T_{x^*} W_\Lambda^s \cap T_{x^*} W_\Lambda^u$$

Moreover, this Γ is $C^{\ell-1}$.

Also by the implicit function theorem, if the transversality condition (5.6) is satisfied for certain x^* in a manifold Γ , then it is satisfied by all $x \in \Gamma$ close enough to x^* .

Given a manifold Γ verifying (5.5), we can consider the wave operators $\Omega_\pm$ of (5.4) restricted to Γ . Under assumption (5.6) we have that $\Omega_\pm$ are local diffeomorphisms from Γ to Λ .

Definition 5.2. We say that Γ is a homoclinic channel if:

1. $\Gamma \subset W_\Lambda^s \cap W_\Lambda^u$ verifies (5.5) and (5.6).
2. The wave operators $(\Omega_\pm)|_\Gamma : \Gamma \longrightarrow \Omega_\pm(\Gamma) \subset \Lambda$ are $C^{\ell-1}$ diffeomorphisms.

Restricting Γ if necessary, from now on we will only consider $\Gamma \subset W_\Lambda^s \cap W_\Lambda^u$ such it verifies Definition 5.2 and then it is a homoclinic channel.

We denote by $\Omega_\pm^\Gamma = \Omega_\pm|_\Gamma$, and $H_\pm^\Gamma = \Omega_\pm^\Gamma(\Gamma) \subset \Lambda$, so that

$$\Omega_\pm^\Gamma : \Gamma \longrightarrow H_\pm^\Gamma$$

are $C^{\ell-1}$ diffeomorphisms. Note that if Γ is a homoclinic channel, so is $f^n(\Gamma)$ for any $n \in \mathbb{Z}$.

Remark 5.2. Using the fact that the foliation W_x^s satisfies $f(W_x^s) = W_{f(x)}^s$, and that, therefore, $f(x)_+ = f(x_+)$, we have (see Figure 5.2)

$$\Omega_+^\Gamma = f^{-1} \circ \Omega_+^{f(\Gamma)} \circ f, \quad (5.7)$$

and analogously

$$\Omega_-^\Gamma = f \circ \Omega_-^{f^{-1}(\Gamma)} \circ f^{-1}. \quad (5.8)$$

Iterating these formulas, we have for every $n \in \mathbb{Z}$,

$$\begin{aligned} \Omega_+^\Gamma &= f^{-n} \circ \Omega_+^{f^n(\Gamma)} \circ f^n, \\ \Omega_-^\Gamma &= f^n \circ \Omega_-^{f^{-n}(\Gamma)} \circ f^{-n}. \end{aligned} \quad (5.9)$$

Definition 5.3. Given a homoclinic channel Γ and $\Omega_\pm^\Gamma : \Gamma \rightarrow H_\pm^\Gamma$ the associated wave operators, we define the scattering map associated to Γ

$$\sigma^\Gamma : H_-^\Gamma \rightarrow H_+^\Gamma$$

by

$$\sigma^\Gamma = \Omega_+^\Gamma \circ (\Omega_-^\Gamma)^{-1} \quad (5.10)$$

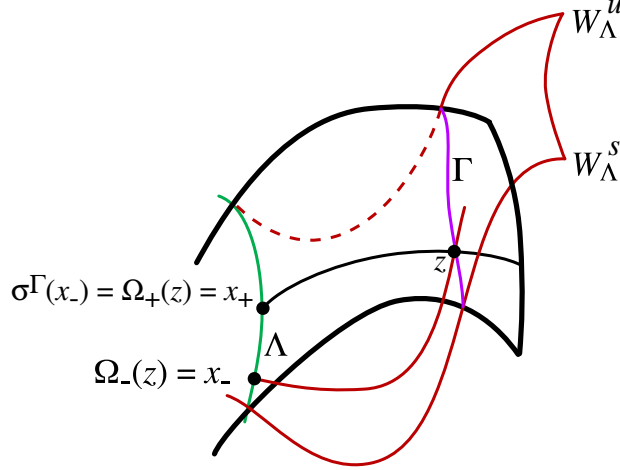


Figure 5.3: Illustration of Definition 5.3 of the scattering map.

5.2.3 Some elementary properties of the scattering map

Regularity properties

We note that, because of the implicit function theorem, the homoclinic channel Γ is as differentiable as the invariant manifolds W_Λ^s, W_Λ^u , that is $C^{\ell-1}$, where ℓ is given in (5.2).

Later, we will consider a family of mappings f_ε which are jointly C^r in all the variables and in the parameter ε . We will show that the scattering map depends on the parameter in a $C^{\ell-j}$ way when we give the maps the C^j topology in a compact neighborhood.

Invariance properties

It is clear from its definition that the scattering map depends on the homoclinic channel considered.

- We note that if Γ satisfies Definition 5.2, so does $f(\Gamma)$ and we can define a scattering map corresponding to $f(\Gamma)$. Using that $f(W_x^{s,u}) = W_{f(x)}^{s,u}$, equalities (5.7) and (5.8) and the Definition 5.3 of the scattering map, we easily obtain:

$$f \circ \sigma^\Gamma = \sigma^{f(\Gamma)} \circ f \quad (5.11)$$

Moreover, iterating f and using (5.9), we have:

$$\sigma^{f^n(\Gamma)} = f^n \circ \sigma^\Gamma \circ f^{-n}. \quad (5.12)$$

We call attention to the fact that in (5.11) and (5.12) the scattering map on both sides is not the same.

- If we exchange the map f by f^{-1} , the manifold Λ is still a normally hyperbolic invariant manifold under f^{-1} . On the other hand, the stable and unstable manifolds are exchanged. Hence, if Γ is an homoclinic channel verifying Definition 5.2 for the $W_\Lambda^{s,(f)}, W_\Lambda^{u,(f)}$, then it is also a homoclinic channel verifying Definition 5.2 for $W_\Lambda^{s,(f^{-1})}, W_\Lambda^{u,(f^{-1})}$, and

$$\Omega_+^{\Gamma,(f)} = \Omega_-^{\Gamma,(f^{-1})}, \quad \Omega_-^{\Gamma,(f)} = \Omega_+^{\Gamma,(f^{-1})} \quad (5.13)$$

and

$$\Omega_\pm^{\Gamma,(f^n)} = \Omega_\pm^{\Gamma,(f)}, \quad n \geq 0.$$

All these properties give

$$\sigma^{\Gamma,(f)} = (\sigma^{\Gamma,(f^{-1})})^{-1}, \quad \sigma^{\Gamma,(f^n)} = \sigma^{\Gamma,(f)}, \quad n \geq 0$$

5.2.4 The scattering map in other contexts

Autonomous flows

The definition of scattering maps for autonomous flows is completely analogous to the definition for diffeomorphisms. In this section, we recall the definitions and introduce the notations needed. We recall

that a manifold Λ is a normally hyperbolic invariant manifold for a flow Φ_t if there exist a constant $C > 0$, exponential rates $0 < \alpha < \beta$ and a splitting for every $x \in \Lambda$

$$T_x M = E_x^s \oplus E_x^u \oplus T_x \Lambda$$

in such a way that

$$\begin{aligned} v \in E_x^s &\Leftrightarrow |D\Phi_t(x)v| \leq Ce^{-\beta t}|v| & t \geq 0 \\ v \in E_x^u &\Leftrightarrow |D\Phi_t(x)v| \leq e^{-\beta|t|}|v| & t \leq 0 \\ v \in T_x \Lambda &\Leftrightarrow |D\Phi_t(x)v| \leq Ce^{\alpha|t|}|v| & t \in \mathbb{R} \end{aligned} \quad (5.14)$$

All the properties and definitions given in section 5.2.1 are analogous in the case of flows. In particular, the stable and unstable manifolds of Λ are given by

$$\begin{aligned} W_\Lambda^s &= \{y \in M \mid d(\Phi_t(y), \Lambda) \leq C_y e^{-\beta t}, t \geq 0\} \\ W_\Lambda^u &= \{y \in M \mid d(\Phi_t(y), \Lambda) \leq C_y e^{-\beta|t|}, t \leq 0\} \end{aligned}$$

and, for each $x \in \Lambda$, we define the stable and unstable manifolds of x as

$$\begin{aligned} W_x^s &= \{y \in M \mid d(\Phi_t(x), \Phi_t(y)) \leq C_{x,y} e^{-\beta t}, t \geq 0\} \\ W_x^u &= \{y \in M \mid d(\Phi_t(y), \Phi_t(x)) \leq C_{x,y} e^{-\beta|t|}, t \leq 0\} \end{aligned}$$

The regularity of the stable and unstable manifolds as well as the regularity of the foliation are the same as in the case of maps.

Another important property is that if Λ is a normally hyperbolic invariant manifold for a flow $\{\Phi_t, t \in \mathbb{R}\}$, so it is for f_T , the time T map, for any $T \in \mathbb{R}$.

In the case of flows we can define analogously the *wave operators*:

$$\begin{aligned} \Omega_\pm : W_\Lambda^{s,u} &\longrightarrow \Lambda \\ x &\longmapsto x_\pm \end{aligned}$$

such that $|\Phi_t(x) - \Phi_t(x_\pm)| \leq C_{x,x_\pm} e^{-\beta|t|}$, as $t \rightarrow \pm\infty$.

To define the scattering map in the case of flows we also assume that there exists a homoclinic channel Γ satisfying Definition 5.2 and then the maps

$$\Omega_\pm^\Gamma : \Gamma \longrightarrow H_\pm^\Gamma \subset \Lambda$$

are diffeomorphisms. Hence, analogously to (5.10), we define the scattering map

$$\sigma^\Gamma = \Omega_+^\Gamma \circ (\Omega_-^\Gamma)^{-1}.$$

It is straightforward to check that these wave operators $\Omega_\pm^\Gamma$ for the flow Φ_t coincide with the wave operators $\Omega_\pm^{\Gamma, f_T}$, for any time T map f_T . That is

$$\Omega_\pm^\Gamma = \Omega_\pm^{\Gamma, f_T} = \Omega_\pm^{\Gamma, f_{T'}}, \quad \forall T, T' \in \mathbb{R}$$

and, consequently:

$$\sigma^\Gamma = \sigma^{\Gamma, f_T} = \sigma^{\Gamma, f_{T'}}, \quad \forall T, T' \in \mathbb{R}. \quad (5.15)$$

From now on, we denote the scattering map for the flow by $\sigma^{\Gamma, \mathcal{H}}$, $\mathcal{H}$ being the vector field generating the flow Φ_t . We have that the following properties, completely analogous to the properties of section 5.2.3, hold:

$$\begin{aligned} \Omega_\pm^{\Gamma, \mathcal{H}} &= \Omega_\pm^{\Gamma, -\mathcal{H}} \\ \Omega_+^{\Gamma, \mathcal{H}} &= \Phi_{-t} \circ \Omega_+^{\Phi_t(\Gamma), \mathcal{H}} \circ \Phi_t, \quad \Omega_-^{\Gamma, \mathcal{H}} = \Phi_t \circ \Omega_-^{\Phi_{-t}(\Gamma), \mathcal{H}} \circ \Phi_{-t} \\ \sigma^{\Gamma, \mathcal{H}} &= (\sigma^{\Gamma, -\mathcal{H}})^{-1} \\ \sigma^{\Phi_t(\Gamma), \mathcal{H}} &= \Phi_t \circ \sigma^{\Gamma, \mathcal{H}} \circ \Phi_{-t} \end{aligned}$$

Non-autonomous flows

One situation that appears in applications is that the vector field $\mathcal{H}$ is a skew product vector field $\mathcal{H} = (\mathcal{G}, \mathcal{L})$ defined in $\tilde{M} = M \times N$ by $\mathcal{H}(x, \theta) = (\mathcal{G}(x, \theta), \mathcal{L}(\theta))$, which happens to be “close” to an autonomous vector field, that is, there exists $\mathcal{G}_0(x)$ such that

$$\|\mathcal{G} - \mathcal{G}_0\|_{C^r} \ll 1 \quad (5.16)$$

We first deal with the product case $\mathcal{H}_0 = (\mathcal{G}_0, \mathcal{L})$, which is very simple.

Proposition 5.1. *Let Λ be a normally hyperbolic invariant manifold under a flow Φ_t on a manifold M . Let $0 < \alpha < \beta$ be the exponential expansion rates corresponding to the normal hyperbolicity of Λ . Let N be another manifold with a flow φ_t with exponential expansion rates less or equal than α . Consider the flow $\tilde{\Phi}_t := (\Phi_t, \varphi_t)$ on the manifold $M \times N$.*

Then the manifold $\tilde{\Lambda} := \Lambda \times N$ is a normally hyperbolic invariant manifold for the flow $\tilde{\Phi}_t$.

Moreover, $W_{\tilde{\Lambda}}^s \times N = W_{\Lambda}^s$ is the stable manifold of $\tilde{\Lambda}$ for the extended flow $\tilde{\Phi}_t$.

For $x \in \Lambda$, $\theta \in N$, we have that $W_{(x, \theta)}^s = W_x^s \times \{\theta\}$ is the stable manifold of the point $(x, \theta) \in M \times \{\theta\}$.

The same results hold for the unstable manifold.

Therefore, in the product case $\mathcal{H}_0 = (\mathcal{G}_0, \mathcal{L})$, we can define a scattering map for the flow. Since the exponential rates in N are smaller or equal than α , we have that $\tilde{W}_{(x, \theta)}^{s, u} = W_x^{s, u} \times \{\theta\}$, so that $\tilde{\Omega}_{\pm}(x, \theta) = (\Omega_{\pm}(x), \theta)$ and the scattering map has the simple form

$$\tilde{\sigma}(x, \theta) = (\sigma(x), \theta).$$

In the skew product case $\mathcal{H} = (\mathcal{G}, \mathcal{L})$, provided that $\mathcal{H}$ is a small perturbation (5.16) of a product flow, we can define a scattering map in the corresponding domain.

The skew product structure of the perturbation implies that the scattering map has the skew product form

$$\tilde{\sigma}(x, \theta) = (\sigma(x, \theta), \theta).$$

In particular, in the case of quasi-periodic flows coming from a non-autonomous Hamiltonian vector field of Hamiltonian $H(x, \theta)$, $\theta = \nu t$, $\nu \in \mathbb{R}^d$, defined in $M \times \mathbb{T}^d$, one can recover the symplectic character of the flow simply by adding d extra actions $A \in \mathbb{R}^d$ conjugated to the angles θ and working with the autonomous flow of the Hamiltonian $H^*(x, \theta, A) = H(x, \theta) + \nu \cdot A$ in the full symplectic space $M^* = M \times T^*N$. When expressing in these complete set of symplectic variables the scattering map, it takes the form

$$\sigma^*(x, \theta, A) = (\sigma(x, \theta), \theta, \mathcal{A}(x, \theta, A)).$$

In the following section we will see that the scattering map for a symplectic map is also symplectic.

Center manifolds

Many of the results discussed above generalize to center manifolds of a fixed point [Gar00] or to locally invariant manifolds with boundary.

The standard method to study locally invariant manifolds (see [Fen72]) is to construct an extended system for which the center manifolds (or the locally invariant manifolds) are invariant.

Unfortunately, the invariant manifolds thus produced and their stable and unstable manifolds depend on the extension considered. Indeed, the stable and unstable manifolds of a point in the center manifold can depend on the extension considered. This is because a trajectory can leave the neighborhood where the original map agrees with the extension. Therefore, the homoclinic intersections and the scattering maps obtained depend on the extension considered. In particular, the symplectic properties stated in Section 5.3 can only be true for center manifolds if the extensions considered are symplectic.

Nevertheless, there are some important cases where there is uniqueness and the results are independent of the extension. For example in Hamiltonian systems with 2-dimensional locally invariant manifolds having KAM tori bounding them. In this case the locally invariant manifolds are indeed invariant and, therefore, unique as well as their stable and unstable manifolds.

Even if the center manifolds are not unique, some of the objects constructed using them (e.g. periodic orbits, KAM tori, Aubry Mather sets) remain in any center manifold and their stable and unstable manifolds are independent of the extension.

5.3 Symplectic properties of the scattering map

The main result of this section is that, in case that f is symplectic and Λ is a symplectic manifold (when endowed with the restriction of the symplectic form), the scattering map preserves the restriction of the symplectic form to Λ . A version of this result for a central manifold of a fixed point with a different proof can be found in [Gar00]. These geometric properties will be very important for the perturbative computations of the scattering map in section 5.4. In this discussion, we will use Cartan calculus and coordinate free calculations. See [AM78, Thi97, BG05].

5.3.1 Notation and some elementary facts on symplectic geometry

When N, M are symplectic manifolds, we say that $f : N \rightarrow M$ is symplectic when

$$f^* \omega_M = \omega_N$$

where f^* is the pull back on forms defined by

$$(f^* \omega_M)(x)(v, w) = \omega_M(f(x))(Df(x)v, Df(x)w) \quad \forall v, w \in T_x N$$

We note that the definition of the pull back for forms does not require that f is a diffeomorphism, but only one to one on N .

When $\omega_N = d\alpha_N$, $\omega_M = d\alpha_M$, we say that f is exact when

$$f^* \alpha_M = \alpha_N + dP^f \tag{5.17}$$

for some function $P^f : N \rightarrow \mathbb{R}$. The function P^f is called the primitive function of f .

If f is a diffeomorphism, an equivalent condition for f to be symplectic is

$$f_* \omega_N = \omega_M$$

where f_* is the push forward on forms defined by

$$(f_* \omega_N)(x)(v, w) = \omega_N(f^{-1}(x))(Df^{-1}(x)v, Df^{-1}(x)w) \quad \forall v, w \in T_x M$$

Remark 5.3. Note that the function P^f is determined uniquely up to constants when N is connected and α_N, α_M are given. When talking about primitive functions, we will identify two functions which differ on a constant. This justifies that we can talk about *the* primitive function of a diffeomorphism.

Specially in the case that $N = M = \mathbb{T}^d \times \mathbb{R}^d$ and that f is a twist map, the primitive function allows us to study several geometric properties of the map. See [LM87] and specially [Har99, Har00] for a systematic study of the primitive function, including numerical applications.

Formulation of the symplectic properties of the scattering map

Theorem 5.4. *Assume that M is endowed with a symplectic (resp. exact symplectic) form ω and that $\omega|_\Lambda$ is also symplectic (hence, in particular, the dimension m of M and the dimension c of Λ are even).*

Assume that f is symplectic (resp. it is exact symplectic).

Assume that there exists a homoclinic channel Γ and so the scattering map σ^Γ is well defined.

Then, the scattering map σ^Γ is symplectic (resp. exact symplectic).

The main technical tool, from which Theorem 5.4 follows almost immediately is:

Lemma 5.5. *Assume that, with the notations above, we have that $\omega|_\Lambda$ is symplectic, and that Γ is C^1 close to Λ on a neighborhood (hence $\omega|_\Gamma$ is also a symplectic form).*

Then,

$$(\Omega_+^\Gamma)_* \omega|_\Gamma = \omega|_\Lambda \tag{5.18}$$

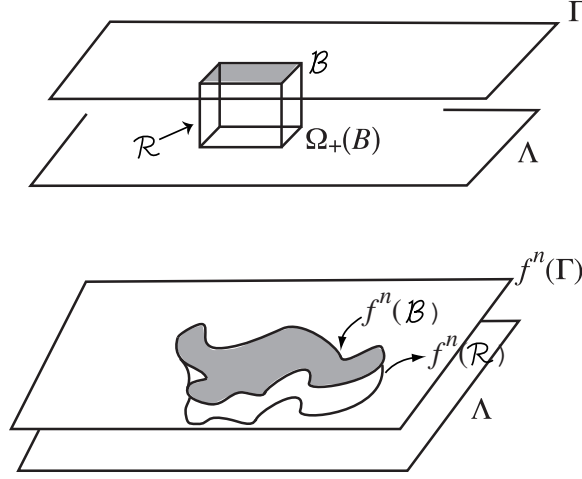


Figure 5.4: Illustration of the proof of Lemma 5.5

5.3.2 Proof of Lemma 5.5

The proof of Lemma 5.5 is very similar to the proof of absolute continuity of Anosov foliation in [PS72].

We will prove that given any two-dimensional cell $\mathcal{B} \subset \Gamma$, we have

$$\int_{\mathcal{B}} \omega = \int_{\Omega_+^\Gamma(\mathcal{B})} \omega \quad (5.19)$$

To prove (5.19), we will consider a 3-cell $\mathcal{C}$ in W_Λ^s whose boundary contains $\mathcal{B}$, $\Omega_+^\Gamma(\mathcal{B})$.

Let $B : [0, 1] \times [0, 1] \rightarrow \Gamma$ be a parameterization of $\mathcal{B}$.

If $z \in [0, 1] \times [0, 1]$, $y = B(z) \in \mathcal{B} \subset \Gamma$ and $\Omega_+^\Gamma(y)$ are, by assumption, close enough, so that there is one shortest γ_z geodesic in $W_{\Omega_+^\Gamma(y)}^s$ joining y and $\Omega_+^\Gamma(y)$. We parameterize these geodesics in such a way that

$$\begin{aligned} \gamma_z(0) &= \Omega_+^\Gamma(y) \\ \gamma_z(1) &= y \end{aligned}$$

We see by the implicit function theorem that the map $C : [0, 1] \times [0, 1] \times [0, 1] \rightarrow W_\Lambda^s$ defined by

$$C(z, t) = \gamma_z(t)$$

is a C^1 map which is a local diffeomorphism and which gives a parameterization of the cell $\mathcal{C}$.

We note that

$$\partial\mathcal{C} = \mathcal{B} - \Omega_+^\Gamma(\mathcal{B}) + \mathbb{R}$$

where $\mathbb{R}$ is the two dimensional cell consisting on a union of geodesics in $W_{\Omega_+^\Gamma(\partial\mathcal{B})}^s$.

By Stokes theorem

$$\int_{\partial\mathcal{C}} \omega = \int_{\mathcal{C}} d\omega = 0$$

We therefore have

$$\int_{\mathcal{B}} \omega = \int_{\Omega_+^\Gamma(\mathcal{B})} \omega - \int_{\mathbb{R}} \omega \quad (5.20)$$

Hence, the desired result (5.19) will be established when we prove $\int_{\mathbb{R}} \omega = 0$.

This is a consequence of the following proposition, which we will also find useful in discussing exactness.

Proposition 5.2. *Let $\mathbb{R}$ be a 2-cell in W_Λ^s parameterized by*

$$R : [0, 1] \times [0, 1] \rightarrow W_\Lambda^s$$

in such a way that

$$R(z, t) \in W_{R(0, t)}^s, \quad R(0, t) \in \Lambda$$

That is, we can think of $\mathbb{R}$ as a union of lines each of which lies in the stable manifold of one point. Then $\int_{\mathbb{R}} \omega = 0$.

Proof. It consists just in observing that, by the invariance of ω under f , we have for every $n \in \mathbb{N}$

$$\int_{\mathbb{R}} \omega = \int_{f^n(\mathbb{R})} \omega$$

and, by the hyperbolicity of Λ , we also have

$$\text{Area}(f^n(\mathbb{R})) \leq C(\lambda\mu)^n,$$

because the stable coordinates contract at least by $C\lambda^n$ and the coordinates along Λ expand by a factor not larger than $C\mu^n$.

By the normal hyperbolicity assumption, $\lambda\mu < 1$, and since $\forall n \in \mathbb{N}$ we have $\int_{f^n(\mathbb{R})} \omega \leq C \text{Area}(f^n(\mathbb{R}))$, Proposition 5.2 is proved. $\square$

Proposition 5.2 finishes the proof of the fact that Ω_+^Γ is symplectic.

To finish the proof of Lemma 5.5, the only thing remaining is to prove the claim of exactness.

If $\omega = d\alpha$ and f is exact, we will show that given a path $\eta : [0, 1] \rightarrow \Gamma$, we have:

$$\int_{\eta} \alpha = \int_{\Omega_+^\Gamma(\eta)} \alpha + \mathcal{G}^\Gamma(\Omega_+(\eta(1)) - \mathcal{G}^\Gamma(\Omega_+(\eta(0))) \quad (5.21)$$

where $\mathcal{G}^\Gamma : \Omega_+(\Gamma) \rightarrow \mathbb{R}$ is an explicit function which we now compute.

Since the path η is arbitrary, (5.21) is equivalent to

$$(\Omega_+^\Gamma)_* \alpha|_\Gamma = \alpha|_\Lambda + d\mathcal{G}^\Gamma \quad (5.22)$$

Given a point $y \in \Omega_+^\Gamma(\Gamma) \subset \Lambda$ we consider a path $\beta \subset W_y^s$ joining y and $(\Omega_+^\Gamma)^{-1}(y) \in \Gamma$. Then, set

$$\mathcal{G}^\Gamma(y) = \int_{\beta} \alpha \quad (5.23)$$

The integral defining $\mathcal{G}^\Gamma$ in (5.23) is independent of the choice of the path β because of Proposition 5.2.

As usual, we argue that given two paths $\beta, \tilde{\beta}$ joining y to $(\Omega_+^\Gamma)^{-1}(y)$, the closing path resulting from going through one and coming back through the other bounds a two cell $\Sigma \subset W_y^s$ such that $\beta - \tilde{\beta} = \partial\Sigma$, hence

$$\int_{\beta} \alpha - \int_{\tilde{\beta}} \alpha = \int_{\Sigma} d\alpha = 0.$$

Since the integral defining $\mathcal{G}^\Gamma$ is independent of the path, it will be advantageous for us to choose a path which depends differentially on the base point. For example, we may choose as β_y the shortest geodesic in W_y^s joining y and $(\Omega_+^\Gamma)^{-1}(y)$.

Denoting $y_0 = \Omega_+^\Gamma(\eta(0))$, $y_1 = \Omega_+^\Gamma(\eta(1))$, the identity (5.21) follows because

$$-\eta + \beta_{y_1} + \Omega_+^\Gamma(\eta) - \beta_{y_0} = \partial\mathbb{R}$$

where $\mathbb{R}$ is a two cell satisfying the assumptions of Proposition 5.2. Then, $\int_{\partial\mathbb{R}} \alpha = \int_{\mathbb{R}} \omega = 0$. $\square$

5.3.3 Proof of Theorem 5.4

By the λ -lemma (see e.g., [PS72]) there is an $n \in \mathbb{N}$ large enough so that $f^n(\Gamma)$ satisfies the assumptions of Lemma 5.5.

Similarly $f^{-n}(\Gamma)$ satisfies the assumptions of Lemma 5.5 for f^{-1} in place of f .

We note that, by equation (5.9) with n and $-n$ respectively

$$\sigma^\Gamma = \Omega_+^\Gamma \circ (\Omega_-^\Gamma)^{-1} = f^{-n} \circ \Omega_+^{f^n(\Gamma)} \circ f^{2n} \circ [\Omega_-^{f^{-n}(\Gamma)}]^{-1} \circ f^{-n} \quad (5.24)$$

Also, by (5.13), we have that

$$\Omega_-^{f^{-n}(\Gamma), (f)} = \Omega_+^{f^{-n}(\Gamma), f^{-1}}$$

Hence, the map σ^Γ is symplectic (resp. exact symplectic) as desired.

5.3.4 The scattering map and the primitive function

The goal of this section is to show that, when the map f is exact symplectic and Λ is an exact symplectic manifold, we can obtain formulas for the primitive function of the scattering map. The main result of this section is formula (5.28), which gives the primitive function of the scattering map in terms of the primitive function of f and formula (5.29) which gives the analogous formula for flows. Formula (5.28) is given by the difference of two sums computed along the homoclinic intersection. In Theorem 5.8, we show that formula (5.28) converges exponentially fast together with some of its derivatives.

Some elementary properties

We recall that in Section 5.3.1, we reviewed the standard definition of primitive function.

The next proposition recalls some elementary properties of the primitive of composition that will be useful in the sequel.

Proposition 5.3. *If $f : N \rightarrow M$ and $g : M \rightarrow V$ are exact symplectic diffeomorphisms with primitives $P^f : N \rightarrow \mathbb{R}$ and $P^g : M \rightarrow \mathbb{R}$, respectively, then we have:*

1. *The primitive $P^{g \circ f}$ of $g \circ f$ is given by*

$$P^{g \circ f} = P^f + P^g \circ f. \quad (5.25)$$

2. *If $g \circ f = \text{Id}$ then*

$$P^g + P^f \circ g = 0 \quad (5.26)$$

- 3.

$$P^{f^n} = \sum_{j=0}^{n-1} P^f \circ f^j \quad (5.27)$$

Proof. The proof of (1) is only the following computation.

$$\begin{aligned} (g \circ f)^* \alpha_V &= f^* g^* \alpha_V = f^* (\alpha_M + dP^g) \\ &= \alpha_N + dP^f + df^* P^g \\ &= \alpha_N + d(P^f + P^g \circ f) \end{aligned}$$

The other parts of the proposition are easy consequences of (5.25). $\square$

We also observe that the primitive function behaves well under restriction to an exact symplectic submanifold invariant under f . The primitive function of the restriction is the restriction of the primitive function in the whole manifold.

Formulas for the primitive function of the scattering map

In this section we study a C^r symplectic diffeomorphism $f : M \rightarrow M$ which has a normally hyperbolic invariant manifold Λ such that $\omega|_{\Lambda}$ is non-degenerate, and also a homoclinic channel Γ verifying Definition 5.2, so that there exists a scattering map $\sigma = \sigma^\Gamma : H^- \rightarrow H^+$ as in (5.10). Again, we are assuming that the map f is uniformly C^r in a neighborhood of the manifold Λ and of the homoclinic channel Γ .

In the case that the map f is exact symplectic we know that the same is true for the scattering map. The next Theorem 5.6 gives us a very effective formula for the primitive of the scattering map σ in terms of the primitive of f .

The main results of this section are Theorem 5.6 which establishes (5.28), a formula for the primitive function of σ , Theorem 5.7, which provides an analogous formula (5.29) for flows, and Theorem 5.8 which guarantees the convergence of the series (and the integrals) defining the primitive function and their derivatives.

As we will see later in Section 5.5, we will obtain formulas very similar to (5.28) and (5.29) for other objects. The results of Theorem 5.8 will therefore, have further applicability.

Theorem 5.6. *Let $f : M \rightarrow M$ be a C^r exact symplectic diffeomorphism which has a normally hyperbolic invariant manifold Λ such that $\omega|_{\Lambda}$ is non-degenerate, and a homoclinic channel Γ verifying Definition 5.2, so that there exists a scattering map $\sigma = \sigma^\Gamma : H^- \rightarrow H^+$ as in (5.10).*

Then, the primitive for σ is given by

$$\begin{aligned} P^\sigma &= \lim_{N_\pm \rightarrow \infty} \sum_{j=1}^{N_-} P^f \circ f^{-j} \circ (\Omega_-^\Gamma)^{-1} - P^f \circ f^{-j} \\ &\quad + \sum_{j=0}^{N_+-1} P^f \circ f^j \circ (\Omega_+^\Gamma)^{-1} \circ \sigma - P^f \circ f^j \circ \sigma \end{aligned} \quad (5.28)$$

In the case that the map f corresponds to the time T flow of a Hamiltonian vector field $\mathcal{H}$ of Hamiltonian H we can adapt the previous result to obtain a formula for the primitive of the scattering map $\sigma = \sigma^{\Gamma, \mathcal{H}}$, that was shown in (5.15) that is independent of T .

Theorem 5.7. *Let $\Phi_t(x)$ be the flow of a Hamiltonian vector field of Hamiltonian $H(x)$ and consider the time T map of this flow, that is, $f(x) = \Phi_T(x)$. Assume that this map has a normally hyperbolic invariant manifold Λ such that $\omega|_\Lambda$ is non-degenerate, and a homoclinic channel Γ verifying Definition 5.2, so that there exists a scattering map $\sigma = \sigma^\Gamma : H^- \rightarrow H^+$ as in (5.10).*

Then, the primitive P^σ is given by

$$\begin{aligned} P^\sigma &= \lim_{T_\pm \rightarrow \infty} \int_{-T_-}^0 (\alpha \mathcal{H} + H) \circ \Phi_t \circ (\Omega_-^\Gamma)^{-1} - (\alpha \mathcal{H} + H) \circ \Phi_t \\ &\quad + \int_0^{T_+} (\alpha \mathcal{H} + H) \circ \Phi_t \circ (\Omega_+^\Gamma)^{-1} \circ \sigma - (\alpha \mathcal{H} + H) \circ \Phi_t \circ \sigma \end{aligned} \quad (5.29)$$

where we denote $\alpha \mathcal{H} = i_{\mathcal{H}} \alpha$.

The convergence of the series in (5.28) and the integrals in (5.29) is guaranteed by the following result.

Theorem 5.8. *Under our standing assumptions let Ψ be a C^m function in a neighborhood of Λ .*

We have the following bounds for all $j \in \mathbb{N}$, $0 \leq k \leq \min(m, \ell, r)$. For any $\tilde{\lambda} > \lambda$, $\tilde{\mu} > \mu$, we have:

$$\begin{aligned} \|D^k(\Psi \circ f^j \circ (\Omega_+^\Gamma)^{-1} \circ \sigma - \Psi \circ f^j \circ \sigma)\|_{C^0(H_-)} &\leq C \|\Psi\|_{C^k} j^k (\tilde{\lambda} \tilde{\mu}^k)^j \\ \|D^k(\Psi \circ f^{-j} \circ (\Omega_-^\Gamma)^{-1} - \Psi \circ f^{-j})\|_{C^0(H_-)} &\leq C \|\Psi\|_{C^k} j^k (\tilde{\lambda} \tilde{\mu}^k)^j \end{aligned} \quad (5.30)$$

Analogous inequalities are valid for the case of flows.

Of course, to apply Theorem 5.8 to (5.28) and (5.29), we just have to take $\Psi = P^f \in C^{r-1}$ (or $\Psi = \alpha \mathcal{H} + H$), hence $m = r - 1$.

A variational interpretation

We recall that the well known Hamilton variational principle states that, under some non-degeneracy condition, $\gamma(t)$ is an orbit of the Hamiltonian flow of Hamiltonian H if and only if it is a stationary point of the formal action

$$\mathcal{L}(\gamma) = \int_{-\infty}^{+\infty} (-\alpha \dot{\gamma}(t) + H \circ \gamma(t)) dt$$

or, if $\alpha = pdq$, and $\gamma(t) = (\gamma^q(t), \gamma^p(t))$,

$$\mathcal{L}(\gamma) = \int_{-\infty}^{+\infty} (-\gamma^p(t) \dot{\gamma}^q(t) + H \circ \gamma(t)) dt$$

Hence, Theorems 5.6 and 5.7 tell us that the primitive function of the scattering map is the limit of the difference between the action of the homoclinic orbit and the action of the asymptotic orbits.

We hope that this variational interpretation of the scattering map can lead to a closer interaction between variational and geometric methods. It seems quite possible that the conditions used in [CY04] can be interpreted as transversality conditions between the scattering map and the inner map.

The difference in action plays a fundamental role in the variational approach to diffusion. Certainly, in the variational theories concerned with local critical points ([Bes96, BCV01, BBB03a]) the difference between primitive functions plays a role.

In more global variational theories, it seems that the definition of Peierls barrier is roughly similar to the infimum of all the differences of action over all homoclinic intersections. Hence, in our language, it would be the infimum of P^σ over all homoclinic intersections ([CI99, CY04, CY09, Mat95, Mat04, Kal03]).

Of course, in the global variational theorems, one assumes that the Lagrangian—and equivalently the Hamiltonian—are convex in the momenta. The version of Hamilton's principle stated here—and the local variational theories—only require some non-degeneracy of the Jacobian so that the Legendre transform is locally defined. That is, it suffices that for each t, γ , the mapping $\dot{\gamma} \mapsto \frac{\partial}{\partial \dot{\gamma}} L$ is invertible. This is significantly weaker than convexity. In particular, it is C^1 dense.

For a comparison between the local and global theories, and in particular a Hamiltonian discussion of barrier functions, see [Ber07].

Proof of Theorem 5.6

The formula (5.28) is closely related to the following formula, which is true for any $N_-, N_+ \in \mathbb{Z}$:

$$\sigma = f^{-N_+} \circ \Omega_+^{\Gamma^{N_+}} \circ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \quad (5.31)$$

where we have denoted $\Gamma^n = f^n(\Gamma)$, for $n \in \mathbb{Z}$.

The formula (5.31) is a consequence of the formula (5.9) for the wave operators.

To compute the primitive function P^σ of the scattering map σ , we start from (5.31) and apply equations (5.25), (5.26) and (5.27). We obtain, for any $N_-, N_+ \in \mathbb{Z}$, the following formula in the reference manifold N .

$$\begin{aligned} P^\sigma &= P^{f^{-N_-}} + P^{(\Omega_-^{\Gamma^{-N_-}})^{-1}} \circ f^{-N_-} + P^{f^{N_++N_-}} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \\ &\quad + P^{\Omega_+^{\Gamma^{N_+}}} \circ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \\ &\quad + P^{f^{-N_+}} \circ \Omega_+^{\Gamma^{N_+}} \circ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \\ &= - \left(P^f \circ f^{-N_-} + \dots + P^f \circ f^{-1} \right) \\ &\quad + P^{(\Omega_-^{\Gamma^{-N_-}})^{-1}} \circ f^{-N_-} \\ &\quad + \left(P^f + \dots + P^f \circ f^{N_++N_- - 1} \right) \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \\ &\quad + P^{\Omega_+^{\Gamma^{N_+}}} \circ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \\ &\quad - \left(P^f \circ f^{-N_+} + \dots + P^f \circ f^{-1} \right) \circ \Omega_+^{\Gamma^{N_+}} \circ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} \end{aligned}$$

Now, we use formula (5.9) for the wave operators, obtaining

$$\begin{aligned} (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} &= f^{-N_-} \circ (\Omega_-^\Gamma)^{-1} \\ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} &= f^{N_+} \circ (\Omega_-^\Gamma)^{-1} \\ \Omega_+^{\Gamma^{N_+}} \circ f^{N_++N_-} \circ (\Omega_-^{\Gamma^{-N_-}})^{-1} \circ f^{-N_-} &= \Omega_+^{\Gamma^{N_+}} \circ f^{N_+} \circ (\Omega_-^\Gamma)^{-1} = f^{N_+} \circ \sigma \end{aligned}$$

which give, using them in the formula for the primitive P^σ :

$$\begin{aligned} P^\sigma &= - \left(P^f \circ f^{-N_-} + \dots + P^f \circ f^{-1} \right) \\ &\quad + P^{(\Omega_-^{\Gamma^{-N_-}})^{-1}} \circ f^{-N_-} \\ &\quad + \left(P^f \circ f^{-N_-} + \dots + P^f \circ f^{-1} \right) \circ (\Omega_-^\Gamma)^{-1} \\ &\quad + \left(P^f + \dots + P^f \circ f^{N_+ - 1} \right) \circ (\Omega_-^\Gamma)^{-1} \\ &\quad + P^{\Omega_+^{\Gamma^{N_+}}} \circ f^{N_+} \circ (\Omega_-^\Gamma)^{-1} \\ &\quad - \left(P^f + \dots + P^f \circ f^{N_+ - 1} \right) \circ \sigma \end{aligned}$$

Now we observe that, by Lemma 5.5 and the λ -Lemma applied to the normally hyperbolic invariant manifold Λ , the wave operators $\Omega_\pm^{\Gamma^{\pm N_\pm}}$ are exact symplectic and converge to the identity map when

$N_{\pm} \rightarrow \infty$. Therefore, we can ensure that the primitives $P(\Omega_-^{\Gamma^{-N_-}})^{-1}$ and $P\Omega_+^{\Gamma^{N_+}}$ converge to zero. So, if we take limits as $N_{\pm} \rightarrow \infty$, we obtain

$$\begin{aligned} P^{\sigma} &= \lim_{N_{\pm} \rightarrow \infty} \sum_{j=-1}^{-N_-} P^f \circ f^j \circ (\Omega_-^{\Gamma})^{-1} - P^f \circ f^j \\ &\quad + \sum_{j=0}^{N_+-1} P^f \circ f^j \circ (\Omega_+^{\Gamma})^{-1} \circ \sigma - P^f \circ f^j \circ \sigma \end{aligned} \quad (5.32)$$

which is formula (5.28). $\square$

Proof of Theorem 5.7

The proof of Theorem 5.7 is an easy consequence of the fact that the primitive of the Hamiltonian flow Φ_t is given by

$$P^{\Phi_T} = \int_0^T (\alpha\mathcal{H} + H) \circ \Phi_t dt$$

where $\mathcal{H}$ is the Hamiltonian vector field of Hamiltonian H . This formula can be obtained, for instance, by differentiating with respect to time the definition of the primitive:

$$\begin{aligned} \frac{d}{dt} P^{\Phi_t} &= \frac{d}{dt} (\Phi_t)^* \alpha \\ &= (\Phi_t)^* (di_{\mathcal{H}} \alpha + i_{\mathcal{H}} d\alpha) = d((\Phi_t)^* (\alpha\mathcal{H} + H)) \end{aligned}$$

Once we know the primitive of the Hamiltonian flow Φ_T , we can consider the corresponding scattering map $\sigma = \sigma^{\Gamma, \mathcal{H}}$ which, by (5.15), is independent of T . We compute the primitive of σ simply applying formula (5.28) for this case and using the following facts:

$$\begin{aligned} P^{\Phi_T} \circ \Phi_{jT} &= \int_0^T (\alpha\mathcal{H} + H) \circ \Phi_t \circ \Phi_{jT} dt = \int_{jT}^{(j+1)T} (\alpha\mathcal{H} + H) \circ \Phi_t dt \\ P^{\Phi_T} \circ \Phi_{-jT} &= \int_0^T (\alpha\mathcal{H} + H) \circ \Phi_t \circ \Phi_{-jT} dt = \int_{-jT}^{-(j-1)T} (\alpha\mathcal{H} + H) \circ \Phi_t dt \\ \sum_{j=0}^{N_+-1} P^{\Phi_T} \circ \Phi_{jT} &= \int_0^{TN_+} (\alpha\mathcal{H} + H) \circ \Phi_t dt \\ \sum_{j=1}^{N_-} P^{\Phi_T} \circ \Phi_{-jT} &= \int_{-TN_-}^0 (\alpha\mathcal{H} + H) \circ \Phi_t dt \end{aligned}$$

With these expressions one easily obtains formula (5.29) by calling $T_{\pm} = TN_{\pm} \rightarrow \pm\infty$.

Proof of Theorem 5.8

We present the proof for the first estimates in (5.30). Then, the second estimate follows by applying the first estimates to a system whose dynamics is given by f^{-1} .

We start by proving the case $k = 0$.

The reason why (5.28) converges exponentially fast is that the general term in the formula is the difference of a function evaluated in two points which are exponentially close. Recall that by the definition of the wave operators and Definition 5.1 we have:

$$\begin{aligned} d(f^j \circ (\Omega_+^{\Gamma})^{-1} \circ \sigma(x), f^j \circ \sigma(x)) &\leq C\lambda^j \\ d(f^{-j} \circ (\Omega_-^{\Gamma})^{-1}(x), f^{-j}(x)) &\leq C\lambda^j \end{aligned}$$

For higher derivatives the argument is more complicated.

We start by choosing a system of coordinates on a neighborhood $\mathcal{U}$ of Λ in W_{Λ}^s . Similar choices are quite standard in [Fen72].

We observe that we can identify $\mathcal{U}$ with a neighborhood of the zero section of the stable bundle. More concretely, we associate to (x, ξ) , with $x \in \Lambda$, $\xi \in E_x^s$, $|\xi| \leq \delta$, the point

$$\exp_x^{W_x^s}(\xi) \quad (5.33)$$

where $\exp_x^{W_x^s}$ denotes the exponential mapping associated to the manifold W_x^s .

We recall that our standing assumptions include that we have a metric which is uniformly differentiable in a neighborhood of Λ and that the map f is also uniformly differentiable in a neighborhood of Λ . These assumptions are automatic if Λ is compact, but they hold in many other situations. As a consequence, $\exp_x^{W_x^s}$ defines a C^r diffeomorphism from a ball $\mathcal{U}$ of radius $\delta > 0$ of Λ in W_Λ^s to its image in W_Λ^s , which is independent of x .

In these system of coordinates, the map f restricted to $\mathcal{U}$ takes the form

$$(x, \xi) \mapsto (f_0(x), f_x(\xi)) \quad (5.34)$$

For the purposes that follow, it is convenient to consider x as a parameter, since we have different mappings for each stable manifold W_x^s . We also note that the points representing Λ have ξ coordinate equal to zero and that the invariance of Λ amounts to $f_x(0) = 0$.

In this system of coordinates, f^j is represented by

$$f^j(x, \xi) = (f_0^j(x), f_{x,j}(\xi)),$$

where we have denoted $f_{f_0^{j-1}(x)} \circ \dots \circ f_x(\xi) \equiv f_{x,j}(\xi)$.

The following adjustments can be made without loss of generality.

1) We can assume that $\|D_\xi f_x(\xi)\|_{C^0(\mathcal{U})} \leq \tilde{\lambda}$, $\|D_x f_x(\xi)\|_{C^0(\mathcal{U})} \leq \tilde{\mu}$, by taking $\mathcal{U}$ sufficiently small, where $\tilde{\lambda}, \tilde{\mu}$ are the numbers appearing in the conclusions.

2) We also note that, by multiplying the metric by a constant, we can assume without loss of generality that $\|D_x^k D_\xi^i f_x(\xi)\|_{C^0(\mathcal{U})} \leq 1$ for $i + j \geq 2$. This will simplify slightly some estimates.

3) We can assume that

$$(\Omega_+^\Gamma)^{-1}(H_+) \subset \mathcal{U}$$

Indeed, by the λ -lemma, we have that for some finite J , $\Gamma^{\pm j} = f^{\pm j}(\Gamma) \subset \mathcal{U}$, for $j \geq J$. Then, we will obtain the estimate (5.30) for $j \geq J$. The desired result follows just changing the constant C .

In the system of coordinates (x, ξ) , we can write $(\Omega_+^\Gamma)^{-1}$ by

$$(x, 0) \mapsto (x, \Phi(x)).$$

Hence, in this system of coordinates, the desired result, formula (5.30), is implied by estimates

$$|D_x^k(\Psi(f_0^j(x), f_{x,j}(\Phi(x)))) - D_x^k \Psi(f_0^j(x), 0)| \leq C \|\Psi\|_{C^k} j^k (\tilde{\lambda} \tilde{\mu}^k)^j \quad (5.35)$$

The main idea in the proof of (5.35) is that, if we apply the Faa-Di-Bruno formula for the derivatives in (5.35) we will obtain derivatives of highly iterated functions (except for one term). The derivatives of highly iterated functions will be estimated in Propositions 5.4 below. The remaining term will be estimated because it is the difference of two terms that have close arguments.

Proposition 5.4. *With the notations above we have:*

For $n \geq 1$:

$$\|D^n f_0^j(x)\|_{C^0(\Lambda)} \leq (n-1)! j^n (\tilde{\mu}^n)^j \quad (5.36)$$

For $m \geq 1$, $n \geq 0$:

$$\|D_x^n D_\xi^m f_{x,j}(\xi)\|_{C^0(\mathcal{U})} \leq C_{n,m} j^{n+m} (\tilde{\lambda} \tilde{\mu}^{n+m})^j \quad (5.37)$$

where $C_{n,m}$ is an explicit expression depending on $n, m, \tilde{\lambda}, \tilde{\mu}$ but independent of j .

Proof. The proof of estimates for highly iterated functions is very similar to estimates appearing in [LMM86]. The dependence on parameters of the derivatives of highly iterated functions were considered in [BLW96, CFL03].

We start by observing that if we apply the chain rule and the product rule to $D^n f_0^j(x)$ we obtain an expression containing T_n terms all of which are factors of the form $D^i f_0 \circ f^k(x)$ for some $1 \leq i \leq n$, $0 \leq k \leq j$. We denote by F_n the maximum number of factors that appear in each of the terms in the expression above.

We observe that the number of factors increases only when we apply the chain rule and the number of terms increases only when we apply the product rule. Therefore,

$$\begin{aligned} T_n &\leq T_{n-1}F_{n-1} \\ F_n &\leq F_{n-1} + j \end{aligned}$$

We also have $T_1 = 1$, $F_1 = j$ from the chain rule. It follows that $F_n \leq nj$, $T_n \leq (n-1)!j^n$.

We also observe that each of the factors can be estimated by $\|D^i f_0 \circ f_0^k(x)\|_{C^0(\mathcal{U})} \leq \tilde{\mu}$. (Recall that $\tilde{\mu} \geq 1$ is an upper bound for the case $i = 1$ and that we have arranged that for $i > 1$ we have $|D^i f_0| < 1$). Therefore, each of the terms can be estimated from above by $\tilde{\mu}^{F_n}$ which in turn is estimated by $(\tilde{\mu}^n)^j$. We obtain the upper estimate (5.36) for the derivative by multiplying the upper estimate for each term by the upper estimate for the number of terms.

The other estimate is proved along similar lines. Again, we observe that, applying the chain rule and the product rule as often as possible, we can express $D_x^n D_\xi^m f_{x,j}(\xi)$ as a sum of $T_{n,m}$ terms, each of which contains not more than $F_{n,m}$ factors. Each of the factors is of the form $D_x^{\tilde{n}} D_\xi^{\tilde{m}} f_{f_0^j(x)}(\xi)$ for some $\tilde{n} \leq n$, $\tilde{m} \leq m$, $\tilde{j} \leq j$.

Again, noting that the number of terms increases only when we apply the product rule, and the number of factors when we apply the chain rule, we obtain:

$$\begin{aligned} T_{n,m} &\leq T_{n-1,m}F_{n-1,m}; & T_{n,m} &\leq T_{n,m-1}F_{n,m-1}; \\ F_{n,m} &\leq F_{n-1,m} + j; & F_{n,m} &\leq F_{n,m-1} + j; \end{aligned}$$

Since

$$D_\xi f_{x,j}(\xi) = D_\xi f_{f_0^j(x)}(\xi) \circ f_{x,j-1}(\xi) \cdot D_\xi f_{f_0^{j-1}(x)}(\xi) \circ f_{x,j-2}(\xi) \cdots D_\xi f_x(\xi)$$

we have that $F_{0,1} = j$, $T_{0,1} = 1$. Hence, we obtain from the recursion relations that $F_{n,m} \leq (n+m)j$ and, therefore, $T_{n,m} \leq (n+m-1)!j^{n+m}$.

In this case, however, we have to observe that there are factors in the terms that can be bounded by $\tilde{\lambda}$. Indeed, these factors are, in some sense rather abundant.

For instance, each of the factors in the derivative $D_\xi f_{x,j}(\xi)$ above can be bounded by $\tilde{\lambda}$ so that we have $\|D_\xi f_{x,j}(\xi)\|_{C^0(\mathcal{U})} \leq \tilde{\lambda}^j$.

We observe that, when we take derivatives (with either x or ξ) we obtain a sum of terms in which only one of the factors is affected.

Therefore, we conclude that in the expression of $D_x^n D_\xi^m f_{x,j}(\xi)$ alluded before, each of the terms contains at least $j - m - n + 1$ factors in which the derivative with respect to ξ is of first order.

We obtain that, therefore, each of the terms is bounded by $\tilde{\lambda}^{j-m-n+1} \tilde{\mu}^{(n+m)j}$. We therefore, obtain the desired bounds (5.37) by multiplying the upper bound for each of the terms by the upper bound on the number of terms. $\square$

The bound (5.35) is an easy consequence of Proposition 5.4.

It follows by induction (or by Faa-Di-Bruno formula) that

$$D_x^m f_{x,j}(\Phi(x)) = \sum_{m_1+m_2=m} C_{m_1,m_2} D_x^{m_1} D_\xi^{m_2} f_{x,j}(\xi)|_{\xi=\Phi(x)} P_{m_1,m_2}$$

where C_{m_1,m_2} is a combinatorial coefficient and P_{m_1,m_2} is a polynomial on the derivatives of Φ up to order m . We call attention that the combinatorial coefficients are independent of j . For the purposes of this calculation we are treating $f_{x,j}$ as a single function.

Therefore, we have

$$\|D_x^m f_{x,j}(\Phi(x))\|_{C^0(\mathcal{U})} \leq C j^m (\tilde{\lambda} \tilde{\mu}^m)^j \quad (5.38)$$

where C depends on the C^m norm of Φ and the combinatorial coefficients, but is independent of j .

Coming back to the proof of inequality (5.35), we compute the derivatives of $\Psi(f_0^j(x), f_{x,j}(\Phi(x)))$ and see that most of the terms that we obtain are already considered in Proposition 5.4 or in (5.38). The terms not considered will exhibit cancellations with the derivatives of $\Psi(f_0^j(x), 0)$.

We will do first the case of first derivatives explicitly. This will be the basis of the induction.

$$\begin{aligned} D_x \Psi(f_0^j(x), f_{x,j}(\Phi(x))) &= (D_1 \Psi)(f_0^j(x), f_{x,j}(\Phi(x))) D_x f_0^j(x) \\ &+ (D_2 \Psi)(f_0^j(x), f_{x,j}(\Phi(x))) D_x f_{x,j}(\Phi(x)) \end{aligned} \quad (5.39)$$

The second term of (5.39) above is controlled in (5.38).

$$|(D_2\Psi)(f_0^j(x), f_{x,j}(\Phi(x)))D_x f_{x,j}(\Phi(x))| \leq C\|\Psi\|_{C^1(\mathcal{U})}j(\tilde{\lambda}\tilde{\mu})^j$$

For the first term, we note that $D_x\Psi(f_0^j(x), 0) = (D_1\Psi)(f_0^j(x), 0)D_x f_0^j(x)$, so that, by the mean value theorem and Proposition 5.4

$$\begin{aligned} |(D_1\Psi)(f_0^j(x), f_{x,j}(\Phi(x)))D_x f_0^j(x) - (D_1\Psi)(f_0^j(x), 0)D_x f_0^j(x)| \\ \leq \|\Psi\|_{C^2(\mathcal{U})}\|f_{x,j} \circ \Phi\|_{C^0(\Lambda)}\|D_x f_0^j\|_{C^0(\mathcal{U})} \\ \leq \|\Psi\|_{C^2(\mathcal{U})}(\tilde{\lambda}\tilde{\mu})^j \end{aligned}$$

These last two bounds imply immediately inequality (5.35) for $k = 1$.

For higher derivatives, we note that all the derivatives of the second term in (5.39) satisfy the desired bounds, so these terms are dealt with.

Hence, when we take higher derivatives, we see that the only terms that we have not shown to satisfy bounds of the desired type are terms in which the second argument of Ψ is not differentiated. The collection of these terms is of the form:

$$\sum_{k=i_1+\dots+i_k} C_{k,i_1,\dots,i_k}(D_1^{i_1}\Psi)(f_0^j(x), f_{x,j}(\Phi(x)))D_x^{i_2}f_0^j(x) \cdots D_x^{i_k}f_0^j(x) \quad (5.40)$$

The combinatorial coefficients $C_{k,i_1,\dots,i_k}$ are the same coefficients that appear in the Faa-di-Bruno expansion of $D_x^k\Psi(f_0^j(x), 0)$. Namely,

$$\begin{aligned} D_x^k\Psi(f_0^j(x), 0) = \\ \sum_{k=i_1+\dots+i_k} C_{k,i_1,\dots,i_k}(D_1^{i_1}\Psi)(f_0^j(x), 0)D_x^{i_2}f_0^j(x) \cdots D_x^{i_k}f_0^j(x) \end{aligned}$$

Therefore, we see that

$$\begin{aligned} D_x^k\Psi(f_0^j(x), f_{x,j}(\Phi(x))) - D_x^k\Psi(f_0^j(x), 0) = \\ \sum_{k=i_1+\dots+i_k} C_{k,i_1,\dots,i_k}[(D_1^{i_1}\Psi)(f_0^j(x), f_{x,j}(\Phi(x))) - (D_1^{i_1}\Psi)(f_0^j(x), 0)] \cdot \\ \cdot D_x^{i_2}f_0^j(x) \cdots D_x^{i_k}f_0^j(x) \\ + O(\|\Psi\|_{C^k(\mathcal{U})}j^k(\tilde{\lambda}\tilde{\mu})^j) \end{aligned}$$

We can use the mean value theorem and (5.38) for $m = 0$, to obtain

$$|(D_1^{i_1}\Psi)(f_0^j(x), 0) - (D_1^{i_1}\Psi)(f_0^j(x), f_{x,j}(\Phi(x)))| \leq C\|\Psi\|_{C^{k+1}(\mathcal{U})}\tilde{\lambda}^j$$

The other factors are bounded in Proposition 5.4.

5.4 A geometric framework for a perturbative calculation of the scattering map

In the applications in [DLS00, DLS03, DLS06a, DLS06b] the scattering map was computed perturbatively in several models.

The goal of this section is to present a geometrically natural set up for a perturbative calculation of the scattering map which will be carried out in next section. As we will see, the final results in Theorem 5.13 and Theorem 5.14 are a generalization and simplification of several results that go under the name of Melnikov theory.

There are two basic ingredients in our calculations that will be developed along this section. First, the theory of normally hyperbolic invariant manifolds shows that the scattering map depends smoothly on parameters. Second, a family of (exact) symplectic mappings σ_ε is conveniently described by observing that $\frac{d}{d\varepsilon}\sigma_\varepsilon$ is a Hamiltonian vector field which, of course, is determined by just a Hamiltonian function.

Along this section we discuss the theory of persistence of normally hyperbolic invariant manifolds and the deformation theory of symplectic mappings. This section does not contain proofs but refers to the literature. The more experienced reader may want to skip them except to get familiar with our notation.

5.4.1 Deformation theory

Deformation theory was introduced in singularity theory [TL71] but soon was used in volume and symplectic geometry [Mos65, Wei79, Ban78]. In [LMM86, BLW96] we can find applications to dynamical systems and normal form theory which are particularly close to our applications.

Let N, M be two connected manifolds. In some applications later, it could happen that $N = M$, but in some other applications, N and M may have different dimensions.

When N, M are assumed to be symplectic (respectively exact symplectic) we will denote the symplectic forms on N, M by ω_N, ω_M (respectively $\omega_N = d\alpha_N, \omega_M = d\alpha_M$).

Given a $\mathbb{C}^r$ family of one to one mappings

$$f_\varepsilon : N \rightarrow M$$

that is, the map $(x, \varepsilon) \mapsto f_\varepsilon(x)$ is a $\mathbb{C}^r$ map in all its arguments for $r \geq 1$, we can define vector fields $\mathcal{F}_\varepsilon$ by

$$\frac{d}{d\varepsilon} f_\varepsilon = \mathcal{F}_\varepsilon \circ f_\varepsilon \quad (5.41)$$

Note that $\mathcal{F}_\varepsilon = (\frac{d}{d\varepsilon} f_\varepsilon) \circ f_\varepsilon^{-1}$ is a vector field defined only on $f_\varepsilon(N)$.

If f_ε is C^r , $r \geq 1$, we can determine a unique $\mathcal{F}_\varepsilon$ which is C^{r-1} . Conversely, from the theory of ODE's, given $f_0 \in C^r$ and $\mathcal{F}_\varepsilon \in C^r$, as above, we can find a unique $f_\varepsilon \in C^r$ satisfying (5.41).

In what follows, we will assume that the regularity is high enough so that we can identify f_ε with the pair $(f_0, \mathcal{F}_\varepsilon)$.

One should heuristically think of $\mathcal{F}_\varepsilon$ as an *infinitesimal deformation*.

We will refer to $\mathcal{F}_\varepsilon$ as the *generator* of the family f_ε . We will use the convention that, given a family denoted by italic letters f_ε , its generator will be denoted by the same letter in calligraphic capitals.

A perturbative calculation of the family f_ε will be for us, a prescription to compute $\mathcal{F}_\varepsilon$.

Remark 5.4. One could think that higher order perturbation theory provides with a way of computing $\frac{d}{d\varepsilon} \mathcal{F}_\varepsilon, \frac{d^2}{d\varepsilon^2} \mathcal{F}_\varepsilon$, etc. We note, however, that in the case that $f_\varepsilon(N)$ is an strict submanifold of M of positive codimension it could well happen that $f_\varepsilon(N) \cap f_{\tilde{\varepsilon}}(N) = \emptyset$ when $\varepsilon \neq \tilde{\varepsilon}$. Hence, the vector fields $\mathcal{F}_\varepsilon$ have disjoint domains. Of course, one can make a geometrically natural definition of these higher derivatives, but it is not quite straightforward.

A Proposition which will be very useful for us is the following

Proposition 5.5. *If $f_\varepsilon : N \rightarrow M$ and $g_\varepsilon : M \rightarrow V$ are one to one mappings and $\mathcal{F}_\varepsilon$ and $\mathcal{G}_\varepsilon$ are their generators, we have:*

1. *If we define $h_\varepsilon = g_\varepsilon \circ f_\varepsilon$, its generator $\mathcal{H}_\varepsilon$ is given by*

$$\mathcal{H}_\varepsilon = \mathcal{G}_\varepsilon + (g_\varepsilon)_* \mathcal{F}_\varepsilon \quad (5.42)$$

where $(g_\varepsilon)_$ is the push-forward:*

$$(g_\varepsilon)_* \mathcal{F}_\varepsilon = Dg_\varepsilon \circ g_\varepsilon^{-1} \mathcal{F}_\varepsilon \circ g_\varepsilon^{-1} = (Dg_\varepsilon \mathcal{F}_\varepsilon) \circ g_\varepsilon^{-1}. \quad (5.43)$$

2. *If $g_\varepsilon \circ f_\varepsilon = \text{Id}$ then*

$$\mathcal{G}_\varepsilon + (g_\varepsilon)_* \mathcal{F}_\varepsilon = 0 \quad (5.44)$$

The proof of the first item of Proposition 5.5 is a simple computation. The second item is a consequence of (5.42) and allows us to compute the generator of the inverses of a family of maps.

It will be important for us to recall that the definition of the push-forward of vector fields (5.43) does not require that g_ε is a diffeomorphism, but only one to one on $f_\varepsilon(N)$.

Note that $\mathcal{H}_\varepsilon$ is defined on $h_\varepsilon(N) = g_\varepsilon(f_\varepsilon(N)) \subset g_\varepsilon(M)$ so, it could well happen that $\mathcal{G}_\varepsilon$ is defined in a larger set than $\mathcal{H}_\varepsilon$.

Note that if f_ε is a smooth family of exact symplectic maps so is dP^{f_ε} . The primitive function P^{f_ε} is defined uniquely up to additive constants. We will assume that these constants are chosen in such a way that P^{f_ε} is also smooth.

To study the relations with geometry, we are interested in studying conditions on $\mathcal{F}_\varepsilon$ that guarantee that f_ε remains symplectic (resp. exact symplectic) when f_0 is.

Proposition 5.6. *Let $f_\varepsilon : N \rightarrow M$ be a smooth family of one to one maps between symplectic manifolds. We have:*

1. If f_0 is symplectic, the necessary and sufficient condition for f_ε to be symplectic is:

$$di_{\mathcal{F}_\varepsilon}\omega_M \in \text{Ker}f_\varepsilon^* \quad (5.45)$$

where we recall that $i_{\mathcal{F}_\varepsilon}\omega_M = \omega_M(\mathcal{F}_\varepsilon, \cdot)$.

2. If f_0 is exact symplectic, the necessary and sufficient condition for f_ε to be exact symplectic is that there exists a family of functions $\psi_\varepsilon : N \rightarrow M$ such that:

$$f_\varepsilon^*(i_{\mathcal{F}_\varepsilon}\omega_M) = d\psi_\varepsilon \quad (5.46)$$

3. In the case that f_ε are diffeomorphisms, we have:

(a) If f_0 is symplectic, f_ε is symplectic if and only if

$$di_{\mathcal{F}_\varepsilon}\omega_M = 0 \quad (5.47)$$

(b) If f_0 is exact symplectic, f_ε is exact symplectic if and only if there exists a family of functions $F_\varepsilon : M \rightarrow \mathbb{R}$ such that:

$$i_{\mathcal{F}_\varepsilon}\omega_M = dF_\varepsilon \quad (5.48)$$

Proof.

If f_0 is symplectic, f_ε is symplectic if and only if $\frac{d}{d\varepsilon}f_\varepsilon^*\omega_M = 0$. Using Cartan's magic formula, we rewrite

$$\begin{aligned} \frac{d}{d\varepsilon}f_\varepsilon^*\omega_M &= f_\varepsilon^*[di_{\mathcal{F}_\varepsilon}\omega_M + i_{\mathcal{F}_\varepsilon}d\omega_M] \\ &= f_\varepsilon^*[di_{\mathcal{F}_\varepsilon}\omega_M] \end{aligned}$$

Hence, f_ε remains symplectic if and only if $f_\varepsilon^*[di_{\mathcal{F}_\varepsilon}\omega_M] = 0$, which is condition (5.45). In the case that f_ε is a diffeomorphism, the necessary and sufficient condition for f_ε to verify (5.45) is (5.47).

In the case that f_0 is exact symplectic, proceeding as before and recalling the definition of the primitive of f_ε (5.17), we see that a necessary and sufficient condition for f_ε to be exact symplectic is that

$$d\left(\frac{d}{d\varepsilon}P^{f_\varepsilon}\right) = \frac{d}{d\varepsilon}f_\varepsilon^*\alpha_M = f_\varepsilon^*[i_{\mathcal{F}_\varepsilon}d\alpha_M + di_{\mathcal{F}_\varepsilon}\alpha_M]$$

That is

$$f_\varepsilon^*[i_{\mathcal{F}_\varepsilon}\omega_M] = d\left[\frac{d}{d\varepsilon}P^{f_\varepsilon} - f_\varepsilon^*i_{\mathcal{F}_\varepsilon}\alpha_M\right] = d\psi_\varepsilon$$

which is condition (5.46) with $\psi_\varepsilon = \frac{d}{d\varepsilon}P^{f_\varepsilon} - f_\varepsilon^*i_{\mathcal{F}_\varepsilon}\alpha_M$.

In the case that f_ε is a diffeomorphism, this is equivalent to (5.48), if we take

$$F_\varepsilon = (f_\varepsilon)_*\left(\frac{d}{d\varepsilon}P^{f_\varepsilon}\right) - i_{\mathcal{F}_\varepsilon}\alpha_M \quad (5.49)$$

□

For exact symplectic deformations, we will refer to F_ε in (5.48) as the *Hamiltonian* for f_ε (note, however that is defined uniquely up to additive constants). We will also use the convention that the Hamiltonian for a family is denoted by the same letter in capitals.

The formula (5.42) simplifies enormously in the case that the two families are exact and admit Hamiltonians.

Proposition 5.7. *If $f_\varepsilon : N \rightarrow M$ and $g_\varepsilon : M \rightarrow V$ are exact symplectic diffeomorphisms generated by their Hamiltonians $F_\varepsilon : M \rightarrow \mathbb{R}$ and $G_\varepsilon : V \rightarrow \mathbb{R}$ respectively, then we have:*

1. If we define $h_\varepsilon = g_\varepsilon \circ f_\varepsilon$, its Hamiltonian H_ε is given by

$$H_\varepsilon = G_\varepsilon + F_\varepsilon \circ g_\varepsilon^{-1} \quad (5.50)$$

2. If $g_\varepsilon \circ f_\varepsilon = \text{Id}$ then

$$G_\varepsilon + F_\varepsilon \circ g_\varepsilon^{-1} = 0 \quad (5.51)$$

In the case of families of exact symplectic diffeomorphisms f_ε , sometimes will be useful to work with the primitive function of the family P^{f_ε} . The next Proposition 5.8 gives us the effect of the deformation on the primitive, and it is a direct consequence of (5.49).

Proposition 5.8. *If $f_\varepsilon : N \rightarrow M$ is a smooth family of exact symplectic diffeomorphisms generated by its Hamiltonian $F_\varepsilon : M \rightarrow \mathbb{R}$ and P^{f_ε} is its primitive, then we have the following formula:*

$$\frac{d}{d\varepsilon} P^{f_\varepsilon} = f_\varepsilon^*(\alpha_M \mathcal{F}_\varepsilon + F_\varepsilon) = f_\varepsilon^*(i_{\mathcal{F}_\varepsilon} \alpha_M + F_\varepsilon) \quad (5.52)$$

5.4.2 Perturbation theory of normally hyperbolic invariant manifolds

The perturbation theory for normally hyperbolic invariant manifolds is a very classical subject [Sac65, Fen72, HPS77, Pes04, Wig94]. In this section we will just summarize the properties of the parameterization method and obtain formulas for geometric objects, especially in the symplectic case.

The goal of this section is to present a convenient framework for the perturbation theory of invariant manifolds.

We recall that the standard perturbation theory of normally hyperbolic invariant manifolds shows that if f_0 has a normally hyperbolic invariant manifold $\Lambda = k_0(N)$, where $k_0 : N \rightarrow \Lambda$ is a diffeomorphism, then there is a C^1 open set of maps that also possess a normally hyperbolic invariant manifold Λ^f . Furthermore, these manifolds are C^1 close to the original one.

It follows from the above considerations, using the implicit function theorem, that given any map f in a C^1 neighborhood of f_0 , one can find a diffeomorphism $k : N \rightarrow \Lambda^f$ in such a way that

$$f \circ k = k \circ r \quad (5.53)$$

where $k : N \rightarrow M$, $r : N \rightarrow N$.

Remark 5.5. Note, however, that the solutions of (5.53) are far from unique. If k, r are solutions of (5.53) and $h : N \rightarrow N$ is any diffeomorphism, we have

$$f \circ (k \circ h) = (k \circ h) \circ (h^{-1} \circ r \circ h)$$

so that

$$\begin{aligned} \tilde{k} &= k \circ h \\ \tilde{r} &= h^{-1} \circ r \circ h \end{aligned} \quad (5.54)$$

is also a solution of (5.53).

The idea is that k is a parameterization of the manifold Λ , r is the dynamics on the manifold in the chosen coordinates, and h represents the possibility of changing coordinates in the *reference manifold* N .

It is a classical result that the manifolds themselves are unique. Hence, all the solutions of (5.53) can be obtained from a solution (k, r) by applying (5.54) with a conveniently chosen h .

Remark 5.6. The study of equation (5.53) provides with an alternative way of establishing the persistence, regularity etc. properties of invariant manifolds.

It is possible to show existence, regularity etc. of normally hyperbolic invariant manifolds by studying the functional analysis properties of (5.53). This method has several desirable properties. For example, it can be used to validate numerical calculations and it leads to efficient algorithms. See [HL06].

For the purposes of this chapter, it is enough to point out that the classical persistence theory of normally hyperbolic invariant manifolds implies the existence of solutions of (5.53). Moreover, the use of (5.53) is very convenient since it is a geometrically natural equation. Hence, it will be very easy to use it to study geometric properties. Also, the geometric naturalness will allow us to compute derivatives in a very efficient manner.

One can study stable and unstable invariant manifolds by studying the equation

$$f \circ k^{s,u} = k^{s,u} \circ r^{s,u} \quad (5.55)$$

where $k^{s,u} : E^{s,u} \rightarrow M$ and $E^{s,u}$ is a bundle over N , $r^{s,u} : E^{s,u} \rightarrow E^{s,u}$ is a bundle map and

$$\begin{aligned} k^{s,u}(\xi, 0) &= k(\xi) \\ r^{s,u}(\xi, 0) &= r(\xi) \\ D_2 k^{s,u}(\xi, 0) E_\xi^{s,u} &= E_x^{s,u} \end{aligned}$$

where E_x^s, E_x^u are the stable and unstable spaces at the point $x = k(\xi)$ in the usual sense of the theory of normally hyperbolic invariant manifolds, see Definition 5.1.

The following is a reformulation of the classical results in the above language (see [Fen72, HPS77]).

Theorem 5.9. *Let $f_\varepsilon : M \rightarrow M$ be a C^r family of diffeomorphisms, $r \geq 2$. Assume that $\Lambda \subset M$ is a normally hyperbolic invariant manifold for f_0 with rates λ, μ as in Definition 5.1. Then for any $\ell < \min(r, \frac{|\log \lambda|}{\log \mu})$ there exists an $\varepsilon_0 > 0$ such that for $|\varepsilon| < \varepsilon_0$ there exist $C^{\ell-1}$ families $k_\varepsilon, r_\varepsilon$ satisfying (5.53), and $C^{\ell-1}$ families $k_\varepsilon^{s,u}, r_\varepsilon^{s,u}$ defined on the unit ball bundle, satisfying (5.55).*

Moreover, there is an open set $U \supset k_0(N) = \Lambda$ in such a way that the set $\Lambda_\varepsilon \equiv k_\varepsilon(N)$ is a normally hyperbolic invariant manifold and verifies

$$\Lambda_\varepsilon \equiv k_\varepsilon(N) = \bigcap_{n \in \mathbb{Z}} f_\varepsilon^n(U) \cap U$$

The parameterizations $k_\varepsilon, r_\varepsilon$ provided by Theorem 5.9 are non unique. We now proceed to fix a suitable ones.

If $f_\varepsilon, k_\varepsilon, r_\varepsilon$ satisfy (5.53), taking derivatives with respect to ε we obtain that their generators (see Proposition 5.5) verify on $k_\varepsilon(N) = \Lambda_\varepsilon$,

$$\mathcal{F}_\varepsilon + (f_\varepsilon)_* \mathcal{K}_\varepsilon = \mathcal{K}_\varepsilon + (k_\varepsilon)_* \mathbb{R}_\varepsilon \quad (5.56)$$

where

$$\begin{aligned} \mathbb{R}_\varepsilon &: N \rightarrow TN \\ \mathcal{F}_\varepsilon &: M \rightarrow TM \\ \mathcal{K}_\varepsilon &: k_\varepsilon(N) = \Lambda_\varepsilon \rightarrow TM \end{aligned}$$

If $x \in \Lambda_\varepsilon$, by Definition 5.1, we have that

$$T_x M = E_x^{s,\varepsilon} \oplus E_x^{u,\varepsilon} \oplus T_x \Lambda_\varepsilon \quad (5.57)$$

If we define the projections $\Pi_x^{s,\varepsilon}, \Pi_x^{u,\varepsilon}, \Pi_x^{c,\varepsilon}$ associated to (5.57), we will call

$$\mathcal{F}_\varepsilon^\alpha(x) = \Pi_x^{\alpha,\varepsilon} \mathcal{F}_\varepsilon(x), \quad \mathcal{K}_\varepsilon^\alpha(x) = \Pi_x^{\alpha,\varepsilon} \mathcal{K}_\varepsilon(x)$$

for $\alpha = s, u, c$.

Due to the fact that (5.57) is invariant under f_ε we have that

$$\Pi^{\alpha,\varepsilon} \circ (f_\varepsilon)_* = (f_\varepsilon)_* \circ \Pi^{\alpha,\varepsilon}.$$

Writing (5.56) as

$$\mathcal{F}_\varepsilon = \mathcal{K}_\varepsilon - (f_\varepsilon)_* \mathcal{K}_\varepsilon + (k_\varepsilon)_* \mathbb{R}_\varepsilon,$$

and taking projections over the splitting (5.57) we obtain that

$$\Pi^{\alpha,\varepsilon} \mathcal{F}_\varepsilon = \Pi^{\alpha,\varepsilon} \mathcal{K}_\varepsilon - \Pi^{\alpha,\varepsilon} (f_\varepsilon)_* \mathcal{K}_\varepsilon + \Pi^{\alpha,\varepsilon} (k_\varepsilon)_* \mathbb{R}_\varepsilon$$

for $\alpha = s, u, c$. Since $(k_\varepsilon)_* \mathbb{R}_\varepsilon$ is tangent to the invariant manifold Λ_ε , (5.56) is equivalent to

$$\begin{aligned} \mathcal{F}_\varepsilon^s &= \mathcal{K}_\varepsilon^s - (f_\varepsilon)_* \mathcal{K}_\varepsilon^s \\ \mathcal{F}_\varepsilon^u &= \mathcal{K}_\varepsilon^u - (f_\varepsilon)_* \mathcal{K}_\varepsilon^u \\ \mathcal{F}_\varepsilon^c &= \mathcal{K}_\varepsilon^c - (f_\varepsilon)_* \mathcal{K}_\varepsilon^c + (k_\varepsilon)_* \mathbb{R}_\varepsilon. \end{aligned} \quad (5.58)$$

We know that $k_\varepsilon, r_\varepsilon$ are not unique. A particularly useful choice of them is the following.

Theorem 5.10. *There exist unique $k_\varepsilon, r_\varepsilon$ such that*

$$\mathcal{K}_\varepsilon^c = 0. \quad (5.59)$$

Proof. If we fix (5.59), then the solution of the third equation in (5.58) is clearly $\mathcal{F}_\varepsilon^c = (k_\varepsilon)_* \mathbb{R}_\varepsilon$. The $\mathcal{K}_\varepsilon^s, \mathcal{K}_\varepsilon^u$ are determined uniquely by (5.58) because, by the definition of the invariant bundles, a sufficiently large power of $f_{\varepsilon*}$ is a contraction on E_ε^s and a sufficiently large power of $f_{\varepsilon*}^{-1}$ is a contraction on E_ε^u . $\square$

One can think that the deformation thus selected is the most economical one since $\mathcal{K}_\varepsilon$, the change of the embedding, moves only on the stable and unstable directions. As we will see in Section 5.4.3 when we discuss symplectic properties, the normalization (5.59) is also natural from the symplectic point of view and leads to interesting symplectic consequences.

Remark 5.7. The equation (5.56) can be used as the basis of a formal perturbation expansion that can be carried out to high orders in ε .

If we assume that $f_\varepsilon, \mathcal{F}_\varepsilon$ can be expanded in powers of ε , we obtain after equating terms of order n in ε

$$(f_0)_*\mathcal{K}^n - \mathcal{K}^n = \mathcal{F}^n + (k_0)_*\mathbb{R}^n + \mathcal{A}_n(\) \quad (5.60)$$

where $\mathcal{A}_n$ is a polynomial expression involving $\mathcal{K}_1, \dots, \mathcal{K}_{n-1}, \mathbb{R}_1, \dots, \mathbb{R}_{n-1}$ and their derivatives up to an order not bigger than $n-1$.

Since $\Lambda = k_0(N)$ is a normally hyperbolic invariant manifold, we know that f_0 verifies (5.1), and then equation (5.60) admits C^0 solutions provided that the right hand side is a C^0 function.

Indeed, the theory of cohomology equations over hyperbolic systems shows that the solutions are C^s when the right hand side is C^s and $s \leq \ell - 1$.

Hence, it follows that the perturbation theory (5.60) can be carried out up to the order $\ell - 1$ which appears as a limit of the regularity of the manifold in Theorem 5.9.

An interesting particular case is when the motion given by f_0 is integrable when restricted to the invariant manifold $\Lambda = k_0(N)$. This situation occurs in the problems considered in [DLS00, DLS03, DLS06a, DLS06b, GL06]. In such a case, the dynamics by f_0 on Λ has a simple expression and one can carry out the perturbation theory to all orders less or equal than r in ε . In those papers, one can find detailed perturbative formulas to order $m \leq r$ with error estimates. However, there are examples that show that, even if the family f_ε is analytic, the manifold Λ_ε is not C^∞ in ε and much less analytic.

5.4.3 Symplectic properties of normally hyperbolic invariant manifolds

In this section we study the effect of symplectic properties of f_ε on the manifold Λ_ε . Since the deformation method deals very well with geometric properties [Ban78, LM87, BLW96], we will obtain very simple formulas.

The main result of this section is:

Theorem 5.11. *In the same conditions of Theorem 5.9, assume furthermore that*

A) *M is endowed with a symplectic form ω (resp. $\omega = d\alpha$ is an exact symplectic form) and $\omega|_\Lambda$ is a symplectic form.*

B) *$(f_\varepsilon)_*\omega = \omega$ (resp. $(f_\varepsilon)_*\alpha = \alpha + dP^f$),*

Let $k_\varepsilon, r_\varepsilon$ be as in Theorem 5.10, that is, $\mathcal{K}_\varepsilon$ satisfies (5.59). Then:

- 1) *$k_\varepsilon^*\omega \equiv \omega_N$ is a symplectic form (resp. exact symplectic form) in N . It is independent of ε .*
- 2) *The vector field $\mathbb{R}_\varepsilon$ is Hamiltonian (resp. exact Hamiltonian) with respect to ω_N . Moreover, its local Hamiltonian (resp. global Hamiltonian) is*

$$R_\varepsilon = F_\varepsilon \circ k_\varepsilon \quad (5.61)$$

where F_ε is a local Hamiltonian for f_ε (resp. a global Hamiltonian).

Formula (5.61) can be considered as a perturbative calculation of the map r_ε since it allows us to compute the Hamiltonian of $\mathbb{R}_0 = \frac{dr_\varepsilon}{d\varepsilon}|_{\varepsilon=0} \circ r_0^{-1}$, the derivative of the map r_ε , once we know the unperturbed manifold and $\mathcal{F}_0 = \frac{df_\varepsilon}{d\varepsilon}|_{\varepsilon=0} \circ f_0^{-1}$.

Remark 5.8. Note that the choice of the identification k_ε in such a way that it is symplectic from N to Λ_ε endowed with the restrictions of the global symplectic forms is a generalization of the constructions in Section 8.1 of [DLS06b]. There, as $\Lambda = N$ and k_0 was simply the trivial inclusion, the system of coordinates on Λ_ε was chosen in such a way that $k_\varepsilon^*\omega|_{\Lambda_\varepsilon}$ took the standard form, which in the case considered was just $\omega|_N$.

Proof

If ω is a 2-form on M invariant under f_ε , for every $u, v \in T_x M$ and $n \in \mathbb{Z}$ we have

$$\omega(x)(u, v) = \omega(f_\varepsilon^n(x))(Df_\varepsilon^n(x)u, Df_\varepsilon^n(x)v) \quad (5.62)$$

Applying repeatedly (5.62) and taking into account the different rates of growth in Definition 5.1, we have that

$$\omega(x)(u, v) = 0$$

in the following cases

$$u \in E_x^{c,\varepsilon} = T_x \Lambda_\varepsilon, v \in E_x^{s,u,\varepsilon} \text{ (or vice versa)}$$

$$u \in E_x^{s,\varepsilon}, v \in E_x^{s,\varepsilon}$$

$$u \in E_x^{u,\varepsilon}, v \in E_x^{u,\varepsilon}$$

So that, with respect to the decomposition

$$T_x M = E_x^{s,\varepsilon} \oplus E_x^{u,\varepsilon} \oplus E_x^{c,\varepsilon}$$

The symplectic form $\omega(x)$ is represented by a matrix

$$\left(\begin{array}{c|c|c} 0 & \omega^{su} & 0 \\ \hline -\omega^{su} & 0 & 0 \\ \hline 0 & 0 & \omega|_{E^c} \end{array} \right) \quad (5.63)$$

Since $d\omega = 0$ (resp. $\omega = d\alpha$) and Λ_ε is an invariant manifold for f_ε we obtain that $d_{\Lambda_\varepsilon} \omega|_{\Lambda_\varepsilon} = 0$ where d_{Λ_ε} denotes the exterior differential in Λ_ε (resp. we have $\omega|_{\Lambda_\varepsilon} = d_{\Lambda_\varepsilon} \alpha|_{\Lambda_\varepsilon}$).

Because of the openness of non-degeneracy and using that $\omega|_{\Lambda}$ is a symplectic form, as well as the stability properties of normally hyperbolic invariant manifolds, we obtain that the perturbed normally hyperbolic invariant manifolds Λ_ε are symplectic.

Hence, we can define a symplectic form $\omega_{\varepsilon,N}$ on N by

$$\omega_{\varepsilon,N} = k_\varepsilon^*(\omega|_{\Lambda_\varepsilon}) \quad (5.64)$$

Note that $\omega_{\varepsilon,N}$ depends on k_ε , which is not uniquely determined. Nevertheless, we will not include the k_ε in the notation unless it can lead to confusion. In Lemma 5.12 we will show that if k_ε is chosen to satisfy (5.59), $\omega_{\varepsilon,N}$ is constant. This reinforces the notion that (5.59) is a very natural normalization to avoid the non-uniqueness in (5.53).

A consequence of (5.53) is that

$$(f_\varepsilon \circ k_\varepsilon)^* \omega = (k_\varepsilon \circ r_\varepsilon)^* \omega.$$

Therefore

$$k_\varepsilon^* f_\varepsilon^* \omega = r_\varepsilon^* k_\varepsilon^* \omega$$

using that $f_\varepsilon^* \omega = \omega$ and the definition of $\omega_{\varepsilon,N}$, we obtain

$$\omega_{\varepsilon,N} = r_\varepsilon^* \omega_{\varepsilon,N} \quad (5.65)$$

In other words, r_ε is a symplectic map with respect to the form $\omega_{\varepsilon,N}$.

If ω is exact and f_ε^* is exact we have

$$k_\varepsilon^* f_\varepsilon^* \alpha = k_\varepsilon^* (\alpha + dP^{f_\varepsilon}) = k_\varepsilon^* \alpha + d_N(k_\varepsilon^* P^{f_\varepsilon})$$

Hence, as $k_\varepsilon^* f_\varepsilon^* \alpha = r_\varepsilon^* k_\varepsilon^* \alpha$, denoting $\alpha_{\varepsilon,N} = k_\varepsilon^* \alpha$,

$$r_\varepsilon^* \alpha_{\varepsilon,N} = \alpha_{\varepsilon,N} + d_N(k_\varepsilon^* dP^{f_\varepsilon}) \quad (5.66)$$

so that r_ε^* is also exact symplectic.

The proof of $R_\varepsilon = F_\varepsilon \circ k_\varepsilon$ is only a computation:

$$\begin{aligned} d(F_\varepsilon \circ k_\varepsilon) &= k_\varepsilon^* dF_\varepsilon = k_\varepsilon^* (i_{\mathcal{F}_\varepsilon} \omega|_{\Lambda_\varepsilon}) \\ &= k_\varepsilon^* (i_{\mathcal{F}_\varepsilon^c} \omega|_{\Lambda_\varepsilon} + i_{\mathcal{F}_\varepsilon^u} \omega|_{\Lambda_\varepsilon} + i_{\mathcal{F}_\varepsilon^s} \omega|_{\Lambda_\varepsilon}) \\ &= k_\varepsilon^* (i_{\mathcal{F}_\varepsilon^c} \omega|_{\Lambda_\varepsilon}) = i_{k_\varepsilon^* \mathcal{F}_\varepsilon^c} k_\varepsilon^* \omega|_{\Lambda_\varepsilon} = i_{\mathbb{R}_\varepsilon} \omega_{\varepsilon,N} \end{aligned}$$

The only thing remaining to obtain Theorem 5.11 is the following:

Lemma 5.12. *With the notations above, if we choose k_ε satisfying (5.59) as in Theorem 5.10, we have that $\omega_{\varepsilon,N}$ is independent of ε , that is*

$$\omega_{\varepsilon,N} = \omega_{0,N}$$

Proof. We compute $\frac{d}{d\varepsilon}\omega_{\varepsilon,N}$ using Cartan's "magic" formula

$$\begin{aligned} \frac{d}{d\varepsilon}\omega_{\varepsilon,N} &= \frac{d}{d\varepsilon}k_\varepsilon^*\omega \\ &= k_\varepsilon^*(i_{\mathcal{K}_\varepsilon}d\omega + di_{\mathcal{K}_\varepsilon}\omega) \\ &= k_\varepsilon^*di_{\mathcal{K}_\varepsilon}\omega \\ &= d_Nk_\varepsilon^*i_{\mathcal{K}_\varepsilon}\omega \end{aligned}$$

Now, we claim that

$$k_\varepsilon^*i_{\mathcal{K}_\varepsilon}\omega = 0.$$

We have that, by definition, the 1-form $k_\varepsilon^*i_{\mathcal{K}_\varepsilon}\omega$ acting on a vector $v \in T_xN$ is defined by

$$(k_\varepsilon^*i_{\mathcal{K}_\varepsilon}\omega(x))v = (i_{\mathcal{K}_\varepsilon}\omega(k_\varepsilon(x)))(dk_\varepsilon(x)v) = \omega(k_\varepsilon(x))(\mathcal{K}_\varepsilon(k_\varepsilon(x)), dk_\varepsilon(x)v)$$

Now, we observe that, by (5.59)

$$\mathcal{K}_\varepsilon \circ (k_\varepsilon(x)) \in E_{k_\varepsilon(x)}^s \oplus E_{k_\varepsilon(x)}^u$$

whereas

$$dk_\varepsilon(x) \in E_{k_\varepsilon(x)}^c$$

By (5.63) we obtain the desired result. $\square$

5.5 Perturbative formulas for the scattering map

In this section we are going to study a $\mathbb{C}^r$ family of symplectic diffeomorphisms $f_\varepsilon : M \rightarrow M$, where f_0 has a normally hyperbolic invariant manifold Λ such that $\omega|_\Lambda$ is non-degenerate and has also a homoclinic channel Γ verifying Definition 5.2, so that, there exists a scattering map $\sigma_0 = \sigma^\Gamma : H^- \rightarrow H^+$ as in (5.10).

Then, if ε is small enough, the theory of normally hyperbolic invariant manifolds (see Theorem 5.9) and the persistence of condition (5.5), (5.6) ensures that there exist a normally hyperbolic invariant manifold Λ_ε and a homoclinic channel Γ_ε and then it is possible to consider the scattering map $\sigma_\varepsilon := \sigma_\varepsilon^{\Gamma_\varepsilon} : H_\varepsilon^- \rightarrow H_\varepsilon^+$ defined in some domain $H_\varepsilon^- \subset \Lambda_\varepsilon$ close to H^- .

Remark 5.9. Note that, from Definition 5.2, smoothness and smoothness with respect to parameters of the scattering map follow using the implicit function theorem from the corresponding properties for the homoclinic channel Γ .

A situation that has been considered very often in the literature is a family of maps indexed by ε such that for $\varepsilon = 0$ the stable and unstable manifolds of Λ coincide.

In such a case, it is natural to consider some first order perturbation theory about the breaking of the connection. Using an adapted Melnikov method, in [DLS06a] it is shown that, under appropriate conditions, for $0 < |\varepsilon| \ll 1$, one can find transversal intersections along a manifold Γ_ε . Furthermore, it is possible to show that the manifold Γ_ε extends smoothly in ε across $\varepsilon = 0$. In this case, it also follows that the scattering map extends also smoothly across $\varepsilon = 0$.

Of course, the limiting manifold Γ_0 is not a transversal intersection. Nevertheless, it follows from the theory in the above reference that the projections $\Omega_\pm^{\Gamma_\varepsilon}$ depend smoothly on parameters and that they extend to $\Omega_\pm^{\Gamma_0}$.

In particular, we note that, when $\Omega_+^{\Gamma_0}$ is invertible in an open domain—this follows from the implicit function theorem under non-degeneracy conditions—then the scattering map has a domain which can be chosen uniform in ε .

By Theorem 5.4, the scattering map σ_ε defined in (5.10) is symplectic, so it is very natural to develop formulas for the Hamiltonian that generates its deformation $\frac{d}{d\varepsilon}\sigma_\varepsilon$.

Unfortunately, in doing so, we are faced with the annoyance that the domain of σ_ε is contained in Λ_ε . Since Λ_ε is a submanifold of positive codimension, it could happen that Λ_ε is disjoint from $\Lambda_{\varepsilon'}$ when $\varepsilon \neq \varepsilon'$, hence there is no common domain for all σ_ε , so that the $\frac{d}{d\varepsilon}\sigma_\varepsilon$ is not easy to interpret.

Fortunately, the cure of this annoyance is rather easy. We have shown in Theorem 5.10 and Theorem 5.11 that there is a unique symplectic parameterization k_ε between the reference manifold N and the normally hyperbolic invariant manifold Λ_ε . So, we consider

$$s_\varepsilon = k_\varepsilon^{-1} \circ \sigma_\varepsilon \circ k_\varepsilon : (k_\varepsilon)^{-1}(H_\varepsilon^-) \subset N \longrightarrow (k_\varepsilon)^{-1}(H_\varepsilon^+) \subset N$$

Hence, our goal in this section is to give formulas for the Hamiltonian function S_ε which generates the deformation $\S_\varepsilon$ of the scattering map s_ε .

The main result of this section is Theorem 5.13, which contains formula (5.67) which expresses the Hamiltonian S_ε of the deformation of the scattering map s_ε in terms of the orbit appearing in the connection, and the Hamiltonian F_ε of the change of the map f_ε . We note that the formula and the calculation leading to it are coordinate independent.

In Section 5.5.2 we derive formula (5.72) which expresses the primitive P^{s_ε} of the deformation of the scattering map s_ε in terms of the primitive P^{f_ε} of the change of the map in the case that f_ε is exact symplectic.

An analogous result to Theorem 5.13 for the case of Hamiltonian flows is provided in Theorem 5.14. The proofs of theorem 5.13 and Theorem 5.14 are given respectively in sections 5.5.1 and 5.5.3, and some heuristic considerations relating the proofs of theorems 5.13 and 5.6 are given in section 5.5.4.

Remark 5.10. From the point of view of applications it is very natural to study the Hamiltonian S_ε . In [DLS00, DLS03, DLS06a, DLS06b] the mechanism of diffusion involved comparing the inner dynamics of the map $r_\varepsilon = k_\varepsilon^{-1} \circ f_\varepsilon \circ k_\varepsilon$ with the outer dynamics of the scattering map s_ε . Roughly, one could get diffusion provided that the inner dynamics and the scattering map were transversal. This comparison can be achieved in any system of coordinates provided that we choose the same coordinates for both maps.

In Theorem 5.11 we computed the Hamiltonian R_ε for r_ε so that, the combination of formula (5.61) for R_ε and formula (5.67) for S_ε will provide the desired comparison. In the above papers one can find calculations up to first order in ε which agree with the ones presented here. See Section 5.6 for a detailed comparison in the case of geodesic flows.

The main result of this section is

Theorem 5.13. *Let $f_\varepsilon : M \rightarrow M$ be a $\mathbb{C}^r$ family of symplectic diffeomorphisms where f_0 has a normally hyperbolic invariant manifold Λ such that $\omega|_\Lambda$ is non-degenerate and also has a homoclinic channel Γ verifying Definition 5.2, so that there exists a scattering map $\sigma_0 = \sigma^\Gamma : H^- \rightarrow H^+$ as in (5.10).*

Assume also that the parameterization k_ε of the perturbed normally hyperbolic invariant manifold Λ_ε verifies (5.59), and denote $s_\varepsilon = k_\varepsilon^{-1} \circ \sigma_\varepsilon \circ k_\varepsilon$, where σ_ε is the perturbed scattering map associated to the perturbed homoclinic channel Γ_ε . Then, denoting $\Gamma_\varepsilon^N = f_\varepsilon^N(\Gamma_\varepsilon)$, the Hamiltonian for s_ε is given by

$$\begin{aligned} S_\varepsilon &= \lim_{N_\pm \rightarrow +\infty} \sum_{j=0}^{N_- - 1} F_\varepsilon \circ f_\varepsilon^{-j} \circ (\Omega_{\varepsilon^-}^{\Gamma_\varepsilon})^{-1} \circ \sigma_\varepsilon^{-1} \circ k_\varepsilon - F_\varepsilon \circ f_\varepsilon^{-j} \circ \sigma_\varepsilon^{-1} \circ k_\varepsilon \\ &\quad + \sum_{j=1}^{N_+} F_\varepsilon \circ f_\varepsilon^j \circ (\Omega_{\varepsilon^+}^{\Gamma_\varepsilon})^{-1} \circ k_\varepsilon - F_\varepsilon \circ f_\varepsilon^j \circ k_\varepsilon \\ &= \lim_{N_\pm \rightarrow +\infty} \sum_{j=0}^{N_- - 1} F_\varepsilon \circ f_\varepsilon^{-j} \circ (\Omega_{\varepsilon^-}^{\Gamma_\varepsilon})^{-1} \circ k_\varepsilon \circ s_\varepsilon^{-1} - F_\varepsilon \circ k_\varepsilon \circ r_\varepsilon^{-j} \circ s_\varepsilon^{-1} \\ &\quad + \sum_{j=1}^{N_+} F_\varepsilon \circ f_\varepsilon^j \circ (\Omega_{\varepsilon^+}^{\Gamma_\varepsilon})^{-1} \circ k_\varepsilon - F_\varepsilon \circ k_\varepsilon \circ r_\varepsilon^j \end{aligned} \tag{5.67}$$

In the case that our family of maps f_ε correspond to the time T flow of a Hamiltonian vector field $\mathcal{H}_\varepsilon$ of Hamiltonian H_ε we can adapt the previous result to obtain a formula for the Hamiltonian S_ε of the scattering map $s_\varepsilon = s^{\Gamma, \mathcal{H}_\varepsilon}$, that was shown in (5.15) that is independent of T .

Concretely, we have the following

Theorem 5.14. *Let $\Phi_{t,\varepsilon}(x)$ be the flow of a Hamiltonian vector field of Hamiltonian $H_\varepsilon(x)$ and consider the family given by the time T map of this flow, that is, $f_\varepsilon(x) = \Phi_{T,\varepsilon}(x)$. Assume that this map has a*

normally hyperbolic invariant manifold Λ_ε and that its parameterization verifies (5.59). Denoting by S_ε the Hamiltonian generating the deformation of s_ε , it is given by

$$\begin{aligned} S_\varepsilon = & \lim_{T_\pm \rightarrow \infty} \int_{-T_-}^0 \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ (\Omega_{\varepsilon_-}^{\Gamma_\varepsilon})^{-1} \circ (\sigma_\varepsilon)^{-1} \circ k_\varepsilon \\ & - \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ (\sigma_\varepsilon)^{-1} \circ k_\varepsilon \\ & + \int_0^{T_+} \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ (\Omega_{\varepsilon_+}^{\Gamma_\varepsilon})^{-1} \circ k_\varepsilon - \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ k_\varepsilon \end{aligned} \quad (5.68)$$

Remark 5.11. We call attention to the similarities between the formulas (5.67) and (5.68) and the formulas (5.28) and (5.29). In Appendix 5.7, we remark the analogy with the perturbative formulas for the scattering matrix in quantum mechanics. Some heuristic reason explaining these similarities is discussed in Section 5.5.4.

It is important to note that the sums and the integrals in (5.67) and (5.68) converge uniformly together with several of their derivatives. The argument, which is given in Theorem 5.8, is the same as in the discussion of Theorem 5.6.

Formula (5.67) is closely related to the following formula, which is true for any $N_-, N_+ \in \mathbb{Z}$:

$$s_\varepsilon = k_\varepsilon^{-1} \circ f_\varepsilon^{-N_+} \circ \Omega_{\varepsilon_+}^{\Gamma_\varepsilon^{N_+}} \circ f_\varepsilon^{N_++N_-} (\Omega_{\varepsilon_-}^{\Gamma_\varepsilon^{-N_-}})^{-1} \circ f_\varepsilon^{-N_-} \circ k_\varepsilon \quad (5.69)$$

The formula (5.69) is a direct consequence of the formula (5.31).

Formulas (5.67) and (5.68) are analogous to formula (5.90) in quantum mechanics in the appendix.

5.5.1 Proof of Theorem 5.13

The proof will be based on studying (5.69), computing the Hamiltonian of its deformation and taking limits when $N_\pm \rightarrow \infty$.

One minor annoyance is that it is hard to adjust the domains because the wave operators $\Omega_{\varepsilon_\pm}^{\Gamma_\varepsilon}$ are defined in Γ_ε and then, their domains depend on ε .

As it turns out, it is possible to introduce identification maps for all the Γ_ε^n with Γ_0^n , so that the calculation can be referred to the Γ_0^n 's. Even if this technology could be interesting on its own right, we have followed another technically simpler route.

We will perform an extension of $\Omega_{\varepsilon_\pm}^{\Gamma_\varepsilon^n}$ to open sets of the manifold M independent of ε . This will allow us to consider the maps in (5.69) as defined in open sets of the whole manifold M and not only in Γ_ε^n . Then, applying Proposition 5.7 we will obtain a formula for finite $N_\pm$. When we take limits as $N_\pm \rightarrow \infty$, we will obtain the desired formula (5.67). In particular, the terms corresponding to the wave operators $\Omega_{\varepsilon_\pm}^{\Gamma_\varepsilon^n}$ will disappear in the limit as $N_\pm \rightarrow \infty$.

We start the proof by establishing a technical extension result that we will use to extend $\Omega_{\varepsilon_\pm}^{\Gamma_\varepsilon}$.

Recall that, by the λ -lemma, the manifolds Γ_ε^n are getting $C^{\ell-1}$ close to Λ_ε when $n \rightarrow \pm\infty$. The dependence on parameters is also $C^{\ell-1}$.

Given a submanifold N , let $\rho > 0$ be small enough such that its exponential mapping is a local diffeomorphism in a neighborhood in any ball of radius ρ centered at any $x \in N$.

We denote $\hat{N}_\rho = \{y \in M \mid \text{dist}(y, N) < \rho\}$.

Proposition 5.9. *Let (M, ω) be a symplectic manifold. Let $N, \Gamma_\varepsilon^n \subset M$ be symplectic submanifolds. Assume that:*

- a) *there exist $\mathbb{C}^r$ families of maps $h_\varepsilon^n : N \rightarrow \Gamma_\varepsilon^n$ such that $\|h_\varepsilon^n\|_{C^r(N)} \leq \delta$. (The C^r -norm is understood in all the variables including ε .)*
- b) *h_ε^n are symplectic from N to Γ_ε^n .*
- c) *$\|\partial_\varepsilon h_\varepsilon^n\|_{C^{r-1}(N)} \rightarrow 0$, when $n \rightarrow \infty$ (as $n \rightarrow -\infty$)*

Then, it is possible to find $\hat{h}_\varepsilon^n : \hat{N}_\rho \rightarrow M$ such that:

- i) $\hat{h}_\varepsilon^n|_N = h_\varepsilon^n$
- ii) $\|\hat{h}_\varepsilon^n\|_{C^r(\hat{N}_\rho)} \leq 2\delta$

iii) $\|\partial_\varepsilon \hat{h}_\varepsilon^n\|_{C^{r-1}(\hat{N}_\rho)} \rightarrow 0$, when $n \rightarrow \infty$ (or $n \rightarrow -\infty$)

iv) $\hat{h}_\varepsilon^n$ are symplectic

Proof. Given $\rho > 0$ small enough, as $T_x M = T_x N \oplus E_x^\perp$ (where we use $E_x^\perp \equiv E_x^s \oplus E_x^u$), we have that given $p \in \hat{N}_\rho$, there exist $x \in N$ and $v \in E_x^\perp$ such that $\exp_x(v) = p$. We can extend the families of diffeomorphisms h_ε^n to some families $\tilde{h}_\varepsilon^n$ satisfying i), ii), iii) using e.g., the identifications given by the exponential mapping and the Levi-Civita connection

$$\tilde{h}_\varepsilon^n(\exp_x(v)) = \exp_{h_\varepsilon^n(x)}(\tilde{v})$$

where $\tilde{v}$ denotes the transportation of v along the shortest geodesic connecting x to $h_\varepsilon^n(x)$.

Of course, the resulting mapping will not be symplectic. Nevertheless we note that

$$\|(\tilde{h}_\varepsilon^n)^* \omega - \omega\|_{C^{\ell-2}(\hat{N}_\rho)} = O(\rho)$$

Now, we can apply the global Darboux theorem with dependence on parameters [BLW96] to find families of diffeomorphisms g_ε^n such that

$$(g_\varepsilon^n)_*(\tilde{h}_\varepsilon^n)_* \omega = \omega$$

The desired diffeomorphism is $\hat{h}_\varepsilon^n = g_\varepsilon^n \circ \tilde{h}_\varepsilon^n$. □

Denoting $h_{\varepsilon\pm}^n = (\Omega_{\varepsilon\pm}^{\Gamma_n})^{-1} \circ k_\varepsilon$ we know, by Lemma 5.5, Theorem 5.11 and the λ -lemma applied to the normally hyperbolic invariant manifold Λ_ε , that the diffeomorphisms $h_{\varepsilon,\pm}^n$ verify the hypotheses of Proposition 5.9. Therefore, we obtain extensions $\hat{h}_{\varepsilon\pm}^n$ and $(\hat{h}_{\varepsilon\pm}^n)^{-1}$ of their inverses.

Using this notation and (5.54), formula (5.69) reads:

$$\begin{aligned} s_\varepsilon &= r_\varepsilon^{-N_+} \circ (k_\varepsilon)^{-1} \circ \Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}^{N_+}} \circ f_\varepsilon^{N_++N_-} (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon-}^{-N_-}})^{-1} \circ k_\varepsilon \circ r_\varepsilon^{-N_-} \\ &= r_\varepsilon^{-N_+} \circ (h_{\varepsilon+}^{N_+})^{-1} \circ f_\varepsilon^{N_++N_-} h_{\varepsilon-}^{-N_-} \circ r_\varepsilon^{-N_-} \end{aligned}$$

As the extensions of $h_{\varepsilon\pm}^{N_\pm}$ coincide with the original functions in their domain of definition N , we have that the formula for the scattering map does not change if we use the extensions $\hat{h}_{\varepsilon\pm}^{N_\pm}$. So we have the diffeomorphism $s_\varepsilon : N \rightarrow N$ defined by

$$s_\varepsilon = r_\varepsilon^{-N_+} \circ (\hat{h}_{\varepsilon+}^{N_+})^{-1} \circ f_\varepsilon^{N_++N_-} \circ \hat{h}_{\varepsilon-}^{-N_-} \circ r_\varepsilon^{-N_-} \quad (5.70)$$

Applying repeatedly Proposition 5.7 to formula (5.70), we obtain that the Hamiltonian of s_ε is

$$\begin{aligned} S_\varepsilon &= - \left(R_\varepsilon \circ r_\varepsilon^{N_+} + \dots + R_\varepsilon \circ r_\varepsilon \right) \\ &\quad - H_{\varepsilon+}^{N_+} \circ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} \\ &\quad + \left(F_\varepsilon + F_\varepsilon \circ f_\varepsilon^{-1} + \dots + F_\varepsilon \circ f_\varepsilon^{-N_+-N_-+1} \right) \circ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} \\ &\quad + H_{\varepsilon-}^{-N_-} \circ f_\varepsilon^{-N_- - N_+} \circ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} \\ &\quad - \left(R_\varepsilon \circ r_\varepsilon^{N_-} + \dots + R_\varepsilon \circ r_\varepsilon \right) \circ (\hat{h}_{\varepsilon-}^{-N_-})^{-1} \circ f_\varepsilon^{-N_- - N_+} \circ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} \end{aligned}$$

As the parameterization for the invariant manifold verifies normalization (5.59), we know that the Hamiltonian of the restricted map r_ε is given in formula (5.61) by $R_\varepsilon = F_\varepsilon \circ k_\varepsilon$. Since S_ε is defined in N , we have that $\hat{h}_{\varepsilon\pm}^n = h_{\varepsilon\pm}^n = (\Omega_{\varepsilon\pm}^{\Gamma_n})^{-1} \circ k_\varepsilon$, and using also formula (5.9) for the wave operators $\Omega_{\varepsilon\pm}^{\Gamma_n}$ and (5.54), we can easily obtain that

$$\begin{aligned} R_\varepsilon \circ r_\varepsilon^n &= F_\varepsilon \circ k_\varepsilon \circ r_\varepsilon^n = F_\varepsilon \circ f_\varepsilon^n \circ k_\varepsilon \\ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} &= (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}^{N_+}})^{-1} \circ k_\varepsilon \circ r_\varepsilon^{N_+} = (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}^{N_+}})^{-1} \circ f_\varepsilon^{N_+} \circ k_\varepsilon \\ &= f_\varepsilon^{N_+} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}})^{-1} \circ k_\varepsilon \\ f_\varepsilon^{-N_- - N_+} \circ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} &= f_\varepsilon^{-N_- - N_+} \circ f_\varepsilon^{N_+} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}})^{-1} \circ k_\varepsilon \\ &= f_\varepsilon^{-N_-} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}})^{-1} \circ k_\varepsilon \\ (\hat{h}_{\varepsilon-}^{-N_-})^{-1} \circ f_\varepsilon^{-N_- - N_+} \circ \hat{h}_{\varepsilon+}^{N_+} \circ r_\varepsilon^{N_+} &= k_\varepsilon^{-1} \circ \Omega_{\varepsilon-}^{\Gamma_{\varepsilon-}^{-N_-}} \circ f_\varepsilon^{-N_-} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}})^{-1} \circ k_\varepsilon \\ &= (k_\varepsilon)^{-1} \circ f_\varepsilon^{-N_-} \circ \Omega_{\varepsilon-}^{\Gamma_{\varepsilon-}} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon+}})^{-1} \circ k_\varepsilon \\ &= (k_\varepsilon)^{-1} \circ f_\varepsilon^{-N_-} \circ \sigma_\varepsilon^{-1} \circ k_\varepsilon \end{aligned}$$

And we obtain the following formula, for any $N_{\pm}$

$$\begin{aligned}
S_{\varepsilon} &= \sum_{j=1}^{N_+} F_{\varepsilon} \circ f_{\varepsilon}^j \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ f_{\varepsilon}^j \circ k_{\varepsilon} \\
&+ \sum_{j=0}^{N_- - 1} F_{\varepsilon} \circ f_{\varepsilon}^{-j} \circ (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}})^{-1} \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ f_{\varepsilon}^j \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon} \\
&- H_{\varepsilon+}^{N_+} \circ f_{\varepsilon}^{N_+} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} \\
&+ H_{\varepsilon-}^{-N_-} \circ f_{\varepsilon}^{-N_-} \circ (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon}
\end{aligned}$$

Now we observe that, by property (iii) in Proposition 5.9, the Hamiltonians $H_{\varepsilon\pm}^{\pm N_{\pm}}$, corresponding to the projections $\hat{h}_{\varepsilon\pm}^{N_{\pm}}$, which are the extensions of $h_{\varepsilon\pm}^{N_{\pm}} = (\Omega_{\varepsilon\pm}^{\Gamma_{\varepsilon}^{N_{\pm}}})^{-1} \circ k_{\varepsilon}$ converge to zero in the sense of families. Then, taking the limit when $N_{\pm} \rightarrow \infty$ we obtain the desired formula (5.67).

The second expression for the Hamiltonian in formula (5.67) is a simple consequence of the fact that $\sigma_{\varepsilon} \circ k_{\varepsilon} = k_{\varepsilon} \circ s_{\varepsilon}$ and that $f_{\varepsilon} \circ k_{\varepsilon} = k_{\varepsilon} \circ r_{\varepsilon}$.

5.5.2 The primitive function of the scattering map s_{ε}

In Theorems 5.6 and 5.7 we have obtained formulas for the primitive P^{σ} of a scattering map σ on a normally hyperbolic invariant manifold for a exact symplectic map f . On the other hand, in applications, it is useful to deal with families of maps (or flows) and invariant manifolds. As we have already mentioned in Section 5.4.2, to deal with functions defined in families of mappings, it is natural to use a parameterization to reduce the family of maps to maps defined on a reference manifold. Moreover, the applications to diffusion in [DLS06a] rely on the interplay between the scattering map and the dynamics restricted to the manifold.

Therefore, the goal of this section is to obtain expressions for the primitive function of the map s_{ε} , which is the expression of the scattering map in the reference manifold.

The primitive function of the inner map r_{ε} is very easy from the properties of restriction. Recall that, since $k_{\varepsilon}^* \alpha_{\Lambda_{\varepsilon}} = \alpha_N$ (see Theorem 5.11), we have that $P^{k_{\varepsilon}} = 0$. Therefore, using the formula (5.25) for the primitive of compositions, we have:

$$P^{r_{\varepsilon}} = P^{f_{\varepsilon}} \circ k_{\varepsilon}. \quad (5.71)$$

Proceeding as in Theorem 5.6 and Theorem 5.7 we obtain the primitive for s_{ε} , using (5.70) instead of (5.31). This gives, in the case of families of maps f_{ε} :

$$\begin{aligned}
P^{s_{\varepsilon}} &= \lim_{N_{\pm} \rightarrow \infty} \sum_{j=0}^{N_+ - 1} P^{f_{\varepsilon}} \circ f_{\varepsilon}^j \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ s_{\varepsilon} \circ k_{\varepsilon} - P^{f_{\varepsilon}} \circ f_{\varepsilon}^j \circ s_{\varepsilon} \circ k_{\varepsilon} \\
&+ \sum_{j=1}^{N_-} P^{f_{\varepsilon}} \circ f_{\varepsilon}^{-j} \circ (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} - P^{f_{\varepsilon}} \circ f_{\varepsilon}^{-j} \circ k_{\varepsilon}
\end{aligned} \quad (5.72)$$

and in the case of a family of flows $\Phi_{t,\varepsilon}$:

$$\begin{aligned}
P^{s_{\varepsilon}} &= \lim_{T_{\pm} \rightarrow \infty} \int_{-T_-}^0 (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} \\
&- (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ k_{\varepsilon} \\
&+ \int_0^{T_+} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ s_{\varepsilon} \circ k_{\varepsilon} \\
&- (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ s_{\varepsilon} \circ k_{\varepsilon}
\end{aligned} \quad (5.73)$$

There are two ways to obtain the derivative of the primitive $P^{s_{\varepsilon}}$ with respect to ε . We can differentiate this formula (5.73) with respect to ε or we can apply Proposition 5.8 to s_{ε} to obtain the derivative of its primitive in terms of its Hamiltonian S_{ε} given in Theorem 5.14. Of course, both formulas give the same result. In general, when we compute the derivative of a sum (or an integral) there are two terms.

One due to the change of the function being integrated and another due to the change of the orbit of intersection. The variational Hamilton principle (see Section 5.3.4) tell us that this second term vanishes. So that, for instance, in the case of flows, one obtains:

$$\begin{aligned}
\left(\frac{d}{d\varepsilon} P^{s_\varepsilon} \right)_{|\varepsilon=0} &= \lim_{T_\pm \rightarrow \infty} \int_{-T_-}^0 \frac{d}{d\varepsilon} (\alpha \mathcal{H}_\varepsilon + H_\varepsilon)_{|\varepsilon=0} \circ \Phi_{t,0} \circ (\Omega_-^\Gamma)^{-1} \circ k_0 \\
&\quad - \frac{d}{d\varepsilon} (\alpha \mathcal{H}_\varepsilon + H_\varepsilon)_{|\varepsilon=0} \circ \Phi_{t,0} \circ k_0 \\
&\quad + \int_0^{T_+} \frac{d}{d\varepsilon} (\alpha \mathcal{H}_\varepsilon + H_\varepsilon)_{|\varepsilon=0} \circ \Phi_{t,0} \circ (\Omega_+^\Gamma)^{-1} \circ s_0 \circ k_0 \\
&\quad - \frac{d}{d\varepsilon} (\alpha \mathcal{H}_\varepsilon + H_\varepsilon)_{|\varepsilon=0} \circ \Phi_{t,0} \circ s_0 \circ k_0
\end{aligned} \tag{5.74}$$

5.5.3 The case of flows: proof of Theorem 5.14

In this section we adapt formula (5.67) for the case of flows. First, we need to know the Hamiltonian F_ε of the deformation in the case that our family f_ε corresponds to the time T flow of a Hamiltonian vector field $\mathcal{H}_\varepsilon$ of Hamiltonian H_ε . Concretely, we have the following

Proposition 5.10. *Let $\Phi_{t,\varepsilon}(x)$ be the flow of a Hamiltonian vector field of Hamiltonian $H_\varepsilon(x)$ and consider the family given by the time T map of this flow, that is, $f_\varepsilon(x) = \Phi_{T,\varepsilon}(x)$. Then, the Hamiltonian $F_{T,\varepsilon}$ of its deformation is given by*

$$F_{T,\varepsilon} = \int_0^T \frac{d}{d\varepsilon} H_\varepsilon \circ \Phi_{s-T,\varepsilon} ds \tag{5.75}$$

Proof. We start from the consideration that the flow $\Phi_{t,\varepsilon}$ verifies the corresponding differential equation

$$\begin{aligned}
\frac{d}{dt} \Phi_{t,\varepsilon} &= \mathcal{H}_\varepsilon \circ \Phi_{t,\varepsilon} \\
\Phi_{0,\varepsilon} &= \text{Id.}
\end{aligned}$$

We will assume that the flow is differentiable enough with respect to the point and with respect to parameters.

Moreover, we have formulas for the derivatives. We denote by $\cdot$ the derivative with respect to ε and D the derivative with respect to x . So, we have the variational equations:

$$\begin{aligned}
\frac{d}{dt} \dot{\Phi}_{t,\varepsilon} &= (D\mathcal{H}_\varepsilon \circ \Phi_{t,\varepsilon}) \dot{\Phi}_{t,\varepsilon} + \dot{\mathcal{H}}_\varepsilon \circ \Phi_{t,\varepsilon} \\
\frac{d}{dt} D\Phi_{t,\varepsilon} &= (D\mathcal{H}_\varepsilon \circ \Phi_{t,\varepsilon}) D\Phi_{t,\varepsilon}
\end{aligned}$$

The proof of (5.75) is based on thinking on $D\Phi_{t,\varepsilon}$ as a set of fundamental solutions of the homogeneous equation associated to the first non-homogeneous equation.

Therefore, we can use the formula of “variation of parameters” obtaining the solution $\dot{\Phi}_{t,\varepsilon}$, using that $\dot{\Phi}_{0,\varepsilon} = 0$ and that $(D\Phi_{t,\varepsilon})^{-1} = D\Phi_{-t,\varepsilon} \circ \Phi_{t,\varepsilon}$:

$$\dot{\Phi}_{t,\varepsilon} = \int_0^t (D\Phi_{t-s,\varepsilon} \circ \Phi_{s,\varepsilon}) \dot{\mathcal{H}}_\varepsilon \circ \Phi_{s,\varepsilon} ds$$

Or, what is the same

$$\dot{\Phi}_{t,\varepsilon} = \left(\int_0^t (\Phi_{t-s,\varepsilon})_* \dot{\mathcal{H}}_\varepsilon ds \right) \circ \Phi_{t,\varepsilon}$$

So that the deformation vector field for $\Phi_{t,\varepsilon}$ is

$$\int_0^t (\Phi_{t-s,\varepsilon})_* \dot{\mathcal{H}}_\varepsilon ds$$

In the Hamiltonian case, to compute the Hamiltonian we just compute the contraction with the symplectic form ω . Using the linearity of the contraction and that $i_{\mathcal{H}_\varepsilon}\omega = dH_\varepsilon$, we have

$$\begin{aligned} i_{\int_0^t (\Phi_{t-s,\varepsilon})_* \mathcal{H}_\varepsilon ds} \omega &= \int_0^t i_{(\Phi_{t-s,\varepsilon})_* \mathcal{H}_\varepsilon} \omega ds = \int_0^t (\Phi_{t-s,\varepsilon})_* i_{\mathcal{H}_\varepsilon} \omega ds \\ &= \int_0^t (\Phi_{t-s,\varepsilon})_* dH_\varepsilon ds = d \int_0^t (\Phi_{t-s,\varepsilon})_* \dot{H}_\varepsilon ds \\ &= d \int_0^t \dot{H}_\varepsilon \circ \Phi_{s-t,\varepsilon} ds \end{aligned}$$

□

Once we know the Hamiltonian of the deformation of the time T map of a flow $f_\varepsilon = \Phi_{T,\varepsilon}$, we can consider the corresponding scattering map $\sigma_\varepsilon = \sigma^{\Gamma, \mathcal{H}_\varepsilon}$, that was shown in Section 5.2.4 that is independent of T . We compute the Hamiltonian S_ε of its deformation simply by “translating” formula (5.67) for this case and using the following facts

$$\begin{aligned} F_{T,\varepsilon} \circ \Phi_{jT,\varepsilon} &= \int_0^T \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{s-T,\varepsilon} \circ \Phi_{jT,\varepsilon} ds = \int_{(j-1)T}^{jT} \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} du \\ F_{T,\varepsilon} \circ \Phi_{-jT,\varepsilon} &= \int_0^T \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{s-T,\varepsilon} \circ \Phi_{-jT,\varepsilon} ds = \int_{-(j+1)T}^{-jT} \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} du \\ \sum_{j=0}^{N_- - 1} F_{T,\varepsilon} \circ \Phi_{-jT,\varepsilon} &= \int_{-TN_-}^0 \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} ds \\ \sum_{j=1}^{N_+} F_{T,\varepsilon} \circ \Phi_{jT,\varepsilon} &= \int_0^{TN_+} \frac{dH_\varepsilon}{d\varepsilon} \circ \Phi_{u,\varepsilon} ds \end{aligned}$$

With these expressions one easily obtains formula (5.68).

5.5.4 Heuristic considerations about the proof of Theorems 5.13 and 5.6

We think that it is quite remarkable that the formulas derived in Theorems 5.13 and 5.6 are so similar. Indeed, it is even much more remarkable that very similar formulas appear in other contexts. Notably, these formulas are very similar to the geometric formulas for the convergent Melnikov functions [Rob88, Tre94, Eli94, DR97, LMS03, DG00], and for the other quantities appearing in variational calculus, [Mat95]. In Appendix 5.7 we also note the similarities between these formulas and the perturbative calculations of Scattering matrices in quantum mechanical scattering theory.

In the following, we present some heuristic argument – still not a proof – that argues that, *all the geometrically natural formulas are determined uniquely up to constant factors*. This would imply that the geometric theories and the variational methods have to agree at least in the perturbative cases.

The scattering map can be considered approximately as the junction of three long trajectories: one going backwards N_- units of time along the manifold Λ_ε , a second one going forward $N_- + N_+$ units of time along the homoclinic trajectory in Γ_ε and a third orbit going backwards N_+ units of time along the manifold Λ_ε .

The following heuristic argument (not a complete proof) will perhaps make reasonable why one can expect formulas such as (5.67) or (5.28).

We make the following observations:

1. By definition, the first order term in perturbation theory has to be linear in the first order term of the perturbing transformation.
2. The first order perturbative term has to depend only on the values of the perturbation on the unperturbed orbit.
3. From the previous two items, it is reasonable to conclude that the Hamiltonian S_0 is expressed as a linear combination of the F_0 evaluated at the points of the unperturbed orbit.

4. By the invariance of the origin of time, we note that the coefficients have to be independent of the index in the homoclinic orbit, and in the forward and backwards orbits.
5. If the coefficients on the forward and backward orbits do not agree up to a sign we do not obtain a convergent sum.

The above heuristic considerations determine the formula up to a constant multiple.

Of course, these arguments, even if we hope illuminating, are not a complete proof.

For example, there are other linear functionals on $f_0^j(x)$ besides $\sum f_0^j(x)w_j$ (e.g. functionals “at infinity” such limits, asymptotic averages).

In item 5, we assume that there is indeed a well defined formula.

Perhaps the above argument can be completed into a complete proof.

We point that the above considerations apply not only to the proof of Theorem 5.13 and Theorem 5.6.

5.6 Example: Scattering maps in geodesic flows

In this section we will describe in greater detail the scattering map of a quasi-periodically perturbed geodesic flow considered in [DLS00, DLS06b].

For this particular example, we will show the existence of a homoclinic channel (see Definition 5.2) that will allow us to define its associated scattering map. In the unperturbed situation we will see that the scattering map of the geodesic flow can be globalized to the whole manifold Λ . Nevertheless, in the perturbed case this globalization leads to monodromies so that the scattering map is not well defined in the whole Λ_ε .

We deal with a n -dimensional manifold M , and we will consider a $\mathbb{C}^r$ metric g on it (r sufficiently large).

We recall that a geodesic “ λ ” is a curve “ λ ” : $\mathbb{R} \rightarrow M$, parameterized by arc length which is a critical point for the length between any two points. It is also possible to consider a dynamical system given by the geodesic flow in $\mathbf{S}_1 M$, the unit tangent bundle of M . We denote the parameterized curve in $\mathbf{S}_1 M$ corresponding to the geodesic “ λ ” as $\lambda(t)$, and we denote by $\hat{\lambda} = \text{Range}(\lambda) \subset \mathbf{S}_1 M$.

We will assume that the metric g verifies:

H1 There exists a closed geodesic “ Λ ” such that its corresponding periodic orbit $\hat{\Lambda}$ under the geodesic flow is hyperbolic.

H2 There exists another geodesic “ γ ” such that $\hat{\gamma}$ is a transversal homoclinic orbit to $\hat{\Lambda}$.

That is, $\hat{\gamma}$ is contained in the intersection of the stable and unstable manifolds of $\hat{\Lambda}$, $W_{\hat{\Lambda}}^s, W_{\hat{\Lambda}}^u$, in the unit tangent bundle. Moreover, we assume that the intersection of the stable and unstable manifolds of $\hat{\Lambda}$ is transversal along $\hat{\gamma}$. That is

$$T_{\gamma(t)}W_{\hat{\Lambda}}^s + T_{\gamma(t)}W_{\hat{\Lambda}}^u = T_{\gamma(t)}\mathbf{S}_1 M, \quad t \in \mathbb{R}. \quad (5.76)$$

Hypotheses **H1**, **H2** are verified in great generality. We refer to [DLS06b, Sec. 2] for a discussion of the abundance. After the publication of [DLS06b], the paper [Con10] established that **H1**, **H2** hold for generic metrics on any manifold.

We will assume without loss of generality and just to avoid typographical clutter that the period of Λ is 1. This, clearly, can be achieved by choosing the units of time.

We recall that the hyperbolicity of $\hat{\Lambda}$ implies that there exist $C > 0, \beta_0 > 0$ such that

$$\text{dist}(\text{“}\Lambda\text{”}(s + a_\pm), \text{“}\gamma\text{”}(s)) \leq Ce^{-\beta_0|s|}, \quad \text{as } s \rightarrow \pm\infty. \quad (5.77)$$

Standard perturbation theory for periodic orbits of ordinary

differential equations (see e.g. [CL55]) shows that the asymptotic phase shift $\Delta := a_+ - a_-$ exists and is unique modulo an integer multiple of the period of “ Λ ”.

We recall that the geodesic flow is Hamiltonian in $\mathbf{T}^*M$ and the Hamiltonian function is

$$H_0(p, q) = \frac{1}{2}g_q(p, p),$$

where g_q is the metric in $\mathbf{T}^*M$. We will denote by Φ_t this geodesic flow.

Since the energy H_0 is preserved and g_q is not degenerate, for each E the energy level $\Sigma_E = \{(p, q), H_0(p, q) = E\}$ is a $(2n - 1)$ -dimensional manifold invariant under the geodesic flow.

Given an arbitrary geodesic “ λ ” : $\mathbb{R} \rightarrow M$ we will denote

$$\lambda_E(t) = (\lambda_E^p(t), \lambda_E^q(t))$$

the orbit such that $H_0(\lambda_E(t)) = E$, $\text{Range}(\lambda) = \text{Range}(\lambda_E^q)$ and “ λ ”(0) = $\lambda_E^q(0)$. It is easy to check that the above conditions determine uniquely the orbit of the geodesic flow in the cotangent bundle corresponding to a geodesic “ λ ”. We use $\hat{\lambda}_E$ to denote the range of the orbit $\lambda_E(t)$.

It is very important to recall that a characteristic property of the geodesic flow is that the orbits rescale with energy as

$$(\lambda_E^p(t), \lambda_E^q(t)) = \left(\sqrt{2E} \lambda_{1/2}^p(\sqrt{2E}t), \lambda_{1/2}^q(\sqrt{2E}t) \right). \quad (5.78)$$

Since $\Lambda_{1/2}$ has period 1 (with our conventions that the geodesic “ Λ ” is normalized to have length 1), Λ_E has period $1/\sqrt{2E}$.

The hypotheses **H1**, **H2** of the geodesic flow when formulated in the Hamiltonian formalism for the Hamiltonian H_0 translate into:

H1’ For any $E > 0$, there exists a periodic orbit $\Lambda_E(t)$, as in (5.78), of the Hamiltonian H_0 whose range $\hat{\Lambda}_E$ is hyperbolic in the energy surface

$$\Sigma_E := \{(p, q) \in \mathbf{T}^*M, H_0(p, q) = E\}. \quad (5.79)$$

H2’ The stable and unstable manifolds $W_{\hat{\Lambda}_E}^{s,u}$ of $\hat{\Lambda}_E$ are n -dimensional, and there exists a homoclinic orbit $\gamma_E(t)$. That is, the range of γ_E satisfies

$$\hat{\gamma}_E \subset \left(W_{\hat{\Lambda}_E}^s \setminus \hat{\Lambda}_E \right) \cap \left(W_{\hat{\Lambda}_E}^u \setminus \hat{\Lambda}_E \right).$$

Moreover, this intersection is transversal as intersection of invariant manifolds in the energy surface Σ_E along $\hat{\gamma}_E$.

As a consequence of the hyperbolicity of $\hat{\Lambda}_{1/2}$, we have that, analogously to (5.77), for some $a_{\pm} \in \mathbb{R}$, there exist $C > 0$ and an *exponential rate* $\beta_0 > 0$, such that

$$\text{dist}(\Lambda_{1/2}(t + a_{\pm}), \gamma_{1/2}(t)) \leq C e^{-\beta_0 |t|}, \quad \text{as } t \rightarrow \pm\infty. \quad (5.80)$$

We consider any fixed value $E_0 > 0$, and introduce the manifold $\Lambda = \bigcup_{E \geq E_0} \hat{\Lambda}_E$ for all values of the energy larger than E_0 which is a 2-dimensional normally hyperbolic invariant manifold with boundary, diffeomorphic to $[E_0, \infty) \times \mathbb{T}^1$. Moreover, its stable and unstable manifolds, W_{Λ}^s and W_{Λ}^u , are $(n+1)$ -dimensional manifolds diffeomorphic to $[E_0, \infty) \times \mathbb{T}^1 \times \mathbb{R}^{n-1}$, intersecting transversally along γ , defined by:

$$\gamma = \bigcup_{E \geq E_0} \hat{\gamma}_E \subset (W_{\Lambda}^s \setminus \Lambda) \cap (W_{\Lambda}^u \setminus \Lambda)$$

which is diffeomorphic to $[E_0, \infty) \times \mathbb{R}$.

By inequality (5.80) and the rescaling properties (5.78) we have:

$$\text{dist} \left(\Lambda_E \left(t + \frac{\varphi_0 + a_{\pm}}{\sqrt{2E}} \right), \gamma_E \left(t + \frac{\varphi_0}{\sqrt{2E}} \right) \right) \leq C \sqrt{2E} e^{-\beta_0 \sqrt{2E} |t|} \quad \text{as } t \rightarrow \pm\infty. \quad (5.81)$$

Given a point $x \in \gamma$, it can be written as $x = \gamma_E(\tau) = \gamma_E(\frac{\varphi}{\sqrt{2E}})$ for some $(\varphi, E) \in \mathbb{R} \times [E_0, \infty]$. Then, by (5.81) the corresponding $x_{\pm} \in \Lambda$ such that $x \in W_{x_+}^s \cap W_{x_-}^u$ are given by

$$x_{\pm} = \Lambda_E \left(\frac{\varphi + a_{\pm}}{\sqrt{2E}} \right),$$

so that the definition (5.4) of the wave operators gives that $\Omega_{\pm}(x) = x_{\pm}$. Indeed, one can easily see that if we move $x_- = \Lambda_E \left(\frac{\varphi + a_-}{\sqrt{2E}} \right)$ around $\hat{\Lambda}_E$ up to $\Lambda_E \left(\frac{\varphi + a_- + 1}{\sqrt{2E}} \right) = x_-$, then $(\Omega_-)^{-1}(x_-)$ moves from the point $x = \gamma_E(\frac{\varphi}{\sqrt{2E}})$ to its image under the time one map $\gamma_E(\frac{\varphi+1}{\sqrt{2E}})$.

In order to make this monodromy more apparent, by using that Λ_E is $1/\sqrt{2E}$ periodic, if we take

$$x^n = \gamma_E \left(\frac{\varphi + n}{\sqrt{2E}} \right) = \Phi_{n/\sqrt{2E}}(x),$$

property (5.81) gives

$$\Omega_{\pm}(x^n) = x_{\pm}^n = x_{\pm}$$

so that the maps $\Omega_{|\gamma}^{\pm} : \gamma \rightarrow \Lambda$ are not global diffeomorphisms.

In order to study the monodromy of these maps, for any $t \in \mathbb{R}$, we define

$$\Gamma^t = \left\{ \gamma_E \left(\frac{\varphi + t}{\sqrt{2E}} \right), |\varphi| < 1/2, E \geq E_0 \right\}$$

which are homoclinic channels, that is

$$\Omega_{\pm}^{\Gamma^t} : \Gamma^t \rightarrow H_{\pm}^t = \Omega_{\pm}^{\Gamma^t}(\Gamma^t)$$

are global diffeomorphisms.

As Λ_E is $1/\sqrt{2E}$ periodic, the sets $H_{\pm}^t$ can be written as $H_{\pm}^t = \Lambda \setminus \cup_{E \geq E_0} \Lambda_E(\frac{1/2+t+a_{\pm}}{\sqrt{2E}})$.

For any fixed t , we can construct the scattering map $\sigma^t = \Omega_{+}^{\Gamma^t}(\Omega_{-}^{\Gamma^t})^{-1}$, which assigns $x_{+} = \Lambda_E(\frac{\varphi+t+a_{+}}{\sqrt{2E}})$ to $x_{-} = \Lambda_E(\frac{\varphi+t+a_{-}}{\sqrt{2E}})$, for $(\varphi, E) \in (-1/2, 1/2) \times [E_0, \infty)$.

It is remarkable that the scattering map in this case is globally defined in the whole manifold γ because the monodromy of $(\Omega_{-})^{-1}$ is exactly canceled out by applying to it Ω_{+} .

The monodromy of $(\Omega_{-})^{-1}$ is precisely an application of Φ_1 , the time 1 map of the geodesic flow. Since $\Omega_{+} \circ \Phi_1 = \Omega_{+}$ we see that σ has no monodromy and is globally well defined in Λ for the geodesic flow.

Concretely, we observe that $\sigma^t = \sigma^{t'}$ in $H_{-}^t \cap H_{-}^{t'}$, and that $\cup_{t \in \mathbb{R}} H_{-}^t = \Lambda$, so it is possible to define globally the scattering map

$$\begin{aligned} \sigma : \Lambda &\rightarrow \Lambda \\ x_{-} = \Lambda_E \left(\frac{\varphi + a_{-}}{\sqrt{2E}} \right) &\mapsto x_{+} = \Lambda_E \left(\frac{\varphi + a_{+}}{\sqrt{2E}} \right) \end{aligned}$$

We use now the notations of Section 5.4.2 for the parameterizations of Λ and introduce the (symplectic) system of coordinates (φ, J) , $J = \sqrt{2E}$ in the reference manifold $N = [E_0, \infty) \times \mathbb{T}$, so that $x = k(\varphi, J) = \Lambda_E(\varphi/\sqrt{2E})$. The scattering map, when written in these coordinates, is given by:

$$\begin{aligned} s : N &\longrightarrow N \\ (\varphi, J) &\mapsto (\varphi + \Delta, J) \end{aligned} \tag{5.82}$$

where $\Delta = a_{+} - a_{-}$ is called the phase shift.

Remark 5.12. It is worth mentioning that the scattering map for the geodesic flow is a very degenerate integrable non-twist map with the same phase shift for all the points. This is a consequence of the fact that the energy H_0 is preserved and the scaling properties (5.78) which are a very particular feature of the geodesic flow. See [CDMR06] for an example, in the planar restricted three body problem, of an integrable scattering map which verifies the twist condition.

5.6.1 Perturbations of geodesic flows

In order to deal with the quasi-periodic perturbations of the geodesic flow of the form $H_{\varepsilon}(p, q, t) = H_0(p, q) + \varepsilon^2 U(q, \varepsilon \nu t)$, for some vector $\nu \in \mathbb{R}^d$ considered in [DLS06b], we first study the product vector field of the geodesic flow $H_0(p, q)$ on $\mathbf{T}^*M$ and the quasi-periodic flow $\dot{\theta} = \varepsilon \nu$ in $\mathbb{T}^d$, defined in the extended phase space $\mathbf{T}^*M \times \mathbb{T}^d$. In (5.82) we have computed the formulas for the scattering map associated to this geodesic flow, and, as we saw in Section 5.2.4, the scattering map on $\tilde{\Lambda} = \Lambda \times \mathbb{T}^d$ is given, in the extended reference manifold $\tilde{N} = N \times \mathbb{T}^d$, by

$$\begin{aligned} \tilde{s} : \tilde{N} &\longrightarrow \tilde{N} \\ (J, \varphi, \theta) &\mapsto (J, \varphi + \Delta, \theta) \end{aligned}$$

If we want to make apparent the symplectic character of the scattering map, we add the extra actions A , conjugated to the angles θ , obtaining the autonomous Hamiltonian $H_0(p, q) + \varepsilon \nu \cdot A$ in the full symplectic space $\mathbf{T}^*M \times \mathbb{R}^d \times \mathbb{T}^d$. We have a $(2d + 2)$ -dimensional manifold $\Lambda^* = \Lambda \times \mathbb{R}^d \times \mathbb{T}^d$ whose projection to the extended phase space $\mathbf{T}^*M \times \mathbb{T}^d$ is $\tilde{\Lambda}$. Using the extended symplectic coordinates (J, φ, A, θ) , the reference manifold of Λ^* is given by $N^* = N \times \mathbb{R}^d \times \mathbb{T}^d$, and its parameterization is given by

$$\begin{aligned} k^* : N^* &\longrightarrow \Lambda^* \\ (J, \varphi, A, \theta) &\mapsto (k(J, \varphi), A, \theta) = (\Lambda_E(\varphi/\sqrt{2E}), A, \theta). \end{aligned}$$

where $E = J^2/2$.

Moreover, the scattering map in this full symplectic space is symplectic and it is given, in the reference manifold N^* , by:

$$\begin{aligned} s^* : N^* &\rightarrow N^* \\ (J, \varphi, A, \theta) &\mapsto (J, \varphi + \Delta, A, \theta). \end{aligned}$$

Before applying perturbation theory we fix some homoclinic channel $\Gamma_0^* = \Gamma_0 \times \mathbb{R}^d \times \mathbb{T}^d$ for some fixed $t_0 \in \mathbb{R}$, in the homoclinic manifold $\gamma^* = \gamma \times \mathbb{R}^d \times \mathbb{T}^d$.

When we consider the perturbed Hamiltonian $H_\varepsilon^*(p, q, \theta, A) = H_0(p, q) + \varepsilon^2 U(q, \theta) + \varepsilon \nu \cdot A$, standard perturbation theory with respect to the parameter ε^2 guarantees the transversal intersection of $W_{\Lambda_\varepsilon^*}^s \cap W_{\Lambda_\varepsilon^*}^u$ along a homoclinic channel Γ_ε^* , ε^2 -close to Γ_0^* , for a normally hyperbolic invariant manifold $\Lambda_\varepsilon^* \subset T^*M \times \mathbb{R}^d \times \mathbb{T}^d$ and the local existence of a perturbed scattering map σ_ε^* . Nevertheless, all the considerations about the global definition of the scattering map σ^* are only valid for the extended geodesic flow $H_0^*(p, q, \theta, A) = H_0(p, q) + \varepsilon \nu \cdot A$. Indeed, the cancellations between the different perturbed maps $(\Omega_{-\varepsilon}^{\Gamma_\varepsilon^*})^{-1}$ and $\Omega_{+\varepsilon}^{\Gamma_\varepsilon^*}$ are not satisfied in general providing an obstruction to the global definition of $\sigma_\varepsilon^* = \sigma_\varepsilon^{*, \Gamma_\varepsilon^*}$ and only guarantee the existence of σ_ε^* in a set $H_{-\varepsilon}^*$, ε^2 -close to $H_-^{*, t_0} = H_-^{t_0} \times \mathbb{R}^d \times \mathbb{T}^d$, of relative measure $1 - \varepsilon^2$ in Λ_ε^* .

We will now compare the perturbative calculation of the scattering map which was already done in [DLS00] and [DLS06b] and formula (5.68).

Remark 5.13. In order to compare the perturbative formulas for the scattering map in [DLS06b] and the ones obtained applying the method of section 5.5 we need to take into account the following fact. In the example considered here, the perturbed Hamiltonian is given by $H_\varepsilon^*(p, q, \theta, A) = H_0(p, q) + \varepsilon^2 V(q, \theta) + \varepsilon \nu \cdot A$, so, it depends on the parameter ε in two different ways. On one side, the term ε^2 in front of the potential makes the perturbation small. On the other hand, the term $\varepsilon \nu \cdot A$ makes the potential slow in the angular variable θ . So, as it was proved in [DLS06b], the perturbation theory is done with respect to the small parameter, which in this case is ε^2 . So, when we apply formula (5.68) we will replace the parameter ε by ε^2 in all the formulas.

In order to perform this comparison, we can choose the parameterization of the perturbed normally hyperbolic invariant manifold Λ_ε^* verifying hypothesis (5.59). In the notation of [DLS06b], any point in this manifold is given by

$$x_\varepsilon^* = (p, q, A, \theta) = k_\varepsilon^*(J, \varphi, B, \theta) = (\mathcal{F}(J, \varphi, \theta, \varepsilon^2), \mathcal{A}(J, \varphi, B, \theta, \varepsilon^2), \theta)$$

for some parameterizations $\mathcal{F} = \Lambda_E(\varphi/\sqrt{2E}) + O(\varepsilon^2)$, $\mathcal{A}$, that, under assumption (5.59), verifies $\mathcal{A}(J, \varphi, B, \theta, \varepsilon^2) = B$.

In those papers, a perturbative formula for the difference of the actions A of the points $x_+^*(\varepsilon) = \sigma_\varepsilon^*(x_-^*(\varepsilon))$ and $x_-^*(\varepsilon)$ were obtained. Concretely, if we call $(J_\pm, \varphi_\pm, B_\pm, \theta_\pm)$ to their coordinates in the reference manifold N^* , we have, first of all, applying standard first order perturbation theory that

$$\begin{aligned} \varphi_\pm &= \varphi + a_\pm + O(\varepsilon^2) \\ J_\pm &= J + O(\varepsilon^2) \\ B_\pm &= B + O(\varepsilon^2) \\ \theta_\pm &= \theta, \end{aligned} \tag{5.83}$$

for some $\varphi \in \mathbb{R}$, $J \in \mathbb{R}$, $B \in \mathbb{R}^d$, and $\theta \in \mathbb{T}^d$, and where $a_\pm$ were introduced in hypotheses **H2'**, in formulas (5.77) and (5.80).

Now, denoting $z^*(\varepsilon) = (\Omega_{\varepsilon+}^{\Gamma_*})^{-1}(x_+^*(\varepsilon)) = (\Omega_{\varepsilon-}^{\Gamma_*})^{-1}(x_-^*(\varepsilon))$ in the homoclinic channel Γ_ε^* , standard first order perturbation theory gives, by (5.81), that $z^*(0) = \gamma_E(\varphi/J)$. Using all these facts, Lemma 4.18 of [DLS06b] gives

$$A(x_+^*(\varepsilon)) - A(x_-^*(\varepsilon)) = \varepsilon^2 \frac{\partial L}{\partial \theta}(E, \varphi, \theta) + O_{\mathbb{C}^1}(\varepsilon^4), \quad (5.84)$$

with $L(E, \varphi, \theta)$ is the Poincaré function given by

$$\begin{aligned} L(E, \varphi, \theta) = & \lim_{T_1, T_2 \rightarrow \infty} \left[- \int_{-T_1}^{T_2} dt \tilde{U} \left(\gamma_E^q \left(t + \frac{\varphi}{\sqrt{2E}} \right), \theta + \varepsilon \nu t \right) \right. \\ & + \int_{-T_1}^0 dt \tilde{U} \left(\Lambda_E^q \left(t + \frac{\varphi + a_-}{\sqrt{2E}} \right), \theta + \varepsilon \nu t \right) \\ & \left. + \int_0^{T_2} dt \tilde{U} \left(\Lambda_E^q \left(t + \frac{\varphi + a_+}{\sqrt{2E}} \right), \theta + \varepsilon \nu t \right) \right] \end{aligned} \quad (5.85)$$

where the functions $\bar{U}(\theta)$ and $\tilde{U}(q, \theta)$ are defined by:

$$\bar{U}(\theta) = \int_0^1 U(\Lambda_{1/2}^q(\varphi), \theta) d\varphi, \quad \tilde{U}(q, \theta) = U(q, \theta) - \bar{U}(\theta). \quad (5.86)$$

Remark 5.14. In this perturbative formula we can see that, in general, $L(E, \varphi + 1, \theta)$ is not equal to $L(E, \varphi, \theta)$. That is, when φ increases by 1, the scattering map changes. Note that changing φ by 1, amounts to shifting the unperturbed homoclinic channel. Therefore, the cancellations on the monodromy that happened in the geodesic flow, are destroyed by perturbations whose effect is different on the shifted orbits.

Indeed, we are going to see that Hamiltonian S_0 of formula (5.68) corresponds to L . Concretely, using that $\sigma_0^* \circ k_0^*(J, \varphi, B, \theta) = k_0^* \circ s_0^*(J, \varphi, B, \theta) = k_0^* \circ (J, \varphi + \Delta, B, \theta)$, with $\Delta = a_+ - a_-$, and $k_0^*(J, \varphi, B, \theta) = (\Lambda_E(\varphi/J), B, \theta)$, where $E = J^2/2$, and $(\Omega_{0\pm}^{\Gamma_*})^{-1} \circ k_0^*(J, \varphi, B, \theta) = (\gamma_E((\varphi - a_{\pm})/J), B, \theta)$,

we have

$$\begin{aligned}
S_0(J, \varphi, B, \theta) &= \lim_{T_{\pm} \rightarrow \infty} \int_{-T_-}^0 U \circ \Phi_{u,0} \circ (\Omega_{0-}^{\Gamma_*})^{-1} \circ (\sigma_0^*)^{-1} \circ k_0^*(J, \varphi, B, \theta) \\
&\quad - U \circ \Phi_{u,0} \circ (\sigma_0^*)^{-1} \circ k_0^*(J, \varphi, B, \theta) \\
&\quad + \int_0^{T_+} U \circ \Phi_{u,0} \circ (\Omega_{0+}^{\Gamma_*})^{-1} \circ k_0^*(J, \varphi, B, \theta) \\
&\quad - U \circ \Phi_{u,0} \circ k_0^*(J, \varphi, B, \theta) \\
&= \lim_{T_{\pm} \rightarrow \infty} \int_{-T_-}^0 U \circ \Phi_{u,0} \circ (\Omega_{0-}^{\Gamma_*})^{-1} \circ k_0^*(J, \varphi - \Delta, B, \theta) \\
&\quad - U \circ \Phi_{u,0} \circ k_0^*(J, \varphi - \Delta, B, \theta) \\
&\quad + \int_0^{T_+} U \circ \Phi_{u,0} \circ (\Omega_{0+}^{\Gamma_*})^{-1} \circ k_0^*(J, \varphi, B, \theta) \\
&\quad - U \circ \Phi_{u,0} \circ k_0^*(J, \varphi, B, \theta) \\
&= \lim_{T_{\pm} \rightarrow \infty} \int_{-T_-}^0 U \circ \Phi_{u,0} \circ (\gamma_E((\varphi - a_+)/J), B, \theta) \\
&\quad - U \circ \Phi_{u,0} \circ (\Lambda_E((\varphi - \Delta)/J), B, \theta) \\
&\quad + \int_0^{T_+} U \circ \Phi_{u,0} \circ (\gamma_E((\varphi - a_+)/J), B, \theta) \\
&\quad - U \circ \Phi_{u,0} \circ (\Lambda_E(\varphi/J), B, \theta) \\
&= \lim_{T_{\pm} \rightarrow \infty} \int_{-T_-}^{T_+} U(\gamma_E^q(u + (\varphi - a_+)/J), \theta + \varepsilon \nu u) \\
&\quad - \int_{-T_-}^0 U(\Lambda_E^q(u + (\varphi - \Delta)/J), \theta + \varepsilon \nu u) \\
&\quad - \int_0^{T_+} U(\Lambda_E^q(u + (\varphi/J)), \theta + \varepsilon \nu u).
\end{aligned}$$

So that, we obtain:

$$S_0(J, \varphi, B, \theta) = -L(J, \varphi - a_+, \theta) \quad (5.87)$$

Observe that $S_0(J, \varphi + a_+, B, \theta) = -L(J, \varphi, \theta)$. So that, taking into account that the perturbation of the geodesic flow is of order ε^2 , the first order perturbative term of the scattering map is

$$s_\varepsilon^*(J, \varphi, B, \theta) = s_0^*(J, \varphi, B, \theta) + \varepsilon^2 s_1^*(J, \varphi, B, \theta) + O(\varepsilon^4)$$

and, deformation theory gives that,

$$s_1^*(J, \varphi, B, \theta) = \mathfrak{S}_0 \circ s_0^*(J, \varphi, B, \theta) = \mathfrak{S}_0(J, \varphi + \Delta, B, \theta) = \mathcal{J} \nabla S_0(J, \varphi + \Delta, B, \theta)$$

where $\mathcal{J}$ is the symplectic matrix.

We denote the coordinates of x_-^* , by $(J, \varphi + a_-, B_-, \theta)$ as in (5.83) and we obtain that $s_1^*(J, \varphi + a_-, B, \theta) = \mathcal{J} \nabla S_0(J, \varphi + a_+, B, \theta) = -\mathcal{J} \nabla L(J, \varphi, \theta)$, and then:

$$s_\varepsilon^*(J, \varphi + a_-, B_-, \theta) = (J, \varphi + a_+, B_-, \theta) - \varepsilon^2 \mathcal{J} \nabla L(J, \varphi, \theta) + O(\varepsilon^4)$$

In particular, for the coordinates B we have

$$B_+ = B_- - \varepsilon^2 \frac{\partial S_0}{\partial \theta}(E, \varphi + a_-, B_-, \theta) + O(\varepsilon^4) = B_- + \varepsilon^2 \frac{\partial L}{\partial \theta}(J, \varphi, \theta) + O(\varepsilon^4)$$

Finally, using that $A_{\pm} = B_{\pm}$ with the normalized parameterization, we obtain that this formula agrees with (5.84) provided in [DLS06b].

The calculations in those papers were done by very different methods using averaging theory which relies on the fact that the energy is a slow variable. The method in [DLS00, DLS06a], also used in [DLS03, DLS06b], allowed only to compute the energy component of the scattering map but it does not allow us to compute the φ component since φ is not a slow variable. The method of this chapter, also gives the φ component of the first order expansion of the scattering map.

$$\mathbb{R}^2 = \widetilde{\mathbb{T}}^2$$

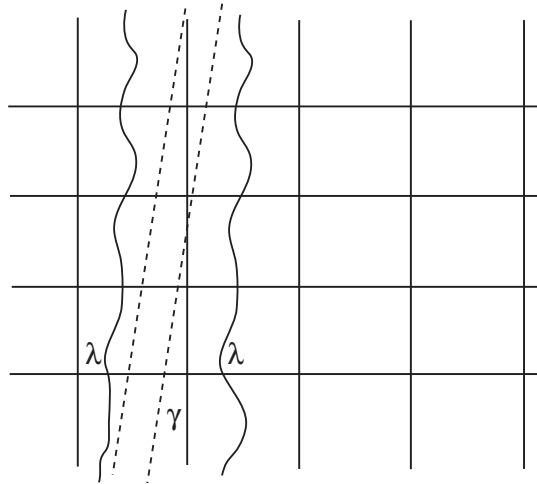


Figure 5.5: Illustration of the closed geodesics.

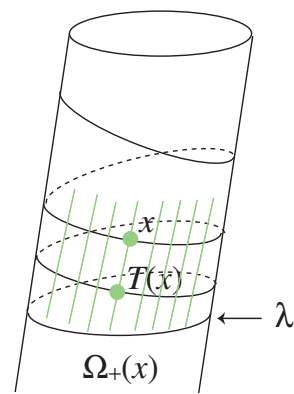


Figure 5.6

The applications in [DLS00, DLS06b] also involve comparing the scattering map with the effect on the KAM tori. This calculation will not be undertaken here, since it involves asymptotic computation of KAM tori and it involves extra cancellations (the leading term in the intersection is $O(\varepsilon^3)$). We nevertheless note that the calculation of intersections simplifies when one uses the geometric properties indicated above. We hope to come back to this application.

We finish the presentation of this example by noting that the primitive function $P_\varepsilon = P_\varepsilon^*$ of the scattering map takes the form:

$$P_\varepsilon = P_0 + \varepsilon^2 P_1 + O(\varepsilon^4)$$

where the leading term P_1 can be controlled from equation (5.74). It is worth noting that $\frac{d}{d(\varepsilon^2)}(\alpha\mathcal{H}_\varepsilon)|_{\varepsilon=0} = 0$, so that $P_1(J, \varphi, \theta) = -L(J, \varphi - a_+, \theta) = S_0(J, \varphi, B, \theta)$ as in the computations that lead to formula (5.87).

The expression L had played an important role in the variational calculation in [Mat95]. This is related to the variational interpretation of the scattering map discussed in Section 5.3.4.

5.7 An informal comparison with quantum mechanical scattering theory

Since quantum mechanical scattering theory has been part of the scientific culture for many decades, it is perhaps useful for some readers, already familiar with quantum mechanical scattering theory, to develop the analogy between this theory and the scattering theory for normally hyperbolic invariant manifolds developed in this chapter.

Of course, readers whose background does not include quantum mechanical scattering theory are urged to skip this section since our treatment will be extremely sketchy and informal.

There are two main versions of quantum scattering theory: time independent and time dependent. We will consider only the time dependent version.

Standard references on quantum mechanical scattering theory are [GW64, New02]. These references emphasize more the time independent scattering theory. Books which emphasize more the time dependent scattering theory are [RS79, Thi81]. We should also mention the papers [Hun68, NT81, Gal82, Thi83, Hub89, FO97] which develop a classical scattering theory for a wide class systems of particles interacting with repulsive potentials, which is somewhat different from our context, but many of the ideas from one context apply in the other. We plan to come back to these issues. Some applications of scattering methods to problems in dynamics appear in [Nel69].

We recall that the time-evolution in quantum mechanics is generated by a self-adjoint operator H . The Schrödinger equation is

$$\frac{d}{dt}U(t) = -iH U(t) ; \quad U(0) = \text{Id}$$

where $U(t)$ is a group of unitary operators implementing the evolution $U(t+s) = U(t)U(s)$.

The classical analogue of H is the vector field generating the evolution and the analogue of $U(t)$ is the flow Φ_t . In particular $U(1)$ will be the analogue of the maps f in the discrete time case.

In the systems considered in quantum scattering theory, particles move freely in the distant future and in the distant past but in the mean time they interact.

The asymptotic free motion in the future is, in general, different from the asymptotic free motion in the past and the relation is given by the scattering operator.

We denote by H_f , H_i the Hamiltonian operators generating the free and interacting dynamics and by U_f , U_i the corresponding free and interacting semigroups.

The wave operators are defined as

$$\Omega_\pm = \lim_{t \rightarrow \pm\infty} U_f(-t)U_i(t)$$

(We ignore, in this sketchy exposition, what is the precise sense in which the limits have to take place. This is also customarily ignored in the Physical literature.)

The intuition is that for large t

$$U_f(t)\Omega_+\psi \approx U_i(t)\psi$$

so that $\Omega_+\psi$ describes the initial condition that, under the free evolution would have behaved as ψ under the interacting evolution.

For example, in the case that the free dynamics is just a particle moving at constant velocity, the $\Omega_+\psi$ gives the asymptotic velocity (and some “initial” position).

Similarly $\Omega_-\psi$ gives the asymptotic behavior in the past.

Note that from the definition it is clear that

$$\begin{aligned}\Omega_\pm U_i(s) &= \lim_{t \rightarrow \pm\infty} U_f(-t)U_i(t+s) \\ &= \lim_{t \rightarrow \pm\infty} U_f(-t+s)U_i(t) \\ &= U_f(s)\Omega_\pm\end{aligned}\tag{5.88}$$

The relations (5.88) are called the intertwining relations. From the dynamical point of view, (5.88) semiconjugate the free dynamics to the interacting dynamics.

This method of producing conjugacies has appeared several times in dynamical systems, e.g., [Ste59]. The analogy with quantum mechanics is emphasized in [Nel69].

Notice that for classical particles interacting with repulsive potential, the existence of wave operators gives a conjugacy to the free particle, so that the results of [Thi83] imply that a wide class of systems interacting by repulsive potentials are integrable. This includes as a particular case the celebrated Calogero-Moser system which can be integrated also by algebraic methods [Cal75, Cal79, Mos75, Mos80]. Relations of this type of algorithms for linearization can be found in [DLT93, DDLT91].

The scattering operator is defined as

$$\sigma = \Omega_+\Omega_-^{-1}$$

and, given the asymptotic state in the past, gives the asymptotic state in the future. We also have

$$\sigma = \lim_{T_\pm \rightarrow \infty} U_f(-T_+)U_i(T_+ + T_-)U_f(-T_-)\tag{5.89}$$

The perturbation theory for the quantum mechanical scattering can be derived very easily. We note that if

$$H_i = H_{i,0} + \varepsilon H_{i,1}(t) + O(\varepsilon^2)$$

is a time dependent perturbation of the interacting Hamiltonian operator the variation of parameters formula gives:

$$U_i(t) = U_{i,0}(t) - \varepsilon U_{i,0}(t) \int_0^t ds U_{i,0}(-s) i H_{i,1}(s) U_{i,0}(s) + O(\varepsilon^2)$$

where we have used the notation $U_i, U_{i,0}$ to denote the evolution groups corresponding to $H_i, H_{i,0}$ respectively.

Substituting in (5.89) we obtain

$$\sigma = \sigma_0 + \varepsilon \lim_{T_\pm \rightarrow \infty} U_f(-T_+) \int_0^{T_+ + T_-} i H_f(s) U_i(s) U_f(-T_0) \tag{5.90}$$

The perturbation from the case in which the unperturbed interaction is the free one is sometimes called Fermi formula and it can be found in most books in quantum mechanics.

For the applications to the scattering map of a normally hyperbolic invariant manifold it is useful to think of the dynamics restricted to the invariant manifold as the free dynamics. The dynamics during the homoclinic excursion is the interacting dynamics.

Both in the future and in the past, there is free dynamics and the scattering map relates the dynamics in the future and in the past.

If we consider the Hamiltonian operator as an analogue of the vector field and the unitary operators as analogues of the flow, we see that many of the formulas for quantum mechanics are analogues to the corresponding formulas in the classical case.

We also note that the proof of the fact that the scattering map is symplectic is very analogous to the proof of unitarity of scattering matrix in quantum mechanics.

One can pursue the analogy between quantum mechanics scattering and classical mechanics scattering. For example, we have emphasized that the scattering map depends on the homoclinic channel $\Gamma \subset W_\Lambda^s \cap W_\Lambda^u$ considered.

One can therefore consider Γ as a rough analogue of the “channels” in quantum scattering theory.

The analogy cannot, however be carried too far. One of the most important properties of the quantum mechanics scattering matrix is that it commutes with the free dynamics.

$$\sigma U_f(t) = U_f(t) \sigma \tag{5.91}$$

The analogue of (5.91) and (5.88) in the context of the scattering map of a normally hyperbolic invariant manifold is more complicated.

In the scattering map for a normally hyperbolic invariant manifold we have

$$\begin{aligned} W_{x-}^u \pitchfork W_{x+}^s &\iff \\ f(W_{x-}^u) \pitchfork f(W_{x+}^s) \\ \iff W_{f(x-)}^u \pitchfork W_{f(x+)}^s \end{aligned}$$

Unfortunately, this does not allow us to conclude that the f commutes with σ^Γ . Note that if the intersection alluded to in the first line occurs in a manifold Γ , the intersection in the last line occurs in a manifold $f(\Gamma)$.

This means that the analogue of (5.88) and (5.91) are

$$\begin{aligned} f \circ \Omega_\pm^\Gamma &= \Omega_\pm^{f(\Gamma)} \circ f \\ f \circ \sigma^\Gamma &= \sigma^{f(\Gamma)} \circ f \end{aligned}$$

Since $f(\Gamma) \neq \Gamma$, in general, when we use only one scattering map, we have $\sigma^\Gamma \circ f \neq f \circ \sigma^\Gamma$.

In the applications to diffusion in [DLS00, DLS03, DLS06a] we have, for the unperturbed system the commutation of the inner map f_0 and the scattering map σ_0 , so

$$\sigma_0^{\Gamma_0} \circ f_0 = f_0 \circ \sigma_0^\Gamma$$

Nevertheless for $0 < |\varepsilon| < 1$ we have:

$$\sigma_\varepsilon^{\Gamma_\varepsilon} \circ f_\varepsilon \neq f_\varepsilon \circ \sigma_\varepsilon^{\Gamma_\varepsilon}$$

provided that the family satisfies some mild non-degeneracy assumptions. (See Section 5.6 for more details of a perturbative computation of σ_ε in these cases.) Note that, if the first order perturbation of both sides do not agree, then the true maps do not commute.

The last of commutation between the inner map and the scattering map is a crucial ingredient in the approach to diffusion in [DLS00, DLS03, DLS06a].

Chapter 6

Complete families of perturbations with few independent harmonics

6.1 Introduction

We are going to see that for any non-trivial perturbation depending on any two independent harmonics of a pendulum and a rotor there is global instability. The proof will be based on the geometrical method and relies on the concrete computation of several scattering maps. A complete description of the different kinds of scattering maps taking place as well as the existence of piecewise smooth global scattering maps is also provided. In an analogous way, for any non-trivial perturbation depending on three independent harmonics of a pendulum and two rotors there is global instability.

6.1.1 Main result

We consider an *a priori unstable* Hamiltonian with $2 + 1/2$ degrees of freedom

$$H_\varepsilon(p, q, I, \varphi, s) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{I^2}{2} + \varepsilon h(q, \varphi, s) \quad (6.1)$$

consisting of a pendulum and a rotor plus a time periodic perturbation depending on two harmonics in the variables (φ, s) :

$$\begin{aligned} h(q, \varphi, s) &= f(q)g(\varphi, s), \\ f(q) &= \cos q, \quad g(\varphi, s) = a_1 \cos(k_1\varphi + l_1s) + a_2 \cos(k_2\varphi + l_2s), \end{aligned} \quad (6.2)$$

with $k_1, k_2, l_1, l_2 \in \mathbb{Z}$.

Our goal is to prove that for *any* non-trivial perturbation $a_1a_2 \neq 0$ depending on *any* two *independent* harmonics $\begin{vmatrix} k_1 & k_2 \\ l_1 & l_2 \end{vmatrix} \neq 0$, there is global instability of the action I for any $\varepsilon > 0$ small enough.

Theorem 6.1. *Assume that $a_1a_2 \neq 0$ and $k_1l_2 - k_2l_1 \neq 0$ in Hamiltonian (6.1)-(6.2). Then, for any $I^* > 0$, there exists $\varepsilon^* = \varepsilon^*(I^*, a_1, a_2) > 0$ such that for any ε , $0 < \varepsilon < \varepsilon^*$, there exists a trajectory $(p(t), q(t), I(t), \varphi(t))$ such that for some $T > 0$*

$$I(0) \leq -I^* < I^* \leq I(T).$$

Remark 6.1. For a rough estimate of $\varepsilon^* \sim \exp(-\pi I^*/2)$ at least for $|a_1/a_2| < 0.625$, $k_1 = l_2 = 1$ and $l_1 = k_2 = 0$, and of the diffusion time $T = T(\varepsilon^*, I^*, a_1, a_2) \sim (T_s(I^*, a_1, a_2)/\varepsilon) \log(C(I^*, a_1, a_2)/\varepsilon)$ the reader is referred to [DS17]. Analogous estimates could be obtained for all the other values of the parameters.

The proof is based on the geometrical method introduced in [DLS00, DLS06a] and relies on the concrete computation of several *scattering maps*. A scattering map is a map of transverse homoclinic orbits to a *normally hyperbolic invariant manifold* (NHIM). For Hamiltonian (6.1), the NHIM turns out to be simply

$$\tilde{\Lambda}_\varepsilon = \tilde{\Lambda} = \left\{ (0, 0, I, \varphi, s) : (I, \varphi, s) \in \mathbb{R} \times \mathbb{T}^2 \right\}. \quad (6.3)$$

In the unperturbed case, i.e., $\varepsilon = 0$, for any $I^* > 0$ the NHIM $\tilde{\Lambda}$ possesses a 4D *separatrix*, that is to say, coincident stable and unstable invariant manifolds

$$W^0 \tilde{\Lambda} = \left\{ (p_0(\tau), q_0(\tau), I, \varphi, s) : \tau \in \mathbb{R}, I \in [-I^*, I^*], (\varphi, s) \in \mathbb{T}^2 \right\},$$

where (p_0, q_0) are the separatrices to the saddle equilibrium point of the pendulum

$$(p_0(t), q_0(t)) = \left(\frac{\pm 2}{\cosh t}, 4 \arctan e^{\pm t} \right).$$

In the perturbed case, i.e., for small $\varepsilon > 0$, $W^u(\tilde{\Lambda}_\varepsilon)$ and $W^s(\tilde{\Lambda}_\varepsilon)$ do not coincide (this is the so-called splitting of separatrices), and every local transversal intersection between them gives rise to a (local) scattering map which is simply the correspondence between a past asymptotic motion in the NHIM to the corresponding future asymptotic motion following a homoclinic orbit. Since the NHIM has also an inner dynamics, an adequate combination of these two dynamics on the NHIM, the inner one and the outer one provided by the scattering map, generates the global instability (also called in short *Arnold diffusion*) as long as the outer dynamics does not preserve the invariant objects of the inner dynamics.

The inner motion is described in Section 6.2, the scattering maps in Section 6.3 and the absence of invariant sets in both dynamics is checked in Section 6.4, which also includes the proof of Theorem 6.1. Section 6.5 deals with the construction of a piecewise smooth global scattering map which is introduced as a possible new tool to design fast and simple paths of global instability. We finish this Introduction with some remarks about the necessity of the assumptions, as well as other features of the scattering map and a discussion of the model chosen and related work.

6.1.2 Necessity of the assumptions

If the determinant $\Delta := k_1 l_2 - k_2 l_1$ or some coefficient a_1, a_2 vanishes, for instance, if there is only one harmonic in g , there is no global instability for the action I . Indeed, looking at the equations associated to Hamiltonian (6.1)

$$\begin{aligned} \dot{q} &= \pm p & \dot{p} &= \left[\pm 1 + \varepsilon (a_1 \cos(k_1 \varphi + l_1 s) + a_2 \cos(k_2 \varphi + l_2 s)) \right] \sin q \\ \dot{\varphi} &= I & \dot{I} &= \varepsilon \cos q (k_1 a_1 \sin(k_1 \varphi + l_1 s) + k_2 a_2 \sin(k_2 \varphi + l_2 s)) \\ \dot{s} &= 1 \end{aligned} \quad (6.4)$$

this is clear for $k_1 = k_2 = 0$, since in this case I is a constant of motion. If k_1 or $k_2 \neq 0$, say $k_1 \neq 0$, the change of variables

$$\bar{\varphi} = k_1 \varphi + l_1 s, \quad r \bar{\varphi} - \bar{s} = k_2 \varphi + l_2 s, \quad \bar{I} = k_1 I + l_1,$$

where $r = k_2/k_1$ can be assumed to satisfy $0 \leq r \leq 1$ without loss of generality, casts system (6.4) into

$$\begin{aligned} \dot{q} &= \pm p & \dot{p} &= \left[\pm 1 + \varepsilon (a_1 \cos \bar{\varphi} + a_2 \cos(r \bar{\varphi} - \bar{s})) \right] \sin q \\ \dot{\bar{\varphi}} &= \bar{I} & \dot{\bar{s}} &= \varepsilon k_1^2 \cos q (a_1 \sin \bar{\varphi} + r a_2 \sin(r \bar{\varphi} - \bar{s})) \\ \dot{\bar{s}} &= \Delta/k_1 \end{aligned}$$

which is a Hamiltonian system with the Hamiltonian given by

$$\bar{H}_\varepsilon(p, q, \bar{I}, \bar{\varphi}, \bar{s}) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{\bar{I}^2}{2} + \varepsilon k_1^2 \cos q (a_1 \cos \bar{\varphi} + a_2 \cos(r \bar{\varphi} - \bar{s})). \quad (6.5)$$

If $\Delta = 0$ Hamiltonian (6.5) is autonomous with 2 degrees of freedom, and therefore a global drift for the action I is not possible. Only drifts of size $\sqrt{\varepsilon}$ are possible due to KAM theorem. Analogously one easily checks that for $a_1 a_2 = 0$ Hamiltonian (6.1) is integrable or autonomous.

6.1.3 Reduction of the harmonic types

Under the hypothesis $(k_1 l_2 - k_2 l_1) a_1 a_2 \neq 0$ of Theorem 6.1, we first notice that the case $k_2 = 0$ of Theorem 6.1 is already proven in [DS17]. Indeed, $k_2 = 0$ implies $r := k_2/k_1 = 0$ and it turns out from (6.5) that Hamiltonian (6.1) is equivalent to the one with $k_1 = 1, k_2 = 0, l_1 = 0, l_2 = 1$:

$$H_\varepsilon(p, q, I, \varphi, t) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{I^2}{2} + \varepsilon \cos q (a_1 \cos \varphi + a_2 \cos s), \quad (6.6)$$

which is just the Hamiltonian studied in [DS17]. Therefore, we only need to prove Theorem 6.1 for $k_1 k_2 \neq 0$ or equivalently for $r \in (0, 1]$. For the sake of clarity we will explain in full detail and prove Theorem 6.1 along Sections 6.2-6.4 just for $r = 1$, which by (6.5) is equivalent to the case $k_1 = 1, k_2 = 1, l_1 = 0, l_2 = -1$:

$$H_\varepsilon(p, q, I, \varphi, t) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{I^2}{2} + \varepsilon \cos q (a_1 \cos \varphi + a_2 \cos(\varphi - s)). \quad (6.7)$$

To finish the proof of Theorem 6.1, in Section 6.4 we will sketch the modifications needed for the case $r \in (0, 1)$.

6.1.4 Scattering map types

By the definition given at the beginning of Section 6.3, a scattering map is in principle only *locally* defined, that is, for a small ball of values of the variables (I, φ, s) or $(I, \theta = \varphi - Is)$, since it depends on a non-degenerate critical point $\tau^* = \tau^*(I, \varphi, s)$ of a real function (6.16), depending smoothly on the variables (I, φ, s) , already introduced in [DLS00]. In the study carried out in Section 6.3, it will be described whether, in terms of the parameter $\mu := a_1/a_2$ and the variable I , a local scattering map can or cannot be smoothly defined for all the values of the angles (φ, s) or $\theta = \varphi - Is$, becoming thus a *global* or *extended* scattering map. This description will depend essentially on a geometrical characterization of the function $\tau^*(I, \varphi, s)$ in terms of the intersection of *crests* and *NHIM lines*, following [DH11]. Any degeneration of the critical point $\tau^* = \tau^*(I, \varphi, s)$ may give rise to more non-degenerate critical points and a bifurcation to *multiple* local scattering maps or to a non global scattering map. Different critical points $\tau^* = \tau^*(I, \varphi, s)$ give rise to different local scattering maps, and putting together different local scattering maps, one can sometimes obtain *piecewise smooth* global scattering maps, which are very useful to design paths of instability for the action I , and are simply called diffusion paths.

For instance, in the paper [DS17] devoted to the Hamiltonian (6.6), it was proven that for $0 < \mu = a_1/a_2 < 0.625$, there exist two different global scattering maps. Among the different kinds of associated orbits of these scattering maps, there appeared two of them called *highways*, where the drift of the action I was very fast and simple. As will be described in Section 6.3, such highways do not appear for Hamiltonian (6.7). Nevertheless, as will be proven in Section 6.5, there exist piecewise smooth global scattering maps, and the possible diffusion along the discontinuity sets opens the possibility of applying the theory of piecewise smooth dynamical systems [Fil88].

6.1.5 About the model chosen and related work

Hamiltonian (6.1) is a standard example of an *a priori unstable* Hamiltonian system [CG94] formed by a pendulum, a rotor and a perturbation. It is usual in the literature to choose a perturbation depending periodically only on the positions—which turn out to be angles in our case—and time. Our perturbation $h(q, \varphi, s)$ (6.2) is a little bit special since it is a product of a function $f(q)$ times a function $g(\varphi, s)$. This choice makes easier the computations of the Poincaré-Melnikov potential (6.17), which is based on the Cauchy's residue theorem. Theorem 6.1 can be easily generalized to any trigonometric polynomial or meromorphic function $f(q)$, although the computations of poles of high order become more complicated. In the same way, it could also be generalized to more general perturbations $h(q, \varphi, s)$, as long that h is a trigonometric polynomial or meromorphic in q . The dependence on more than two harmonics gives rise to the appearance of more resonances in the inner dynamics, which requires more control of their sizes, see for instance [DS97, DH09]. Apart from more difficulty in the computations of the Poincaré-Melnikov potential and the inner Hamiltonian, we do not foresee substantial changes, so we believe that Hamiltonian (6.1) could be considered as a paradigmatic example of an *a priori unstable* Hamiltonian system.

The model considered is a natural culmination of [DS17], which dealt with the simpler Hamiltonian (6.6), and where a detailed description of NHIM lines and crests was carried out. An “optimal” estimate of the diffusion time close to some special orbits of the scattering map, called *highways*, was also given there. The study in our case of Hamiltonian (6.7) is more complicated, due to a greater complexity of the evolution of the NHIM lines and crests with respect to the action I and the parameters of the system. In particular, the absence of highways prevents us of showing an estimate of diffusion time close to them.

The paper [DS17] also contains a fairly extensive list of references about global instability. Let us simply mention some new references that are not there, like [DT16] which contains a similar approach

to the function τ^* of [DLS00] and the crests of [DH11], and the recent papers [GT17, LMS19, Mar24, GM22, Che17] involving the geometrical method or variational methods.

We finish this introduction by noticing that we stress the interaction between NHIM lines and crests, since this allows us to describe the diverse scattering maps, as well as their domains, that appear in our problem. In more complicated models of Celestial Mechanics the Melnikov potential is not available. In these cases the computations of scattering maps rely on the numerical computation of invariant manifolds of a NHIM or some of its selected invariant objects, and the search of diffusion orbits is performed in a more crafted way (see [CDMR06, DMR08, DGR13, CGL17a, DGR16, DGR26]).

6.2 Inner dynamics

The inner dynamics is derived from the restriction of H_ε in (6.7) and its equations to $\tilde{\Lambda}$, that is,

$$K(I, \varphi, s) = \frac{I^2}{2} + \varepsilon (a_1 \cos \varphi + a_2 \cos(\varphi - s)), \quad (6.8)$$

and differential equations

$$\dot{\varphi} = I \quad \dot{s} = 1 \quad \dot{I} = \varepsilon (a_1 \sin \varphi + a_2 \sin(\varphi - s)). \quad (6.9)$$

Note that in this case the inner dynamics is slightly more complicated to describe than in [DS17] where there was just one resonance, namely, in $I = 0$. In the current case we have two resonant regions of size $\mathcal{O}(\sqrt{\varepsilon})$ where secondary KAM tori appear. To describe these regions, we use normal forms as in [DLS00].

Consider the autonomous extended Hamiltonian

$$\overline{K}(I, A, \varphi, s) = \frac{I^2}{2} + A + \varepsilon (a_1 \cos \varphi + a_2 \cos(\varphi - s)), \quad (6.10)$$

with the differential equations

$$\begin{aligned} \dot{\varphi} &= I & \dot{I} &= \varepsilon (a_1 \sin \varphi + a_2 \sin(\varphi - s)) \\ \dot{s} &= 1 & \dot{A} &= -\varepsilon a_2 \sin(\varphi - s). \end{aligned}$$

This system is equivalent to the system represented by (6.8)+(6.9). We wish to eliminate the dependence on the angle variables. Consider a change of variables ε -close to the identity

$$(\varphi, s, I, A) = g(\phi, \sigma, J, B) = (\phi, \sigma, J, B) + \mathcal{O}(\varepsilon)$$

such that it is the one-time flow for a Hamiltonian εG , i.e., $g = g_{t=1}$, where g_t is solution of

$$\frac{dg_t}{dt} = J_0 \nabla \varepsilon G \circ g_t, \text{ where } J_0 \text{ is the symplectic matrix } \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Composing $\overline{K}$ with g and expanding in a Taylor series around $t = 0$, one obtains

$$\overline{K} \circ g = \overline{K} + \left\{ \overline{K}, \varepsilon G \right\} + \frac{1}{2} \left\{ \left\{ \overline{K}, \varepsilon G \right\}, \varepsilon G \right\} + \dots,$$

where $\{\cdot\}$ is the Poisson bracket. Using the expansion (6.10) of $\overline{K}$, the equation above can be written as

$$\begin{aligned} \overline{K} \circ g &= \frac{J^2}{2} + B + \varepsilon \left(a_1 \cos \phi + a_2 \cos(\phi - \sigma) + \left\{ \frac{J^2}{2} + B, G \right\} \right) \\ &\quad + \frac{\varepsilon^2}{2} \left\{ \left\{ \frac{J^2}{2} + B, G \right\}, G \right\} + \mathcal{O}(\varepsilon^3). \end{aligned} \quad (6.11)$$

We want to find G such that $a_1 \cos \phi + a_2 \cos(\phi - \sigma) + \left\{ \frac{J^2}{2} + B, G \right\} = 0$, or equivalently,

$$J \frac{\partial G}{\partial \phi} + \frac{\partial G}{\partial \sigma} = a_1 \cos \phi + a_2 \cos(\phi - \sigma).$$

Given $a < b < 1$, consider any function $\Psi \in C^\infty(\mathbb{R})$ satisfying $\Psi(x) = 1$ for $x \in [-a, a]$ and $\Psi(x) = 0$ for $|x| > b$ and introduce

$$G(J, B, \phi, \sigma) := \frac{a_1}{J} (1 - \Psi(J)) \sin \phi + \frac{a_2}{J-1} (1 - \Psi(J-1)) \sin(\phi - \sigma),$$

Substituting the above function $G(J, B, \phi, \sigma)$ in (6.11) we have

$$\overline{K} \circ g = \frac{J^2}{2} + B + \mathcal{O}(\varepsilon^2), \quad (6.12)$$

for $J, J-1 \notin [-b, b]$. For $J \in [-a, a]$,

$$\overline{K} \circ g = \frac{J^2}{2} + B + \varepsilon a_1 \cos \phi + \mathcal{O}(\varepsilon^2). \quad (6.13)$$

Finally, for $J-1 \in [-a, a]$,

$$\overline{K} \circ g = \frac{J^2}{2} + B + \varepsilon a_2 \cos(\phi - \sigma) + \mathcal{O}(\varepsilon^2). \quad (6.14)$$

From (6.13) and (6.14), one sees that on $J = 0$ and $J = 1$ there are resonances of first order in ε with a pendulum-like behavior.

Coming back to the original variables, three kinds of invariant tori are obtained. For the first order resonance $I = 0$, there is a positive $\bar{a}$ such that the invariant tori are given by $F^0(I, \varphi, s) = \text{constant}$ with

$$F^0(I, \varphi, s) = \frac{I^2}{2} + \varepsilon a_1 \cos \varphi + \mathcal{O}(\varepsilon^2). \quad (6.15)$$

for $I \in [-\bar{a}, \bar{a}]$

Analogously, for the first order resonance $I = 1$, with

$$F^1(I, \varphi, s) = \frac{(I-1)^2}{2} + \varepsilon a_2 \cos(\varphi - s) + \mathcal{O}(\varepsilon^2),$$

for $I-1 \in [-\bar{a}, \bar{a}]$.

Remark 6.2. As commented in [DLS00], there exists a *secondary* resonance in $I = 1/2$, but the size of the gap in its resonant region is much smaller than the size of gaps in resonant regions associated to $I = 0$ and $I = 1$.

Remark 6.3. In a more general case with $r \neq 1$, the resonances take place in $I = 0$ and $I = 1/r$.

From (6.12), on the non-resonant region the invariant tori has equations $F^{\text{nr}}(I) = \text{constant}$ with

$$F^{\text{nr}}(I) = \frac{I^2}{2} + \mathcal{O}(\varepsilon^2).$$

An illustration of the inner dynamics is displayed in Figure 6.1.

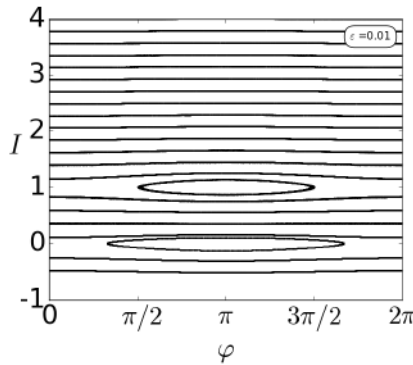


Figure 6.1: Plane $\varphi \times I$ of inner dynamics for $\mu = 0.75$ and $\varepsilon = 0.01$.

6.3 Scattering map

6.3.1 Definition of scattering map

We are going to explore the properties of the scattering maps of Hamiltonian (6.7). The notion of scattering map on a NHIM was introduced in [DLS00]. Let W be an open set of $[-I^*, I^*] \times \mathbb{T}^2$ such that the invariant manifolds of the NHIM $\tilde{\Lambda}$ introduced in (6.3) intersect transversally along a homoclinic manifold $\Gamma = \{\tilde{z}(I, \varphi, s; \varepsilon), (I, \varphi, s) \in W\}$ so that for any $\tilde{z} \in \Gamma$ there exist unique $\tilde{x}_{+,-} = \tilde{x}_{+,-}(I, \varphi, s; \varepsilon) \in \tilde{\Lambda}$ such that $\tilde{z} \in W_\varepsilon^s(x_-) \cap W_\varepsilon^u(\tilde{x}_+)$. Let

$$H_{+,-} = \bigcup \{\tilde{x}_{+,-}(I, \varphi, s; \varepsilon) : (I, \varphi, s) \in W\}.$$

The scattering map associated to Γ is the map

$$\begin{aligned} S : H_- &\longrightarrow H_+ \\ \tilde{x}_- &\longmapsto S(\tilde{x}_-) = \tilde{x}_+. \end{aligned}$$

For the characterization of the scattering maps, it is required to select the homoclinic manifold Γ and this is done using the Poincaré-Melnikov theory. From [DLS00, DH11], we have the following proposition

Proposition 6.2. *Given $(I, \varphi, s) \in [-I^*, I^*] \times \mathbb{T}^2$, assume that the real function*

$$\tau \in \mathbb{R} \longmapsto \mathcal{L}(I, \varphi - I\tau, s - \tau) \in \mathbb{R} \quad (6.16)$$

has a non degenerate critical point $\tau^ = \tau^*(I, \varphi, s)$, where*

$$\mathcal{L}(I, \varphi, s) := \int_{-\infty}^{+\infty} (f(q_0(\sigma)) - f(0)) g(\varphi + I\sigma, s + \sigma; 0) d\sigma.$$

Then, for $0 < \varepsilon$ small enough, there exists a unique transversal homoclinic point $\tilde{z}$ to $\tilde{\Lambda}_\varepsilon$ of Hamiltonian (6.1), which is ε -close to the point $\tilde{z}^(I, \varphi, s) = (p_0(\tau^*), q_0(\tau^*), I, \varphi, s) \in W^0(\tilde{\Lambda})$:*

$$\tilde{z} = \tilde{z}(I, \varphi, s) = (p_0(\tau^*) + O(\varepsilon), q_0(\tau^*) + O(\varepsilon), I, \varphi, s) \in W^u(\tilde{\Lambda}_\varepsilon) \cap W^s(\tilde{\Lambda}_\varepsilon).$$

The function $\mathcal{L}$ is called the *Melnikov potential* of Hamiltonian (6.1). For the concrete Hamiltonian (6.7) it takes the form

$$\mathcal{L}(I, \varphi, s) = A_1(I) \cos \varphi + A_2(I) \cos(\varphi - s), \quad (6.17)$$

where

$$A_1(I) = \frac{2\pi I a_1}{\sinh(\pi I/2)} \quad \text{and} \quad A_2(I) = \frac{2\pi(I-1)a_2}{\sinh(\pi(I-1)/2)}.$$

The homoclinic manifold Γ is characterized by the function $\tau^*(I, \varphi, s)$. Once a $\tau^*(I, \varphi, s)$ is chosen, which under the conditions of Proposition 6.2, is locally smoothly well defined, by the geometric properties of the scattering map, see [DLS06a, DLS08, DH11], the scattering map has the explicit local form

$$S(I, \varphi, s) = \left(I + \varepsilon \frac{\partial \mathcal{L}^*}{\partial \varphi}(I, \varphi, s) + \mathcal{O}(\varepsilon^2), \varphi - \varepsilon \frac{\partial \mathcal{L}^*}{\partial I}(I, \varphi, s) + \mathcal{O}(\varepsilon^2), s \right),$$

where

$$L^*(I, \varphi, s) = \mathcal{L}(I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s)). \quad (6.18)$$

Notice that the variable s is fixed under the scattering map. As a consequence [DH11, DS17], introducing the variable

$$\theta = \varphi - Is$$

and defining the *reduced Poincaré function*

$$\mathcal{L}^*(I, \theta) := L^*(I, \varphi - Is, 0) = L^*(I, \varphi, s), \quad (6.19)$$

in the variables (I, θ) , the scattering map has the simple form

$$S(I, \theta) = \left(I + \varepsilon \frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) + \mathcal{O}(\varepsilon^2), \theta - \varepsilon \frac{\partial \mathcal{L}^*}{\partial I}(I, \theta) + \mathcal{O}(\varepsilon^2) \right),$$

so up to $\mathcal{O}(\varepsilon^2)$ terms, $S(I, \theta)$ is the ε times flow of the *autonomous* Hamiltonian $-\mathcal{L}^*(I, \theta)$. In particular, the iterates under the scattering map follow the level curves of $\mathcal{L}^*$ up to $\mathcal{O}(\varepsilon^2)$.

6.3.2 Crests and NHIM lines

We have seen that the function τ^* plays a central role in our study. Therefore, we are interested in finding the critical points $\tau^* = \tau^*(I, \varphi, s)$ of function (6.16). For our concrete case (6.17), τ^* is a solution of

$$IA_1(I) \sin(\varphi - I\tau^*) + (I - 1)A_2(I) \sin(\varphi - s - (I - 1)\tau^*) = 0. \quad (6.20)$$

This equation can be viewed from two equivalently geometrical viewpoints. The first one is that to find $\tau^* = \tau^*(I, \varphi, s)$ satisfying (6.20) for any $(I, \varphi, s) \in [-I^*, I^*] \times \mathbb{T}^2$ is the same as to look for the extrema of $\mathcal{L}$ on the *NHIM line*

$$R(I, \varphi, s) = \{(I, \varphi - I\tau, s - \tau) : \tau \in \mathbb{R}\}. \quad (6.21)$$

Remark 6.4. Since $(\varphi, s) \in \mathbb{T}^2$, $R(I, \varphi, s)$ is a closed line if $I \in \mathbb{Q}$ and it is a dense line on $\{I\} \times \mathbb{T}^2$ if $I \notin \mathbb{Q}$.

The other viewpoint is that, fixing (I, φ, s) , a solution τ^* of (6.20) is equivalent to finding intersections between a NHIM line (6.21) and a curve defined by

$$IA_1(I) \sin \varphi + (I - 1)A_2(I) \sin(\varphi - s) = 0. \quad (6.22)$$

These curves are called *crests* or *ridges*, and in a general way can be defined as follows.

Definition 1. [DH11] We define by Crests $\mathcal{C}(I)$ the curves on (I, φ, s) , $(\varphi, s) \in \mathbb{T}^2$, such that

$$\frac{\partial \mathcal{L}}{\partial \tau}(I, \varphi - I\tau, s - \tau)|_{\tau=0} = 0, \quad (6.23)$$

or equivalently,

$$I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi, s) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi, s) = 0.$$

As in our case $\mathcal{L}(I, \varphi - I\tau, s - \tau) = A_1(I) \cos(\varphi - I\tau) + A_2(I) \cos(\varphi - s - (I - 1)\tau)$, equation (6.23) takes the form (6.22). Introducing

$$\sigma = \varphi - s, \quad (6.24)$$

equation (6.22) can be rewritten as

$$\mu \alpha(I) \sin \varphi + \sin \sigma = 0, \quad (6.25)$$

for $I \neq 1$, where

$$\mu = \frac{a_1}{a_2} \quad \text{and} \quad \alpha(I) = \frac{I^2 \sinh(\frac{\pi}{2}(I - 1))}{(I - 1)^2 \sinh(\frac{\pi I}{2})}. \quad (6.26)$$

From now on, when we refer to crests $\mathcal{C}(I)$ we mean the set of points (I, φ, σ) satisfying equation (6.25). See an illustration in Fig. 6.3.

Remark 6.5. In [DS17] the crests were described on the plane (φ, s) , whereas now such curves lie on the plane (φ, σ) . Besides, differently from the cases studied in [DH11, DS17], the function $\alpha(I)$ is not defined for all I . More precisely, it is not defined for $I = 1$. For this value of I , equation (6.25) is not adequate, and one has to use (6.22) to check that for $I = 1$ the crests are just two vertical straight lines on the plane (φ, σ) given by $\varphi = 0$ and $\varphi = \pi$.

Remark 6.6. For Hamiltonian (6.5) and $r \in (0, 1)$, $\alpha_r(I)$ is not defined for $I = 1/r$ and is given by

$$\alpha_r(I) = \frac{I^2 \sinh(\frac{\pi}{2}(rI - 1))}{(rI - 1)^2 \sinh(\frac{\pi I}{2})}.$$

We are interested in understanding the behavior of these crests because, as we have seen in previous works [DH11, DS17], their intersection with the NHIM lines determine the existence and behavior of scattering maps.

From (6.25), when $|\alpha(I)| < 1/|\mu|$, σ can be written as a function of φ for all $\varphi \in \mathbb{T}$ on the crest $\mathcal{C}(I)$. On the other hand, if $|\alpha(I)| > 1/|\mu|$, φ can be written as a function of σ for all $\sigma \in \mathbb{T}$. These two conditions give us two kinds of crests: *horizontal* for $|\alpha(I)| < 1/|\mu|$ and *vertical* for $|\alpha(I)| > 1/|\mu|$. These names are due to their forms on the plane (φ, σ) . We consider the same characterization used in [DS17]:

- For $|\alpha(I)| < 1/|\mu|$, there are two horizontal crests $\sigma = \xi_{M,m}(I, \varphi)$

$$\mathcal{C}_{M,m}(I) = \{(I, \varphi, \xi_{M,m}(I, \varphi)) : \varphi \in \mathbb{T}\},$$

$$\begin{aligned} \xi_M(I, \varphi) &= -\arcsin(\mu\alpha(I) \sin \varphi) \quad \text{mod } 2\pi \\ \xi_m(I, \varphi) &= \arcsin(\mu\alpha(I) \sin \varphi) + \pi \quad \text{mod } 2\pi. \end{aligned} \quad (6.27)$$

- For $|\alpha(I)| > 1/|\mu|$, there are two vertical crests $\varphi = \eta_{M,m}(I, \sigma)$

$$\mathcal{C}_{M,m}(I) = \{(I, \eta_{M,m}(I, \sigma), \sigma) : \sigma \in \mathbb{T}\},$$

$$\begin{aligned} \eta_M(I, \sigma) &= -\arcsin(\sin \sigma / (\mu\alpha(I))) \quad \text{mod } 2\pi \\ \eta_m(I, \sigma) &= \arcsin(\sin \sigma / (\mu\alpha(I))) + \pi \quad \text{mod } 2\pi. \end{aligned}$$

Remark 6.7. $|\alpha(I)| = 1/|\mu|$ is a singular or bifurcation case. In this case, the crests are straight lines and are not differentiable in $\varphi = \pi/2$ and $\varphi = 3\pi/2$. See Fig. 6 of [DS17].

Remark 6.8. The crest containing the point $(\varphi, \sigma) = (0, 0)$ will be denoted by $\mathcal{C}_M(I)$ and the crest containing the point $(\varphi, \sigma) = (\pi, \pi)$ by $\mathcal{C}_m(I)$.

Note that the function $|\alpha(I)|$ is not bounded, indeed

$$\lim_{I \rightarrow 1} |\alpha(I)| = +\infty.$$

This implies that for any μ there exists a neighborhood U of $I = 1$ such that for all $I \in U$ the crests are vertical. On the other hand, since $\alpha(0) = 0$ there exists a neighborhood V of $I = 0$ such that for all $I \in V$ the crests are horizontal. We notice here a remarkable difference with the Hamiltonians studied in [DH11, DS17], where, for $|\mu| \leq 0.97$, all the crests are horizontal for all I .

Now take a look at the properties of the function $\alpha(I)$ introduced in (6.26) to describe under which conditions in μ the crests are horizontal or vertical. First of all, observe that for $I \neq 1$, $\alpha(I)$ is smooth and $\alpha'(I) \neq 0$, and for $I = 1$ $\alpha(I)$ is not bounded, indeed it has a vertical asymptote

$$\lim_{I \rightarrow 1^-} \alpha(I) = -\infty \quad \text{and} \quad \lim_{I \rightarrow 1^+} \alpha(I) = +\infty.$$

Given a $\mu \neq 0$, since $\alpha(0) = 0$, there exists a unique $I_c \in (0, 1)$ such that $|\alpha(I)| = 1/|\mu|$. So, the crests are horizontal for $I \in [0, I_c]$ and vertical for $I \in (I_c, 1)$.

Others important limits are

$$\lim_{I \rightarrow -\infty} \alpha(I) = \exp(\pi/2) \quad \text{and} \quad \lim_{I \rightarrow +\infty} \alpha(I) = \exp(-\pi/2).$$

The first limit implies that $|\alpha(I)| < \exp(\pi/2)$ for $I \in (-\infty, 0)$. Thus, if $\exp(\pi/2) \leq 1/|\mu|$ the crests are horizontal for $I \in (-\infty, 0)$. Otherwise, if $1/|\mu| < \exp(\pi/2)$, there exists a unique $I_1 \in (-\infty, 0)$ such that $|\alpha(I)| = 1/|\mu|$ and the crests are vertical for $I \in (-\infty, I_1)$ and horizontal for $I \in (I_1, 0)$.

The second limit implies that $|\alpha(I)| > \exp(-\pi/2)$ for $I \in (1, +\infty)$. Then, if $\exp(-\pi/2) \geq 1/|\mu|$, the crests are vertical for $I \in [1, +\infty)$. if $\exp(-\pi/2) < 1/|\mu|$, there exists a unique $I_r \in (1, +\infty)$, such that the crests are vertical for any I in $[1, I_r)$ and horizontal for $I \in (I_r, +\infty)$.

Summarizing, for $1/|\mu| \geq \exp(\pi/2)$, crests are horizontal for $I \in (-\infty, I_c) \cup (I_r, +\infty)$ and vertical for $I \in (I_c, I_r)$. For $\exp(-\pi/2) < 1/|\mu| < \exp(\pi/2)$, crests are horizontal for $I \in (I_1, I_c) \cup (I_r, +\infty)$ and vertical for $I \in (-\infty, I_1) \cup (I_c, I_r)$. Finally, if $1/|\mu| < \exp(-\pi/2)$, crests are horizontal for $I \in (I_1, I_c)$ and vertical for $I \in (-\infty, I_1) \cup (I_c, +\infty)$.

Remark 6.9. For $r \in (0, 1)$, $\alpha_r(I)$ is not bounded on a neighbourhood of the resonance $I = 1/r$, i.e., $\lim_{I \rightarrow 1/r^-} \alpha_r(I) = -\infty$ and $\lim_{I \rightarrow 1/r^+} \alpha_r(I) = +\infty$. The same behavior takes place for $r = 1$ and close to $I = 1$. On the other hand, for $I \rightarrow \pm\infty$, $\alpha_r(I)$ has the same behavior as in the case for $r = 0$, $\lim_{I \rightarrow \pm\infty} \alpha_r(I) = 0$. This implies that for any value of μ , for I close enough to $I = 1/r$ the crests are vertical, and for $|I|$ large enough the crests are horizontal.

Example To illustrate this discussion, we present a concrete example. Taking $\mu = 0.5$, we have $\exp(-\pi/2) < 1/\mu = 2 < \exp(\pi/2)$. In this case we have $I_l \approx -1.807$, $I_c \approx 0.701$ and $I_r \approx 1.367$. The crests are horizontal in $(-1.807, 0.701) \cup (1, 367, +\infty)$ and vertical in $(-\infty, -1.807) \cup (0.701, 1.367)$. We emphasize that this scenario is very different from the case in [DS17]. There, for $\mu = 0.5$ the crests are horizontal for all I .

Now, we are going to focus on the transversality of the intersection between NHIM lines $R(I, \varphi, s)$ and crests $\mathcal{C}(I)$. On the plane (φ, σ) the NHIM lines can be written as

$$R_I(\varphi, \sigma) = \{(\varphi - I\tau, \sigma - (I - 1)\tau), \tau \in \mathbb{R}\}, \quad (6.28)$$

so that its slope is $(I - 1)/I$ in such plane. Therefore, there exists an intersection between NHIM lines and crests that is not transversal if, and only if, there exists a tangent vector of $\mathcal{C}(I)$ at a point that is parallel to $(I, I - 1)$, or, using the parameterizations,

$$\frac{\partial \xi}{\partial \varphi}(I, \varphi) = \frac{I - 1}{I} \quad \text{or} \quad \frac{\partial \eta}{\partial \sigma}(I, \sigma) = \frac{I}{I - 1}.$$

Considering a *horizontal* parameterization of $\mathcal{C}(I)$, the tangency condition is equivalent to

$$\frac{\pm \alpha(I) \mu \cos \varphi}{\sqrt{1 - \mu^2 \alpha^2(I) \sin^2 \varphi}} = \frac{I - 1}{I}.$$

Therefore, there exists a φ satisfying the above condition if, and only if,

$$|\beta(I)| \geq \frac{1}{|\mu|}, \quad \text{where} \quad \beta(I) = \frac{I \alpha(I)}{I - 1}$$

and φ takes the form

$$\varphi = \pm \arctan \left(\sqrt{\frac{\beta(I)^2 - (1/\mu)^2}{(1/\mu)^2 - \alpha(I)^2}} \right).$$

In an analogous way, for a *vertical* parameterization $\eta(I, \sigma)$, there are tangencies if, and only if,

$$|\beta(I)| \leq \frac{1}{|\mu|} \quad \text{with} \quad \sigma = \pm \arctan \left(\left| \frac{I - 1}{I} \right| \sqrt{\frac{(1/\mu)^2 - \beta(I)^2}{\alpha(I)^2 - (1/\mu)^2}} \right).$$

Remark 6.10. Observe that in both cases, horizontal and vertical crests, there are tangencies if, and only if,

$$\left(|\alpha(I)| - \frac{1}{|\mu|} \right) \left(|\beta(I)| - \frac{1}{|\mu|} \right) < 0.$$

The function $|\beta(I)|$ is smooth in $\mathbb{R} \setminus \{1\}$ and $d|\beta(I)|/dI = 0$ only for $I = 0$. Besides, we have

$$\lim_{I \rightarrow 1} |\beta(I)| = +\infty, \quad \lim_{I \rightarrow -\infty} |\beta(I)| = \exp(\pi/2) \quad \text{and} \quad \lim_{I \rightarrow +\infty} |\beta(I)| = \exp(-\pi/2).$$

Therefore, there are three possibilities:

- for $1/|\mu| \geq \exp(\pi/2)$, there exist $I_0 \in (1/2, 1)$ and $I_+ \in (1, +\infty)$ such that I_0 and I_+ are solutions of $|\beta(I)| - 1/|\mu| = 0$. Besides, $|\beta(I)| < 1/|\mu|$ for $I \in (-\infty, I_0) \cup (I_+, +\infty)$ and $|\beta(I)| > 1/|\mu|$ for $I \in (I_0, 1) \cup (1, I_+)$.
- for $\exp(-\pi/2) < 1/|\mu| < \exp(\pi/2)$, there exist $I_- \in (-\infty, 0)$, $I_0 \in (0, 1)$ and $I_+ \in (1, +\infty)$ such that I_- , I_0 and I_+ are solutions of $|\beta(I)| - 1/|\mu| = 0$. Besides, $|\beta(I)| < 1/|\mu|$ for $I \in (I_-, I_0) \cup (I_+, +\infty)$ and $|\beta(I)| > 1/|\mu|$ for $I \in (-\infty, I_-) \cup (I_0, 1) \cup (1, I_+)$.
- For $1/|\mu| \leq \exp(-\pi/2)$, there exist $I_- \in (-\infty, 0)$ and $I_0 \in (0, 1/2)$ such that I_- and I_0 are solutions of $|\beta(I)| - 1/|\mu| = 0$. Besides, $|\beta(I)| < 1/|\mu|$ for $I \in (I_-, I_0)$ and $|\beta(I)| > 1/|\mu|$ for $I \in (-\infty, I_-) \cup (I_0, 1) \cup (1, \infty)$.

Putting together this description of $|\beta(I)|$ with the study about vertical and horizontal crests and adding that

$$\begin{aligned} |\beta(I)| &< |\alpha(I)| & \forall I \in (-\infty, 0) \cup (0, 1/2); \\ |\beta(I)| &> |\alpha(I)| & \forall I \in (1/2, 1) \cup (1, +\infty); \\ |\beta(0)| &= |\alpha(0)| = 0 & |\beta(1/2)| = |\alpha(1/2)| = 1 \end{aligned}$$

we can state the proposition below.

Proposition 6.3. *Consider the two crests $\mathcal{C}(I)$ defined by (6.25) and the NHIM line $R_I(\varphi, \sigma)$ defined in (6.21) for Hamiltonian (6.7).*

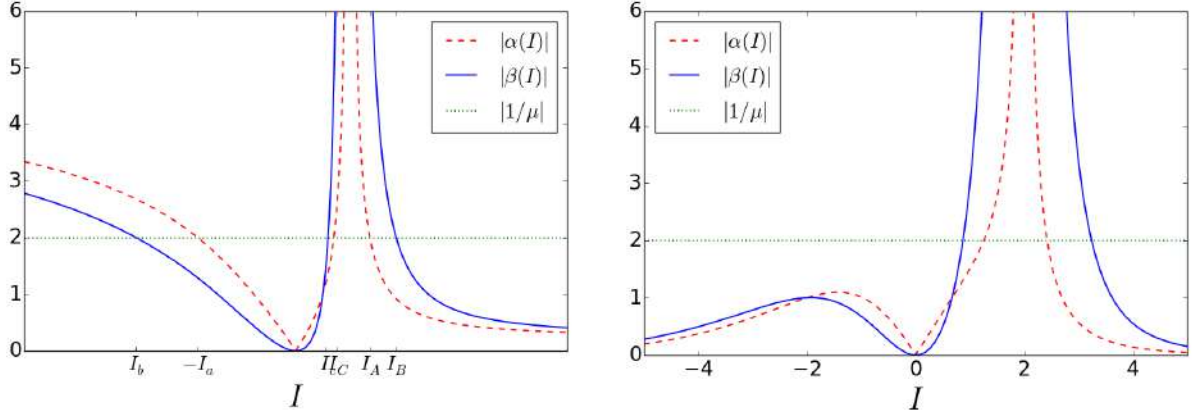
- For $|\mu| \leq \exp(-\pi/2)$, there exist $I_b < I_a < I_A < I_B$ such that
 - for $I < I_b$ or $I_B < I$, $\mathcal{C}(I)$ are horizontal and intersect transversally any $R_I(\varphi, \sigma)$;
 - for $I_b \leq I < I_a$ or $I_A < I \leq I_B$, the crests $\mathcal{C}(I)$ are horizontal, but now, there exist tangencies between $\mathcal{C}(I)$ and two NHIM lines $R_I(\varphi, \sigma)$;
 - for $I_a < I < I_A$, the crests $\mathcal{C}(I)$ are vertical and intersect transversally any $R_I(\varphi, \sigma)$.
- For $\exp(-\pi/2) < |\mu| < \exp(\pi/2)$ there exist $I_b < I_a < I_c \leq I_C < I_A < I_B$ such that
 - for $I < I_b$ or $I_C < I < I_A$, $\mathcal{C}(I)$ are vertical and intersect transversally any $R_I(\varphi, \sigma)$;
 - for $I_b \leq I < I_a$, the crests $\mathcal{C}(I)$ are vertical and there exist tangencies between $\mathcal{C}(I)$ and two NHIM lines $R_I(\varphi, \sigma)$;
 - for $I_a < I < I_c$ or $I_B < I$, $\mathcal{C}(I)$ are horizontal and intersect transversally any $R_I(\varphi, \sigma)$;
 - for $I_A \leq I \leq I_B$, the crests $\mathcal{C}(I)$ are horizontal and there exist tangencies between $\mathcal{C}(I)$ and two NHIM lines $R_I(\varphi, \sigma)$;
 - for $I_c \leq I \leq I_C$, if $I_c < 1/2$, the crests $\mathcal{C}(I)$ are vertical and there exist tangencies between $\mathcal{C}(I)$ and $R_I(\varphi, \sigma)$. If $I_c = 1/2$, from the properties of $\alpha(I)$ and $\beta(I)$ this interval is just one point. If $I_c > 1/2$, the crests $\mathcal{C}(I)$ are horizontal and there exist tangencies.
- For $|\mu| \geq \exp(\pi/2)$ there exist $I_b < I_a < I_A < I_B$ such that
 - for $I < I_b$ or $I_B < I$, $\mathcal{C}(I)$ are vertical and intersect transversally any $R_I(\varphi, \sigma)$;
 - for $I_b \leq I < I_a$ or $I_A < I \leq I_B$, the crests $\mathcal{C}(I)$ are vertical and there exist tangencies between $\mathcal{C}(I)$ and two NHIM lines $R_I(\varphi, \sigma)$;
 - for $I_a < I < I_A$, the crests $\mathcal{C}(I)$ are horizontal and intersect transversally any $R_I(\varphi, \sigma)$.

Remark 6.11. Note that we are not considering the singular case $|\alpha(I)| = 1/|\mu|$ described in Remark 6.7.

Example Again, to illustrate this proposition, we take the case with $\mu = 0.5$, see Fig. 6.2a. In this case, we have $|\beta(I)| = 1/\mu$ for $I \approx -2.942, 0.595, 1.85$ and

- for $I \in (-\infty, -2.942) \cup (0.701, 1) \cup (1, 1.367) \Rightarrow \begin{cases} |\alpha(I)| > 1/|\mu| \Rightarrow \text{vertical crests} \\ |\beta(I)| > 1/|\mu| \Rightarrow \text{no tangencies} \end{cases}$
- for $I \in [-2.942, -1.807] \Rightarrow \begin{cases} |\alpha(I)| > 1/|\mu| \Rightarrow \text{vertical crests} \\ |\beta(I)| \leq 1/|\mu| \Rightarrow \text{tangencies} \end{cases}$
- for $I \in (-1.807, 0.595) \cup (1.85, +\infty) \Rightarrow \begin{cases} |\alpha(I)| < 1/|\mu| \Rightarrow \text{horizontal crests} \\ |\beta(I)| < 1/|\mu| \Rightarrow \text{no tangencies} \end{cases}$
- for $I \in [0.595, 0.701] \cup (1.367, 1.85] \Rightarrow \begin{cases} |\alpha(I)| < 1/|\mu| \Rightarrow \text{horizontal crests} \\ |\beta(I)| \geq 1/|\mu| \Rightarrow \text{tangencies} \end{cases}$

Once more, we compare with the Hamiltonian (6.6) studied in [DS17]. For Hamiltonian (6.6) and $\mu = 0.5$ there is no tangency, but for Hamiltonian (6.7) we can find tangencies for horizontal and vertical crests. Indeed, for Hamiltonian (6.6) and any $0 < |\mu| < 0.625$ there is no tangency, whereas for any $\mu \neq 0$ there are tangencies for Hamiltonian (6.7).



(a) $|\alpha(I)|$ and $|\beta(I)|$: $\mu = 0.5$, $I_b \approx -2.942$, $I_a \approx -1.807$, $I_c \approx 0.595$, $I_c \approx 0.701$, $I_A \approx 1.367$ and $I_B \approx 1.85$

(b) $|\alpha_r(I)|$ and $|\beta_r(I)|$: $\mu = 0.5$ and $r = 0.5$.

Figure 6.2: $|\alpha(I)|$ and $|\beta(I)|$: Behavior of the crests and tangencies.

Remark 6.12. For $r \in (0, 1)$, $\beta_r(I)$ is defined by $\beta_r(I) = I\alpha_r(I)/(rI - 1)$. In this case, $\lim_{I \rightarrow 1/r} |\beta_r(I)| = +\infty$ and $\lim_{I \rightarrow \pm\infty} |\beta_r(I)| = 0$. In Fig. 6.2b, a comparison between the functions $\alpha_r(I)$, $\beta_r(I)$ and the straight line $1/|\mu|$ for $r = 1/2$ is displayed.

For each crest, where it is well defined, there exists, at least, a value τ^* such that

$$(\varphi - I\tau^*, \sigma - (I - 1)\tau^*) = (\varphi - I\tau^*, \xi(I, \varphi - I\tau^*)) \text{ or } (\eta(I, \sigma - (I - 1)\tau^*), \sigma - (I - 1)\tau^*),$$

which means that $R_I(\varphi, \sigma) \cap \mathcal{C}(I) \neq \emptyset$. This intersection is intrinsically associated to a homoclinic orbit to the NHIM. To make a choice about how to take such τ^* is to choose in which homoclinic manifold Γ the homoclinic points $\tilde{z}^*$ lie. Even more, it is to choose what scattering map we are going to use.

6.3.3 Construction of scattering maps

We have now several goals. First, to explain, given (I, θ) , how to find the intersection between one of the NHIM lines and one of the two crests, and consequently, to define the function τ^* . Second, to show how each crest can give rise to many scattering maps. And third, to explain the different scattering maps or combinations of them that can be defined.

Let us first study the intersection between NHIM lines and crests. From the definition of the function $\tau^* = \tau^*(I, \varphi, s)$ in equation (6.20) and the definition of a NHIM line $R(I, \varphi, s)$ in (6.21) and a crest $\mathcal{C}(I)$ in Definition 1, it turns out that

$$R(I, \varphi, s) \cap \mathcal{C}(I) = \left\{ (I, \varphi - I\tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s)) \right\}.$$

Moreover, from the equation satisfied by the function τ^* , one can get (see Eq. (3.12) in [DS17]) that for any γ

$$\tau^*(I, \varphi - I\gamma, s - \gamma) = \tau^*(I, \varphi, s) - \gamma.$$

In particular, for the change (6.24) $s = \varphi - \sigma$ and $\gamma = \varphi - \sigma$ one gets

$$\tau^*(I, \varphi, \varphi - \sigma) = \tau^*(I, \theta) + \varphi - \sigma, \quad (6.29)$$

where $\theta = \varphi - Is = (1 - I)\varphi + I\sigma$. In the variables (I, φ, σ) , taking into account the expression (6.28) for the NHIM lines $R(I, \varphi, \varphi - \sigma)$ and again equation (6.20) satisfied by the $\tau^*(I, \varphi, s)$, we have that

$$\begin{aligned} R(I, \varphi, \varphi - \sigma) \cap \mathcal{C}(I) &= \left\{ (I, \varphi - I\tau^*(I, \varphi, \varphi - \sigma), \sigma - (I - 1)\tau^*(I, \varphi, \varphi - \sigma)) \right\} \\ &= \left\{ (I, \theta - I\tau^*(I, \theta), \theta - (I - 1)\tau^*(I, \theta)) \right\}, \end{aligned}$$

where (6.29) has been used, and $\theta = (1 - I)\varphi + I\sigma$.

From a geometrical point of view, to find an intersection between a NHIM line and a crest, one throws from a point (θ, θ) on the plane (φ, σ) a straight line with slope $(I-1)/I$, until it touches the crest $\mathcal{C}(I)$. The function $\tau^*(I, \theta)$ is the time spent to go from a point (θ, θ) in the diagonal $\sigma = \varphi$ up to $\mathcal{C}(I)$ with a velocity vector $\mathbf{v} = -(I, I-1)$, see Fig. 6.3.

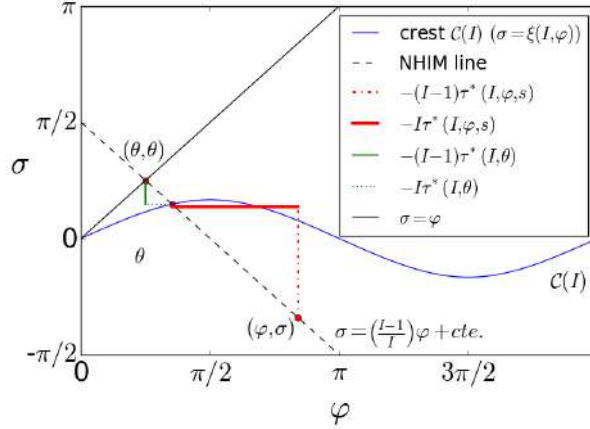


Figure 6.3: Finding $\tau^*(I, \theta)$ using the straight line $\sigma = \varphi$.

One has to decide the direction for τ^* using the idea explained above. For example, if we are on a point on the straight line $\sigma = \varphi$, we have to decide if we go up or go down along the NHIM line, i.e., to look for a negative or a positive $\tau^*(I, \theta)$ (to look at the past or the future). In both cases we are going to detect an intersection with the desired crest, but, in general, different choices give rise to different scattering maps, because we are looking for different homoclinic invariant manifolds Γ .

To show another difference between scattering maps from the choice of τ^* we begin by introducing each kind of scattering map. The first one is inspired in [DH11] and [DS17] for $|\mu| < 0.97$. In these cited cases all scattering maps studied were associated to one of the horizontal crests like in (6.27). In the same way, we can separate completely the scattering maps associated to the horizontal crests and the scattering maps associated to the vertical crests. Notice that the scattering maps associated to horizontal crests are defined only for values of I satisfying $|\alpha(I)| < 1/|\mu|$ whereas the scattering maps associated to the vertical crests are defined only for values of I satisfying $|\alpha(I)| > 1/|\mu|$.

As noted previously, crests are vertical in a neighborhood of $I = 1$ for any value of μ . Therefore, there is no scattering map associated to a horizontal crest close to $I = 1$. Analogously, since $|\alpha(0)| = 0$, crests are horizontal in a neighborhood of $I = 0$ for any value of μ and, therefore, there is no scattering map associated to a vertical crest close to $I = 0$. This implies that these “horizontal” or “vertical” scattering maps are just locally defined, in other words, they are not defined on the whole plane (θ, I) . This motivates to define *global scattering maps*. Global scattering maps are important because they describe the outer dynamics for large intervals of I and are defined as follows

Definition 2. A scattering map $\mathcal{S}(I, \theta)$ is called a global scattering map if it is defined on all $\theta \in \mathbb{T}$ for any fixed I .

Note that $\mathcal{S}(I, \theta)$ is a global scattering map as long as $\tau^*(I, \theta)$ is a global function, i.e., defined on all $\theta \in \mathbb{T}$ for any fixed I . If $\tau^*(I, \theta)$ is smoothly defined, the same will happen to $\mathcal{S}(I, \theta)$. Tangencies between NHIM lines and crests, as well as discontinuities in their intersections give rise to non-smooth scattering maps.

Remark 6.13. For instance, in the paper [DS17] devoted to the Hamiltonian (6.6), it was proven that for $0 < \mu = a_1/a_2 < 0.625$, there exist two different global scattering maps. Let us add that for $0.625 \leq \mu < 0.97$, due to the existence of tangencies between the NHIM lines and the crests, there appear two or six scattering maps. Such *multiple* scattering maps are indeed piecewise smooth global scattering maps, see Figs. 9–11 of [DS17]. Their discontinuities lie along the *tangency locus* and were avoided there to construct diffusion paths, just for the sake of simplicity.

For Hamiltonian (6.7), to extend scattering maps which are in principle only locally defined we have now two options: to combine a scattering map associated to a horizontal crest with a scattering map associated to a vertical crest or to extend the previously called “horizontal” or “vertical” scattering maps.

Although the first option may provide a global scattering map, they may appear complex discontinuity sets which give rise to a complicated phase space.

The second option is to apply the same idea used in [DS17] when we defined the scattering map “with holes”. When $|\alpha(I)| > 1/|\mu|$, the horizontal crests are no longer defined for all $\varphi \in \mathbb{T}$, indeed, they become vertical crests defined for all $\sigma \in \mathbb{T}$. Nevertheless, the vertical crests are formed by pieces of horizontal crests. This implies that even for these values of I we can use ξ given in (6.27) to parameterize some intersections between $R(I, \varphi, \sigma)$ and $\mathcal{C}(I)$. As we can see in Fig. 6.4, the vertical and horizontal crest $\mathcal{C}_M$ are very close in a neighbourhood of $\varphi = 0$. When we have a bifurcation from horizontal to vertical crests (or vice versa), it is natural just to change the parameterization from ξ_M to η_M for these values of φ . With this choice the orbits of the scattering map are continuous for θ close to 0 or 2π . The same happens with ξ_m and η_m for values of φ close to π . Scattering maps associated to horizontal crests for values of I satisfying $|\mu\alpha(I)| < 1$ are defined for all $\varphi \in \mathbb{T}$. The extension of them to values of I for $\varphi \in \mathbb{T}$ such that $|\mu\alpha(I) \sin \varphi| < 1$ are called *extended scattering maps*.

Definition 3. A scattering map $\mathcal{S}(I, \theta)$ is called an *extended scattering map* if it is associated to horizontal crests for which $|\mu\alpha(I)| < 1$, and is continuously extended to the pieces of the vertical crests where they behave as horizontal crests, that is, for the values φ such that $|\mu\alpha(I) \sin \varphi| < 1$.

Since we have already seen in Proposition 6.3 that there exist tangencies between NHIM lines and crests for any value of μ , there are no global scattering maps for Hamiltonian (6.7). However, there exist extended scattering maps with a domain large enough to provide diffusion paths.

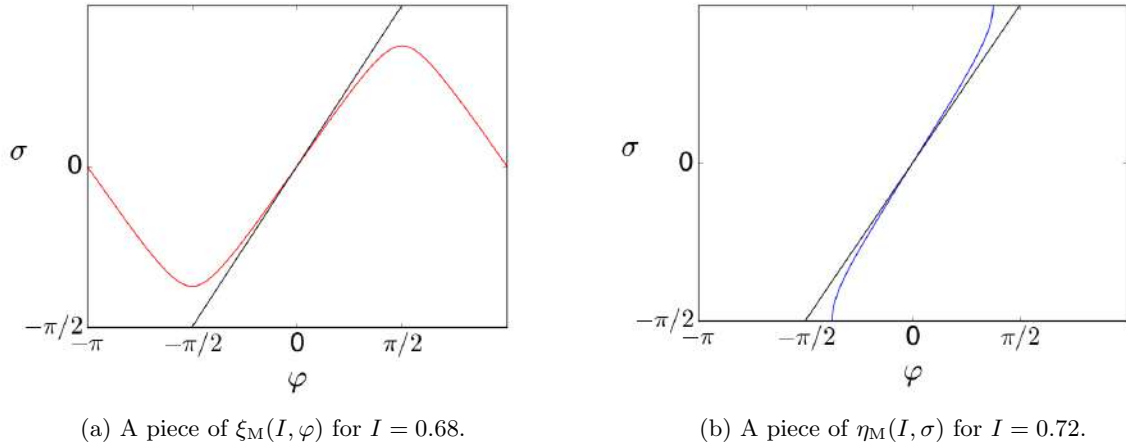


Figure 6.4: Comparison between $\xi_M(I, \varphi)$ and $\eta_M(I, \sigma)$ for $\mu = 0.5$, $I = 0.68$ and $I = 0.72$ respectively.

To illustrate the current scenario we will display the level curves of the reduced Poincaré function $\mathcal{L}^*(I, \theta)$ defined in (6.19), which up to $\mathcal{O}(\varepsilon^2)$ contain orbits of the scattering map $\mathcal{S}(I, \theta)$. We begin by considering $\mu = 0.6$ and the horizontal crest $\mathcal{C}_M(I)$. In Fig. 6.5a we display the scattering map built using τ^* defined by the first intersection between $R_I(\varphi, \sigma)$ and $\mathcal{C}_M(I)$ from $\sigma = \varphi$ going down along $R_I(\varphi, \sigma)$. In Fig. 6.5b, we use a similar idea, but now, from $\sigma = \varphi$ going up along $R_I(\varphi, \sigma)$. Alternatively, if we choose τ^* with minimal absolute value, independently of going up or down, we obtain the scattering map plotted on Fig. 6.5c. In this last case, there are orbits of the scattering maps that are not smooth in $\theta = \pi$. This happens because we change the homoclinic manifold Γ , so we are using, indeed, two different scattering maps. In [DS17] we chose scattering maps associated to a function τ^* with the minimal absolute value, which were called *primary* scattering maps. This example shows us that is not enough to say what crest is associated to a scattering map, but it is also necessary to make explicit the criterion used for τ^* (going up or down along the NHIM lines, or choosing a minimal $|\tau^*|$).

The next lemma is a good example about the criteria for $\tau^*(I, \theta)$ and its consequences, and is used to prove Proposition 6.5. Before, a new notation is introduced. An *even* subindex k is assigned to the branches $\mathcal{C}_k(I)$ of $\mathcal{C}_M(I)$ when considering $\sigma, \varphi \in \mathbb{R}$

$$\xi_k(I, \varphi) = -\arcsin(\alpha(I)\mu \sin \varphi) + k\pi \quad \text{and} \quad \eta_k = -\arcsin\left(\frac{\sin \sigma}{\alpha(I)\mu}\right) + k\pi$$

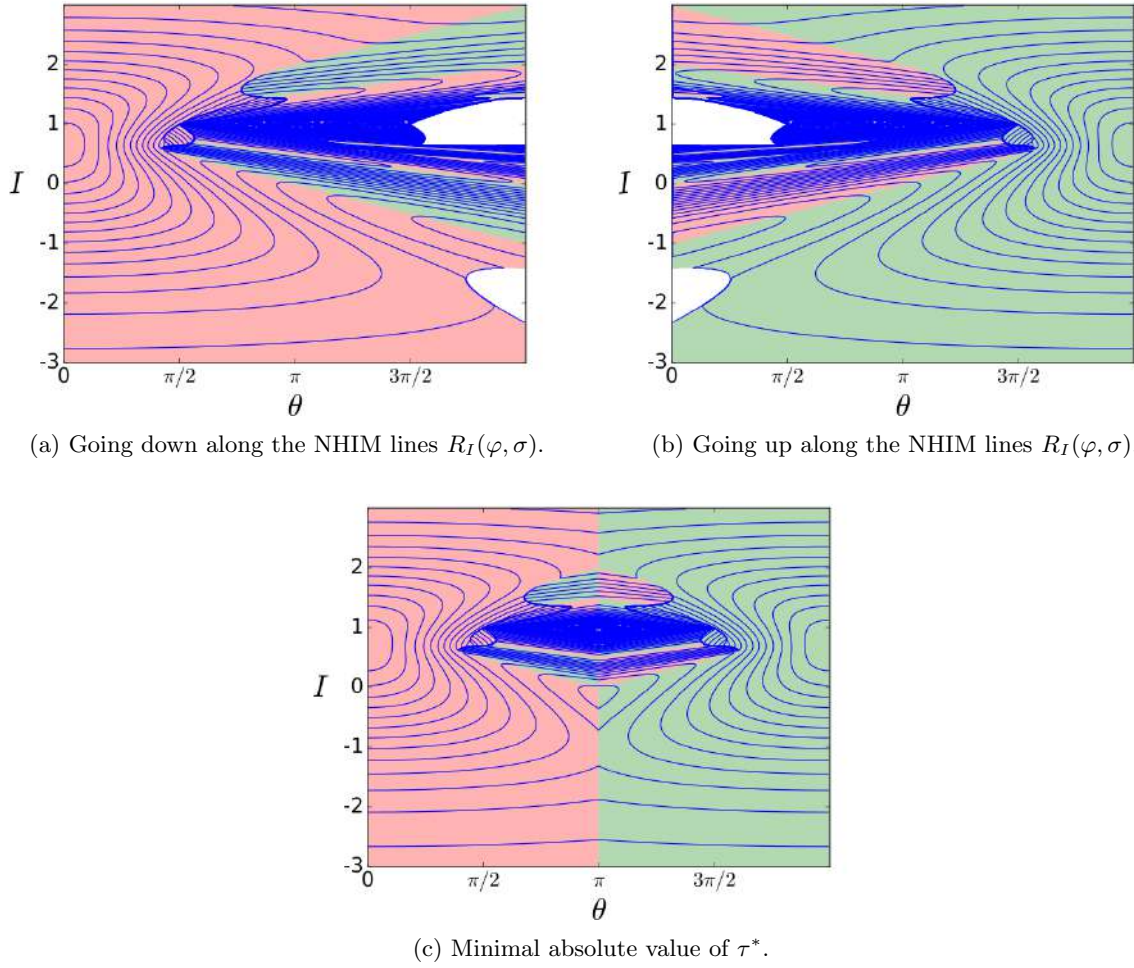


Figure 6.5: Different phase space of scattering maps $\mathcal{S}(I, \theta)$ associated to the same horizontal crest $C_M(I)$, for $\mu = 0.6$ and $\varepsilon = 0.01$. The orbits of scattering maps are represented by the blue lines which are, up to $\mathcal{O}(\varepsilon^2)$, level sets of the reduced Poincaré function $\mathcal{L}^*(I, \theta)$. In the red zones the values of I on such orbits decrease, in the green one the values of I increase. The white regions are regions where $|\mu\alpha(I)\sin\varphi| > 1$ is satisfied.

and an *odd* subindex k to the branches $\mathcal{C}_k(I)$ of $\mathcal{C}_m(I)$ when considering $\sigma, \varphi \in \mathbb{R}$

$$\xi_k(I, \varphi) = \arcsin(\alpha(I)\mu\sin\varphi) + k\pi \quad \text{and} \quad \eta_k = \arcsin\left(\frac{\sin\sigma}{\alpha(I)\mu}\right) + k\pi.$$

We notice that the crests $\mathcal{C}(I)$ are naturally defined for $(\varphi, \sigma) \in \mathbb{T}^2$ and give rise to two different crests $\mathcal{C}_M(I)$, $\mathcal{C}_m(I)$ (except for the singular case $|\mu\alpha(I)| = 1$). When we run now over real values of φ, σ , we may have an *infinite* number of crests $\mathcal{C}_k(I)$, where even (odd) values of k are assigned to the branches of $\mathcal{C}_M(I)$ ($\mathcal{C}_m(I)$). Among them, we are going to use $\mathcal{C}_0(I)$, $\mathcal{C}_1(I)$ and $\mathcal{C}_2(I)$.

Lemma 6.4. *Let $\mathcal{L}_0^*$ and $\mathcal{L}_2^*$ be reduced Poincaré functions associated to the same crest $\mathcal{C}(I)$, where for $\mathcal{L}_0^*$ we look at the first intersection points “under” $\sigma = \varphi$, that is, with $\mathcal{C}_0(I)$, and for $\mathcal{L}_2^*$ we look at the first intersection points “over” $\sigma = \varphi$, that is, with $\mathcal{C}_2(I)$. Then we have*

$$\frac{\partial \mathcal{L}_0^*}{\partial \theta}(I, \theta) = -\frac{\partial \mathcal{L}_2^*}{\partial \theta}(I, 2\pi - \theta). \quad (6.30)$$

Remark 6.14. We say “under” $\sigma = \varphi$ and “over” $\sigma = \varphi$ for intersection points going down or up along $R_I(\varphi, \sigma)$, respectively on $(\varphi, \xi_0(I, \varphi))$ and $(\varphi, \xi_2(I, \varphi))$, because when the horizontal crest $\mathcal{C}_M(I)$ is defined for all $\varphi \in \mathbb{T}$ the graphs $(\varphi, \xi_0(I, \varphi))$ of $\mathcal{C}_0(I)$ and $(\varphi, \xi_2(I, \varphi))$ of $\mathcal{C}_2(I)$ are under and over the straight line $\sigma = \varphi$.

Proof. Let $\mathcal{L}^*$ be a reduced Poincaré function (6.19)-(6.17), then

$$\frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) = \frac{A_1(I) \sin(\theta - I\tau^*(I, \theta))}{I - 1}.$$

So, equation (6.30) is satisfied if, and only if

$$\sin(\theta - I\tau_0^*(I, \theta)) = \sin(\theta - I(-\tau_2^*(I, 2\pi - \theta))). \quad (6.31)$$

We assume that the crest is horizontal and given by the graph of ξ_M , the other cases are analogous. Indeed, we are going to use

$$\xi_0(I, \varphi) = -\arcsin(\mu\alpha(I) \sin \varphi) \quad \text{and} \quad \xi_2(I, \varphi) = \xi_0(I, \varphi) + 2\pi. \quad (6.32)$$

This implies that the intersection point “under” $\sigma = \varphi$ is a point on the curve parameterized by $\xi_0(I, \varphi)$. Otherwise, the intersection “over” $\sigma = \varphi$ is a point on the curve parameterized by $\xi_2(I, \varphi)$. As the slope of the NHIM lines is $(I - 1)/I$, given a point (θ, θ) , we obtain

$$\frac{\xi_2(I, \theta - I\tau_2^*(I, \theta)) - \theta}{\theta - I\tau_2^*(I, \theta) - \theta} = \frac{I - 1}{I},$$

which can be rewritten as

$$\frac{2\pi + \xi_0(I, \theta - I\tau_2^*(I, \theta)) - \theta}{-I\tau_2^*(I, \theta)} = \frac{I - 1}{I}.$$

From this equation, we obtain an expression for $\tau_2^*(I, \theta)$

$$\tau_2^*(I, \theta) = \frac{-(2\pi + \xi_0(I, \theta - I\tau_2^*(I, \theta)) - \theta)}{I - 1}.$$

From the expressions of $\tau_2^*(I, \theta)$ above and (6.32),

$$\tau_2^*(I, 2\pi - \theta) = \frac{(\xi_0(I, \theta - I(-\tau_2^*(I, 2\pi - \theta))) + \theta)}{I - 1},$$

and therefore

$$\theta - (I - 1)(-\tau_2^*(I, 2\pi - \theta)) = \xi_0(I, \theta - (I - 1)(-\tau_2^*(I, 2\pi - \theta))),$$

which implies that $-\tau_2^*(I, 2\pi - \theta)$ is a time of intersection between the NHIM line and the curve parameterized by ξ_0 . In the case that there exists only one intersection point, this implies

$$\tau_0^*(I, \theta) = \tau_2^*(I, 2\pi - \theta).$$

So, condition (6.31) is satisfied. □

Proposition 6.5. *Let $\mathcal{S}_1(I, \theta)$ be the scattering map associated to the graphs of ξ_1 and η_1 of $\mathcal{C}_1(I)$. Assuming $a_1, a_2 > 0$, for any I there exists a θ_+ such that $\dot{I} > 0$ for $\theta \in (\pi, \theta_+)$. Moreover, $\theta_+ \geq 3\pi/2$ for $I \notin (-1/2, 1/2)$.*

Proof. A proof is given in Appendix 6.7. □

Remark 6.15. If $a_1 < 0$, we have that there exists a θ_- such that $\dot{I} > 0$ for any $\theta \in (\theta_-, \pi)$.

Remark 6.16. An analogous proposition holds for $\mathcal{S}_2(I, \theta)$, the scattering map associated to the graphs of ξ_2 and η_2 of $\mathcal{C}_2(I)$. In such case, there is a θ_+ such that $\dot{I} \geq 0$ for any $\theta \in (\theta_+, 2\pi)$ where $\theta \geq 3\pi/2$ for $I \in (1/2, 3/2)$.

Note that this proposition leads us to ensure the diffusion in an analogous way to the one used to prove Theorem 4 in [DS17]. Next, the diffusion mechanism is stated and the Arnold diffusion is proven.

6.4 Arnold Diffusion

In this section we are going to complete our goal proving the existence of global instability or Arnold diffusion, that is, Theorem 6.1.

We begin by presenting some general geometrical properties of the scattering maps that we have to take into account to prove the theorem of diffusion. The first one reduces the study of scattering maps to positive values of μ . More precisely, we have the lemma below

Lemma 6.6. *The scattering map for a value of μ and $s = \pi$, associated to the intersection between $R(I, \varphi, s)$ and $C_m(I)$ ($C_M(I)$) has the same geometrical properties as the scattering map for $-\mu$ and $s = 0$, associated to the intersection between $R_\theta(I)$ and $C_m(I)$ ($C_M(I)$), i.e.,*

$$S_{m(M)}^\mu(I, \varphi, \pi) = S_{M(m)}^{-\mu}(I, \varphi, 0) = S_{M(m)}^{-\mu}(I, \theta)$$

Proof. First, we look for τ_m^* such that the NHIM segment $R(I, \varphi, s)$ intersects the crest $C_m(I)$. If we fix $s = \pi$, we have from (6.17) and (6.18):

$$L_{\mu,m}^*(I, \varphi, \pi) = A_1(I) \cos(\varphi - I\tau_m^*(I, \varphi, \pi)) + A_2(I) \cos(\varphi - \pi - (I-1)\tau_m^*(I, \varphi, \pi)). \quad (6.33)$$

Besides, τ^* satisfies

$$\mu\alpha(I) \sin(\varphi - I\tau_m^*) + \sin(\varphi - \pi - (I-1)\tau_m^*) = 0,$$

or

$$-\mu\alpha(I) \sin(\varphi - I\tau_m^*) + \sin(\varphi - (I-1)\tau_m^*) = 0.$$

We have that $\varphi - \pi - (I-1)\tau_m^* \pmod{2\pi} = \xi_m(I, \varphi - I\tau_m^*)$ with $\pi/2 \leq \xi_m \leq 3\pi/2$. Then, for each τ_m^* there exists a $K \in \mathbb{Z}$ such that

$$\frac{\pi}{2} < \varphi - \pi - (I-1)\tau_m^* + 2\pi K < \frac{3\pi}{2}.$$

This implies

$$\frac{3\pi}{2} < \varphi - (I-1)\tau_m^* + 2\pi K \quad \text{and} \quad \varphi - (I-1)\tau_m^* + 2\pi(K-1) < \frac{\pi}{2}.$$

Therefore,

$$\varphi - (I-1)\tau_m^* \pmod{2\pi} < \frac{\pi}{2} \quad \text{or} \quad \varphi - (I-1)\tau_m^* \pmod{2\pi} > \frac{3\pi}{2}.$$

We can conclude that $\varphi - (I-1)\tau_m^* \pmod{2\pi} = \xi_m(I, \varphi - I\tau_m^*)$. Therefore $\tau_m^*(I, \varphi, \pi)$ for μ is equal to $\tau_m^*(I, \varphi, 0)$ for $-\mu$. From (6.33), $L_{\mu,m}^*(I, \varphi, \pi)$ satisfies

$$\begin{aligned} L_{\mu,m}^*(I, \varphi, \pi) &= A_1(I) \cos(\varphi - \tau_m^*(I, \varphi, 0)) + (-A_2(I)) \cos(\varphi - (I-1)\tau_m^*(I, \varphi, 0)) \\ &= L_{-\mu,M}^*(I, \varphi, 0). \end{aligned}$$

Since $L_{\mu,m}^*(\cdot, \cdot, \pi)$ and $L_{-\mu,M}^*(\cdot, \cdot, 0)$ coincide, their derivatives too and this implies that

$$S_m^\mu(I, \varphi, \pi) = S_M^{-\mu}(I, \varphi, 0) = S_M^{-\mu}(I, \theta).$$

□

From now on, just to simplify the exposition, a_1 and a_2 are considered positive. The same strategy used in [DS17] is applied to prove the existence the diffusion: we combine the scattering map in an interval of θ where $I > 0$ and the inner map to build a diffusion pseudo-orbit. Then we apply shadowing results to get the existence of a diffusion orbit.

Since $I = 0$ and $I = 1$ are resonance values, the application of the inner map must be more careful, because in these resonance regions, for some orbits, the value of I decreases in order $\mathcal{O}(\sqrt{\varepsilon})$, i. e., the tori cannot be considered flat. We study the transversality between the foliations of invariant sets of the inner and the scattering map in resonant and non-resonant regions and its image under the scattering map $\mathcal{S}$. For more details and a more general case, the reader is referred to [DH09].

Consider the resonant region associated to $I = 0$. In such region, the tori can be approximated by $F^0(I, \varphi)$ given in (6.15). The transversality between invariant sets of the inner and the scattering map holds if the gradient vectors of the level curves of F^0 and $\mathcal{L}^*$ are not parallel vectors, or equivalently,

$$\{F^0(I, \theta), \mathcal{L}^*(I, \theta)\} \neq 0,$$

where $\{, \}$ is the Poisson bracket,

$$\{F^0, \mathcal{L}^*\} = \frac{\partial F^0}{\partial \theta} \frac{\partial \mathcal{L}}{\partial I} - \frac{\partial F^0}{\partial I} \frac{\partial \mathcal{L}}{\partial \theta}.$$

From (6.15), the partial derivatives of F^0 are

$$\frac{\partial F^0}{\partial I} = I \quad \text{and} \quad \frac{\partial F^0}{\partial \theta} = -\varepsilon a_1 \sin \theta,$$

and since $\mathcal{L}^*(I, \theta) = A_1(I) \cos(\theta - I\tau^*(I, \theta)) + A_2(I) \cos(\theta - (I-1)\tau^*(I, \theta))$, we have the partial derivatives given by

$$\frac{\partial \mathcal{L}^*}{\partial \theta} = \frac{A_1(I) \sin(\theta - I\tau^*)}{I-1},$$

$$\frac{\partial \mathcal{L}^*}{\partial I} = A'_1(I) \cos(\theta - I\tau^*) + A'_2(I) \cos(\theta - (I-1)\tau^*) + A_1(I)\tau^* \sin(\theta - I\tau^*) + A_2(I)\tau^* \sin(\theta - (I-1)\tau^*).$$

Note that if $|I| > \mathcal{O}(\varepsilon)$, $\partial F^0/\partial I$ dominates $\partial F^0/\partial \theta$, so the Poisson bracket above can be reduced to

$$\{F^0, \mathcal{L}^*\} \simeq -\frac{\partial F^0}{\partial I} \frac{\partial \mathcal{L}}{\partial \theta} = \frac{-IA_1(I) \sin(\theta - I\tau^*)}{I-1}$$

Expanding $\sin(\theta - I\tau^*)$ in Taylor's series around $I = 0$, we have

$$\sin(\theta - I\tau^*) = \sin \theta + \mathcal{O}(I),$$

which implies $\{F^0, \mathcal{L}^*\} = 0$ if, and only if, $\theta \approx 0, \pi$, assuming that $\mathcal{O}(I)$ is small enough.

Now, we consider $I = \mathcal{O}(\varepsilon)$ and look at the intersections between the NHIM lines and the graph of ξ_1 . Note that as the value of I is close to 0 we can assume that the crests are horizontal. Using Taylor's series we can write

$$\begin{aligned} \sin(\theta - I\tau^*) &= \sin \theta + \mathcal{O}(I) & \cos(\theta - I\tau^*) &= \cos \theta + \mathcal{O}(I) \\ \sin(\theta - (I-1)\tau^*) &= \mathcal{O}(I) & \cos(\theta - (I-1)\tau^*) &= -1 + \mathcal{O}(I). \end{aligned}$$

This implies

$$\{F^0, \mathcal{L}^*\} = -\frac{IA_1(I) \sin \theta}{I-1} - \varepsilon a_1 \sin \theta (A'_1(I) \cos \theta - A'_2(I) + A_1(I)\tau^* \sin \theta) + \mathcal{O}(I^2, \varepsilon I). \quad (6.34)$$

Taylor expanding the functions $A_1(I)$, $A'_1(I)$ and $A'_2(I)$ around $I = 0$, we obtain

$$A_1(I) = 4a_1 + \mathcal{O}(I^2), \quad A'_1(I) = \mathcal{O}(I) \quad \text{and} \quad A'_2(I) = a_2\pi(\pi \coth \pi/2 - 2)\text{csch}(\pi/2) + \mathcal{O}(I)$$

Plugging these expressions in (6.34), we set

$$\{F^0, \mathcal{L}^*\} = -\frac{4a_1 I \sin \theta}{I-1} - \varepsilon a_1 \sin \theta [a_2\pi(\pi \coth \pi/2 - 2)\text{csch}(\pi/2) + 4a_1(\pi - \theta) \sin \theta] + \mathcal{O}(I^2, I\varepsilon).$$

So, $\{F^0, \mathcal{L}^*\} = 0 \Leftrightarrow a_1 \sin \theta \left[\frac{-4I}{I-1} - \varepsilon a_2\pi(\pi \coth \pi/2 - 2)\text{csch}(\pi/2) + \varepsilon 4(\pi - \theta) \sin \theta \right] = 0$. In other words, we do not have transversality if, and only if, $\theta = 0, \pi$ or satisfies

$$(\pi - \theta) \sin \theta = \frac{I}{\varepsilon a_1} + \frac{\pi(\coth \pi/2 - 2)\text{csch}(\pi/2)}{4},$$

which is not an horizontal curve in the plane (θ, I) and is transversal to an invariant torus of the inner dynamics.

For the other resonant region $I = 1$, F^1 is very similar. Assuming $I - 1 = \mathcal{O}(\varepsilon)$, we have

$$\{F^1, \mathcal{L}^*\} = a_2 \sin \theta \left\{ 4 \left(\frac{I-1}{I} \right) - \varepsilon [\pi a_1(2 - \pi \coth(\pi/2))\text{csch}(\pi/2) + 4a_2 \sin \theta] \right\}.$$

Applying the same methodology, we obtain an analogous result for the other resonant region F^1 . In short, we conclude that the image $\mathcal{S}(\mathcal{T}_i)$ of an invariant torus $\mathcal{T}_i$ of the inner map under the scattering map intersects transversally another invariant torus $\mathcal{T}_{i+1}$ of the inner map.

Finally, in the non-resonant region, we notice that

$$\{F^{\text{nr}}, \mathcal{L}^*\} = -\frac{\partial F^{\text{nr}}}{\partial I} \frac{\partial \mathcal{L}^*}{\partial \theta} = -\frac{IA_1(I) \sin(\theta - I\tau^*)}{I - 1},$$

just the same expression as the one for the resonance $I = 0$, so the transversality between invariant sets of the inner and the scattering map follows.

Now, a constructive proof of Theorem 6.1 is presented. This proof is similar to the proof presented in [DS17], but now, there is no any piece of “highway” or fast vertical lines where $|I|$ is large. So, the inner map is applied more times.

6.4.1 Proof of Theorem 6.1

Proof. First of all we have to choose what scattering map we use. This choice depends on the sign of μ as explained in Lemma 6.6. Assuming $\mu > 0$, we take $\mathcal{S}_1(I, \theta)$, the global scattering map associated to the graphs of ξ_1 and η_1 . If $a_1 > 0$, by Proposition 6.5 for any I there exists an interval $\theta \in (\pi, \theta_+)$ where $I > 0$. Define H_r the set $(\rho, \theta_+) \times [-I^*, I^*]$, where $\rho = \pi + \delta$ is such that $\pi < \rho < \theta_+$ and the transversality between NHIM lines and $\mathcal{L}_1^*$ holds. We first construct a pseudo-orbit $\{(I_i, \theta_i) : i = 0, \dots, N_1\} \subset H_r$ with $I_0 = -I^*$ and θ_{N_1} as close as possible to ρ . Note that all these points lie in the same level curve of $\mathcal{L}_1^*$, that is, $\mathcal{L}_1^*(I_0, \theta_0) = \mathcal{L}_1^*(I_i, \theta_i)$, $i = 1, \dots, N_1$. Applying the inner dynamics, we get $(I_{N_1+1}, \theta_{N_1+1}) = \phi_{t_{N_1}}(I_{N_1}, \theta_{N_1})$ with $\theta_{N_1+1} \in (\rho, \theta_+)$ and then we construct a pseudo-orbit $\{(I_i, \theta_i) : i = N_1 + 1, \dots, N_1 + M_1\} \subset \mathcal{L}_1^*(I_{N_1+1}, \theta_{N_1+1}) = l_{N_1+1}$ with $\theta_i \in (\rho, \theta_{N_1+1})$, $\theta_+ - \theta_{N_1+M_1} = \mathcal{O}(\varepsilon^2)$. Applying the inner dynamics, we get $(I_{N_1+M_1+1}, \theta_{N_1+M_1+1}) = \phi_{t_{N_1+M_1}}(I_{N_1+M_1}, \theta_{N_1+M_1})$ with $\theta_{N_1+M_1+1} \in (\rho, \theta_+)$. Recursively, we construct a pseudo-orbit $\{(I_i, \theta_i) : i = N_1 + 1, \dots, N_2\}$ such that $I_{N_2} \geq I^*$. In the same ways as in [DS17] (Theorem 4), we can apply shadowing techniques of [FM00, FM03, GLMS20], due to the fact that the inner dynamics is simple enough to satisfy the required hypothesis of these references, to prove the existence of a diffusion trajectory. If $a_{10} < 0$, changing H_r to $H_l = (\theta_+, \pi)$ all the previous reasoning applies. $\square$

Remark 6.17. Considering Remark 6.3, Remark 6.6, Remark 6.9 and Remark 6.12, for any $r \in (0, 1)$, an equivalent diffusion result is readily obtained.

6.5 Piecewise smooth global scattering maps

In this section, the geometric freedom of the choice of τ^* is explored. Until now, only two different scattering maps have been used to build a global one, and this was enough to ensure diffusion. But, with this approach, finding a diffusion pseudo-orbit is not always easy enough and this pseudo-orbit can be also complicated. This depends simply on the “aspect” of the scattering map obtained.

We now suggest a new criterion to choose τ^* : to take the minimal value for $|\tau^*|$ for any (θ, I) . This provides us with a piecewise smooth global scattering map with a good property: the phase space of this scattering map which is $\mathcal{O}(\varepsilon^2)$ -close to the level sets of the reduced Poincaré function $\mathcal{L}^*(I, \theta)$ associated to the chosen τ^* is simpler and “cleaner” than the phase spaces of other scattering maps displayed up to now. By a cleaner scattering map, we mean that we can easily identify and understand the orbits of the scattering maps, except for a small region which contains the tangency locus.

Besides, the zones where the value of I is increased or decreased under the scattering map is well behaved. I decreases for $\theta \in (0, \pi)$ (the red region on all pictures in Fig. 6.6) and I increases for $\theta \in (\pi, 2\pi)$ (the green region on all pictures in Fig. 6.6). So it is easy to infer that for finding a diffusion pseudo-orbit it is enough to build a combination between the inner map and this scattering map restricted to $(\pi, 2\pi)$, for example if an increased value of I is wished. The same idea used in the proof of Theorem 6.1.

Observe that the scattering maps we are now considering are a mix of the scattering maps studied previously. As an example, we illustrate the scattering map obtained for $\mu = 0.9$. Such scattering map can be divided into three regions and in each region, the scattering map coincides with a scattering map studied before.

In Fig. 6.7, for regions I ($0 < \theta < \pi/2$), II ($\pi/2 < \theta < 3\pi/2$) and III ($3\pi/2 < \theta < 2\pi$) the scattering map has the following correspondence:

I Extended scattering map $\mathcal{S}_0(I, \theta)$ associated to the horizontal $\mathcal{C}_M(I)$ “under” $\sigma = \varphi$.

II Extended scattering map $\mathcal{S}_1(I, \theta)$ associated to the horizontal $\mathcal{C}_m(I)$.

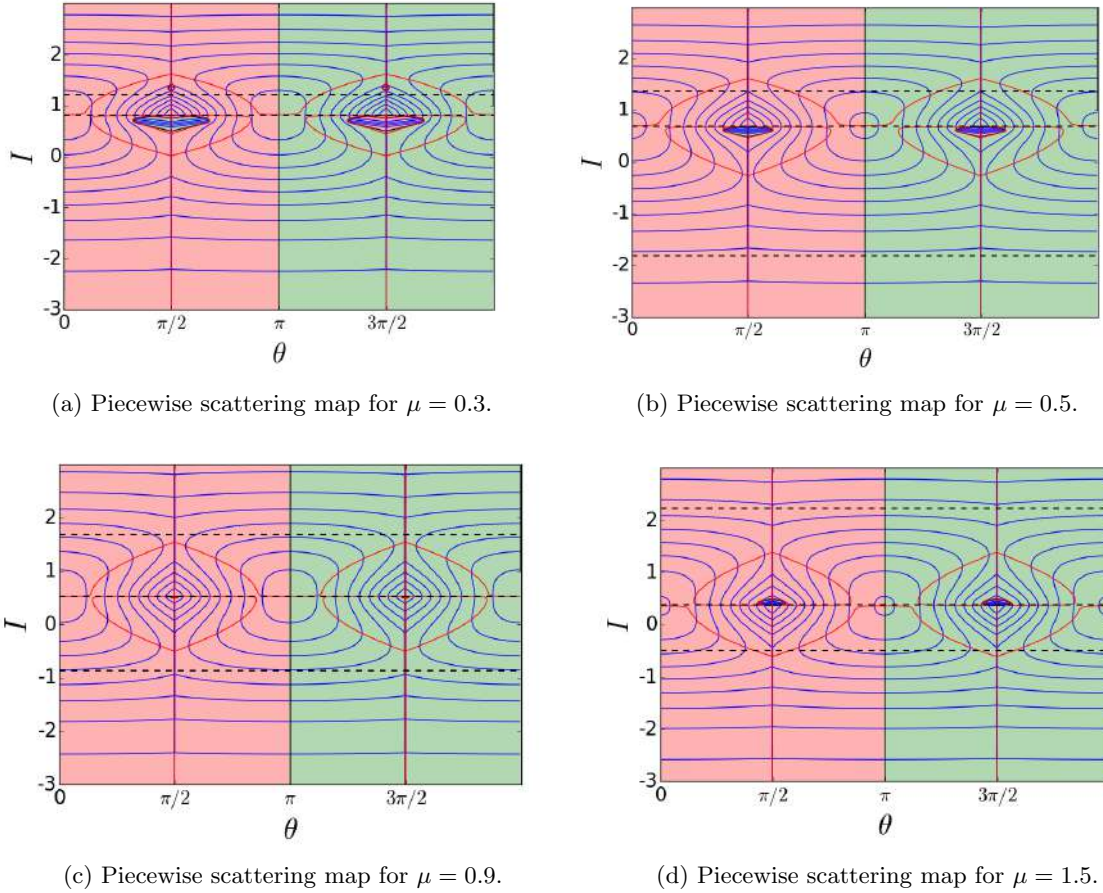


Figure 6.6: Examples of piecewise smooth global scattering maps. The orbits of scattering maps are represented by the blue lines. In the red zones the values of I on such orbits decrease, in the green one the values of I increase.

III Extended scattering map $\mathcal{S}_2(I, \theta)$ associated to the horizontal $\mathcal{C}_M(I)$ “over” $\sigma = \varphi$.

If extended scattering maps are not considered and we just use scattering maps associated to horizontal and vertical crests, one can see that these scattering maps can be divided into 6 regions, i.e., they can be viewed as a combination of up to 6 scattering maps.

Another property of these scattering maps is the loss of differentiability on the straight lines $\theta = \pi/2$ and $\theta = 3\pi/2$. The vector field associated to the Hamiltonian $-\mathcal{L}_i^*$ defined around these discontinuity lines behaves as the vector fields studied in non-smooth dynamics theory. More precisely, we can find regions with slide and unstable slide behavior [Fil88]. In a future work, we envisage to design special pseudo-orbits along these discontinuity lines using such theory. Note that these pseudo-orbits would be very similar to the “highways” defined in [DS17], so in principle, one can expect fast and simple diffusion along these discontinuity lines.

6.6 Sketch of the simplest case $k_1 = l_2 = 1, k_2 = l_1 = 0$

Consider now a pendulum and a rotor plus a time periodic perturbation depending on two harmonics in the variables (φ, s) depending separately on the variables φ and s (case $k_1 = l_2 = 1, k_2 = l_1 = 0$):

$$H_\varepsilon(p, q, I, \varphi, s) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{I^2}{2} + \varepsilon h(q, \varphi, s) \quad (6.35)$$

$$\begin{aligned} h(q, \varphi, s) &= f(q)g(\varphi, s), \\ f(q) &= \cos q, \quad g(\varphi, s) = a_1 \cos \varphi + a_2 \cos s. \end{aligned} \quad (6.36)$$

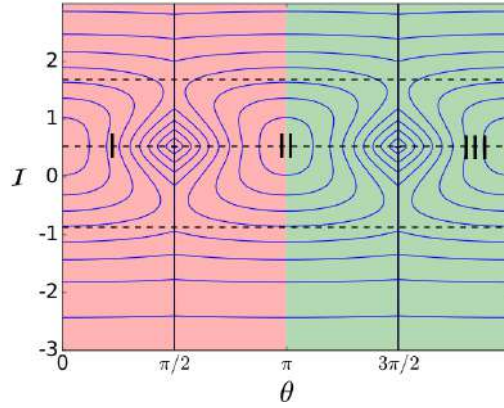


Figure 6.7: A piecewise smooth global scattering map divided into 3 regions. The vertical black lines are the boundaries of the domains of smooth scattering maps.

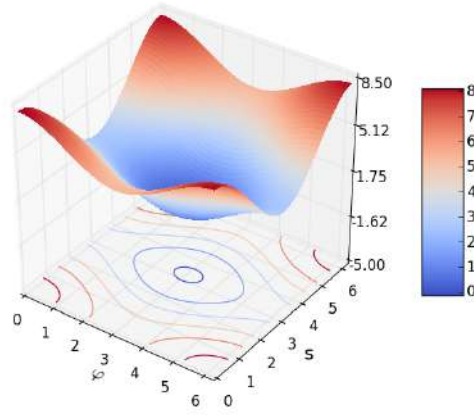


Figure 6.8: The Melnikov Potential $\mathcal{L}(I, \varphi, s)$ for $I = 1$, $\mu = a_0/a_1 = 0.6$, $k_1 = l_2 = 1$ and $k_2 = l_1 = 0$.

The Melnikov potential becomes

$$\mathcal{L}(I, \varphi, s) = A_0(I) \cos \varphi + A_1 \cos s,$$

where $A_0(I) = \frac{2\pi I a_0}{\sinh(\pi I/2)}$ and $A_1 = \frac{2\pi a_1}{\sinh(\pi/2)}$. For $\theta = \varphi - I s$, the *Reduced Poincaré function* is

$$\mathcal{L}^*(I, \theta) = \mathcal{L}(I, \varphi - I \tau^*(I, \varphi, s), s - \tau^*(I, \varphi, s)),$$

so we have to look for τ^* such that $\frac{\partial \mathcal{L}}{\partial \tau}(I, \varphi - I \tau^*, s - \tau^*) = 0$. Recall the two different view-points for $\tau^* = \tau^*(I, \varphi, s)$:

- Look for critical points of $\mathcal{L}$ on the straight line $R(I, \varphi, s) = \{(\varphi - I \tau, s - \tau), \tau \in \mathbb{R}\}$.
- Look for intersections between $R(I, \varphi, s) = \{(\varphi - I \tau, s - \tau), \tau \in \mathbb{R}\}$ and a *crest* which is a curve of equation

$$\frac{\partial \mathcal{L}}{\partial \tau}(I, \varphi - I \tau, s - \tau)|_{\tau=0} = 0.$$

For each I , the *crest* $\mathcal{C}(I)$ is the set of curves in the variables (φ, s) of equation

$$I \frac{\partial \mathcal{L}}{\partial \varphi}(I, \varphi, s) + \frac{\partial \mathcal{L}}{\partial s}(I, \varphi, s) = 0. \quad (6.37)$$

which in this case can be rewritten as

$$\mu\alpha(I) \sin \varphi + \sin s = 0, \quad \text{with } \alpha(I) = \frac{\sinh(\frac{\pi}{2}) I^2}{\sinh(\frac{\pi I}{2})}, \quad \mu = \frac{a_{10}}{a_{01}}. \quad (6.38)$$

- For any I , the critical points of the Melnikov potential $\mathcal{L}(I, \cdot, \cdot)$ $((0, 0)$, $(0, \pi)$, $(\pi, 0)$ and (π, π) : one maximum, one minimum point and two saddle points) always belong to the crest $\mathcal{C}(I)$.
- $\mathcal{L}^*(I, \theta)$ is nothing else but $\mathcal{L}$ evaluated on the crest $\mathcal{C}(I)$.
- $\theta = \varphi - Is$ is constant on the straight line $R(I, \varphi, s)$

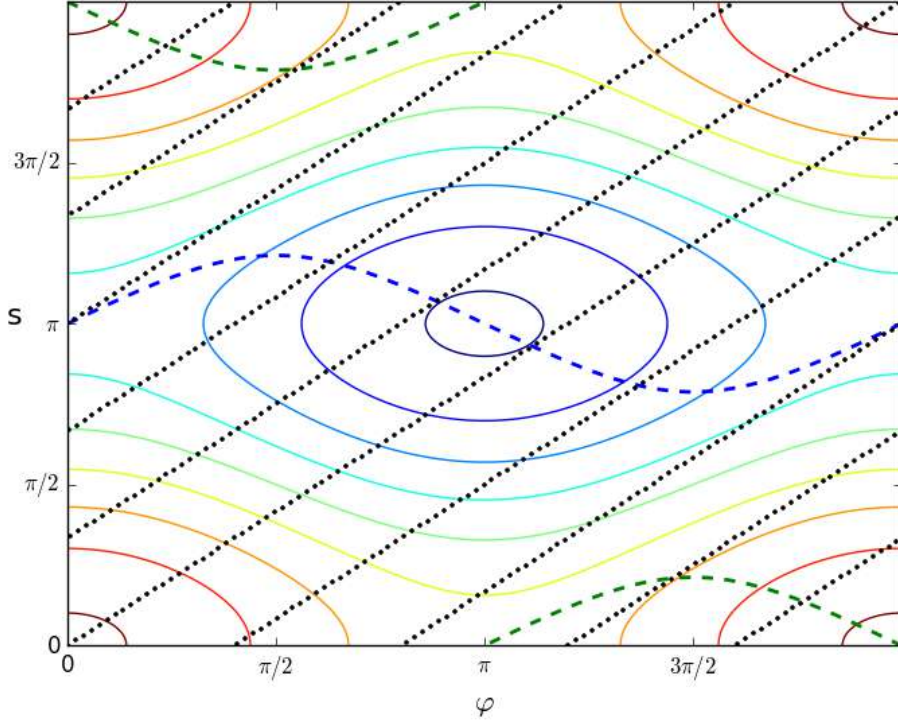
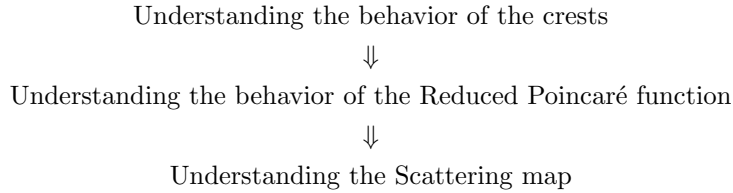


Figure 6.9: Level curves of $\mathcal{L}$ for $\mu = a_0/a_1 = 0.5$, $I = 1.2$, $k_1 = l_2 = 1$ and $k_2 = l_1 = 0$.

Crests are important:



In this simple case ($k_1 = l_2 = 1$ and $k_2 = l_1 = 0$) there appear *Highways*.

Definition 6.1 (Highways). Highways are the level curves of $\mathcal{L}^*$ such that

$$\mathcal{L}^*(I, \theta) = \frac{2\pi a_0}{\sinh(\pi/2)}.$$

- The highways are “vertical” in the variables (φ, s) .
- We always have a pair of highways. One goes up, the other goes down (this depends on the sign of $\mu = a_0/a_1$)
- The highways give rise to fast diffusing pseudo-orbits.

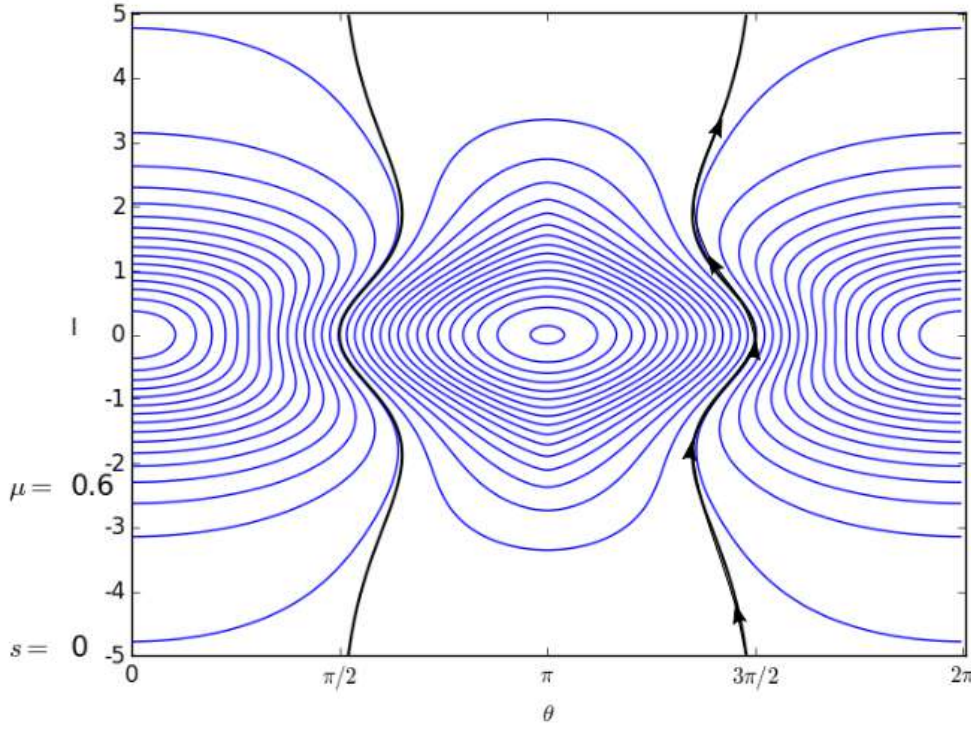


Figure 6.10: The scattering map jumps $\mathcal{O}(\varepsilon)$ distances along the level curves of $\mathcal{L}^*(I, \theta)$

6.6.1 Case $0 < |\mu| < 0.97$

- For $|\mu\alpha(I)| < 1$, there are two “horizontal” crests $\mathcal{C}_{M,m}(I)$ parameterized by:

$$\begin{aligned} s = \xi_M(I, \varphi) &= -\arcsin(\mu\alpha(I) \sin \varphi) \quad \text{mod } 2\pi, \\ \xi_m(I, \varphi) &= \arcsin(\mu\alpha(I) \sin \varphi) + \pi \quad \text{mod } 2\pi. \end{aligned} \quad (6.39)$$

6.6.2 Case $0 < |\mu| < 0.625$

- For each I , the line $R(I, \varphi, s)$ and the crest $\mathcal{C}_{M,m}(I)$ have only one intersection point.
- The scattering map S_M associated to the intersections between $\mathcal{C}_M(I)$ and $R(I, \varphi, s)$ is well defined for any $\varphi \in \mathbb{T}$. Analogously for S_m , changing M to m . In the variables $(I, \theta = \varphi - Is)$, both scattering maps $\mathcal{S}_M, \mathcal{S}_m$ are globally well defined.

6.6.3 Case $0.625 < |\mu|$

- There are *tangencies* between $\mathcal{C}_{M,m}(I, \varphi)$ and $R(I, \varphi, s)$. For some value of (I, φ, s) , there are 3 points in $R(I, \varphi, s) \cap \mathcal{C}_{M,m}(I)$.
- This implies that there are 3 scattering maps associated to each crest with different domains. (*Multiple Scattering maps*)

6.6.4 $0.97 < |\mu|$

- For some values of I , $|\mu\alpha(I)| > 1$, the two crests $\mathcal{C}_{M,m}$ are parameterized by:

$$\begin{aligned} \varphi = \eta_M(I, s) &= -\arcsin(\mu\alpha(I) \sin s) \quad \text{mod } 2\pi, \\ \eta_m(I, s) &= \arcsin(\mu\alpha(I) \sin s) + \pi \quad \text{mod } 2\pi, \end{aligned} \quad (6.40)$$

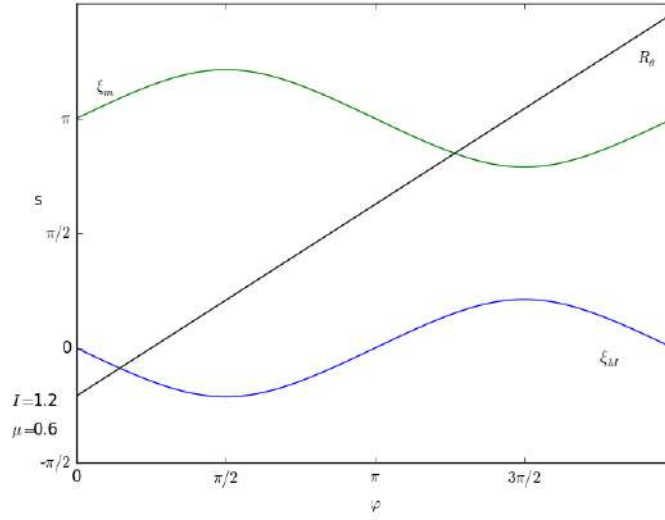
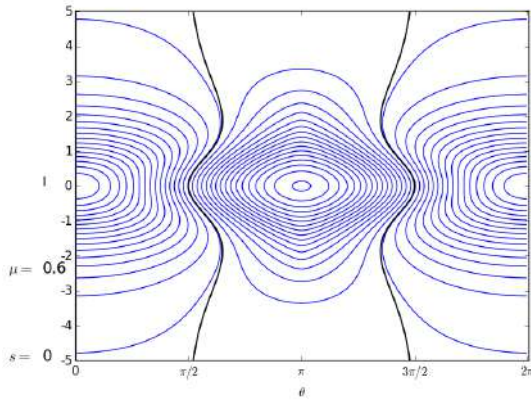
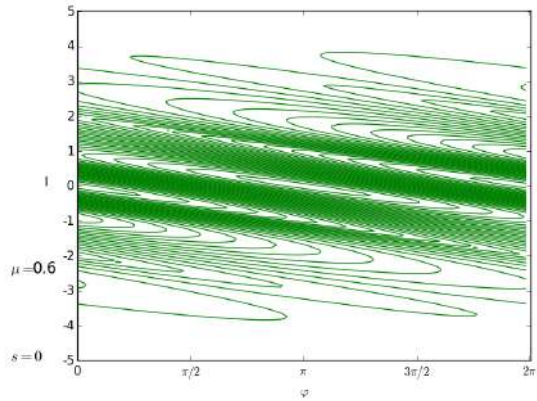


Figure 6.11: Two horizontal crests $\mathcal{C}_{M,m}(I)$ having each one only one intersection point with the line $R(I, \varphi, s)$ for $\mu = 0.6$, $I = 1.2$.



(a) Level curves of $\mathcal{L}_M^*(I, \theta)$



(b) Level curves of $\mathcal{L}_m^*(I, \theta)$

so they are “vertical” crests.

For the values of I when horizontal crests become vertical, it is not always possible to prolong in a continuous way the scattering maps, so the domain of the scattering map has to be restricted.

6.6.5 An example of pseudo-orbit

An estimate of the total time of diffusion between $-I^*$ and I^* , along the highway, is

$$T_d = \frac{T_s}{\varepsilon} \left[2 \log \left(\frac{C}{\varepsilon} \right) + \mathcal{O}(\varepsilon^b) \right], \text{ for } \varepsilon \rightarrow 0, \text{ where } 0 < b < 1,$$

with

$$T_s = T_s(I^*, a_{10}, a_{01}) = \int_0^{I^*} \frac{-\sinh(\pi I/2)}{\pi a_{10} I \sin \psi_h(I)} dI,$$

where $\psi_h = \theta - I\tau^*(I, \theta)$ is the parameterization of the highway $\mathcal{L}^*(I, \psi_h) = A_{00} + A_{01}$, and

$$C = C(I^*, a_{10}, a_{01}) = 16 |a_{10}| \left(1 + \frac{1.465}{\sqrt{1 - \mu^2 A^2}} \right)$$

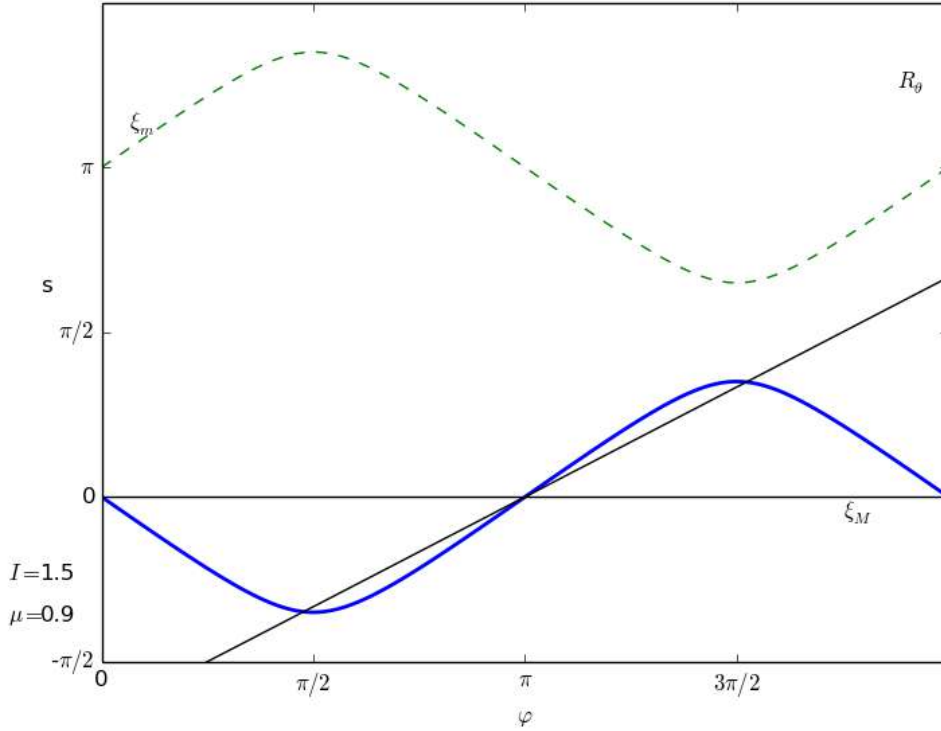


Figure 6.13: For $I = 1.5$, $\mu = 0.9$, there are 3 points in $R(I, \varphi, s) \cap \mathcal{C}_{M,m}(I)$ so there are 3 scattering maps associated to each crest with different domains

where $A = \max_{I \in [0, I^*]} \alpha(I)$, with $\alpha(I) = \frac{\sinh(\frac{\pi}{2}) I^2}{\sinh(\frac{\pi I}{2})}$ and $\mu = a_{10}/a_{01}$.

Note: This estimate quantifies the general optimal diffusion estimate $\mathcal{O}\left(\frac{1}{\varepsilon} \log \frac{1}{\varepsilon}\right)$ of [BB02, CG03a, Tre04].

6.7 Proof of Proposition 6.5

Proposition 6.5. *Let $\mathcal{S}_1(I, \theta)$ be the scattering map associated to the graphs ξ_1 and η_1 . Assuming $a_1, a_2 > 0$, then for any I , there exists a θ_+ such that $\dot{I} > 0$ for $\theta \in (\pi, \theta_+)$. Moreover, $\theta_+ \geq 3\pi/2$ for $I \notin (-1/2, 1/2)$.*

Proof. We have

$$\dot{I} = \frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) = \frac{A_1(I) \sin(\theta - I\tau^*(I, \theta))}{I - 1} = -\frac{A_2(I) \sin(\theta - (I - 1)\tau^*(I, \theta))}{I}. \quad (6.41)$$

where $A_1(I)$ and $A_2(I)$ are positive, because $a_1, a_2 > 0$. Notice that $\mu = a_1/a_2 > 0$.

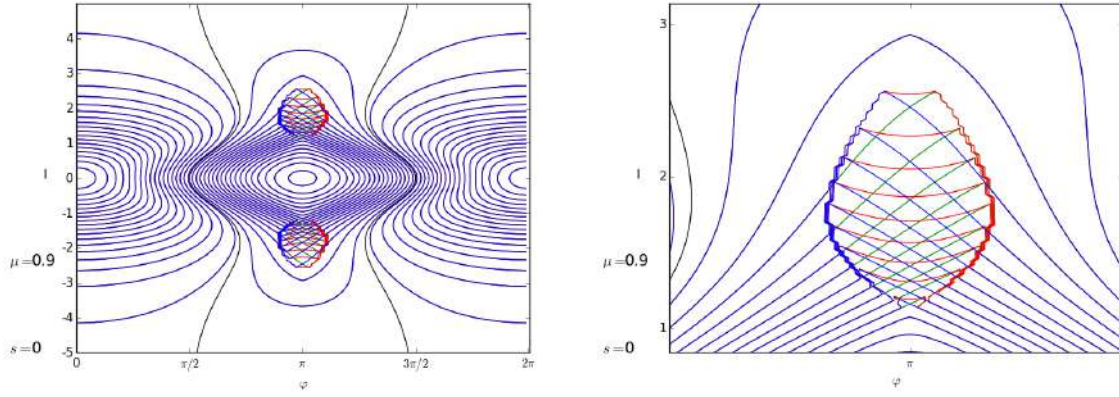
Note that as $(I, \varphi = \pi, \theta = \pi)$ is always on the crest $\mathcal{C}_m(I)$, $\tau^*(I, \pi) = 0$ for all I .

Consider first the case of horizontal crests ($|\alpha(I)\mu| < 1$).

- a) For $I < 0$, the function $\alpha(I)$ introduced in (6.26) satisfies $\alpha(I) > 0$, and from (6.40), $\sin(\xi_1(I, \varphi)) \sin \varphi = -\mu \alpha(I) \sin \varphi \leq 0$. Take $\theta = \frac{3\pi}{2}$; since $I < 0$, the slope $m = (I - 1)/I$ of the NHIM lines is greater than 1. Therefore, $3\pi/2 - I\tau_1^*(I, 3\pi/2) \in (\pi, 3\pi/2)$. This implies that for any $\theta \in (\pi, 3\pi/2)$, $\theta - I\tau_1^*(I, \theta) \in (\pi, 3\pi/2)$, so $\sin(\theta - I\tau_1^*) < 0$. From (6.41), $\dot{I} > 0$.

- b) For $0 < I < 1$, $\alpha(I) < 0$, so $\sin \xi_1(I, \varphi) \sin \varphi \geq 0$. Besides, $m < 0$, so if we look for θ_* satisfying

$$\begin{aligned} \theta - I\tau &= 2\pi \\ \theta - (I - 1)\tau &= \pi, \end{aligned} \quad (6.42)$$



(a) The three types of level curves.

(b) Zoom where the scattering maps are different.

Figure 6.14: Level curves of $\mathcal{L}_M^*(I, \theta)$, $\mathcal{L}_M^{*(1)}(I, \theta)$ and $\mathcal{L}_M^{*(2)}(I, \theta)$.

we have that for any $\theta \in (\pi, \theta_*)$, $\theta - I\tau_1^* \in (\pi, 2\pi)$. By solving (6.42) and defining $\theta_+ := \theta_*$, we obtain $\theta_+ = (2-I)\pi$. Then, $\sin(\theta - I\tau_1^*(I, \theta)) < 0$ and therefore $\dot{I} > 0$ for any $\theta \in (\pi, \theta_+ = (2-I)\pi)$. In particular, $\theta_+ < 3\pi/2$ if, and only if, $I \in (1/2, 1)$.

- c) For $I > 1$, one more time $\alpha(I) > 0$ and $\sin \xi_1(I, \varphi) \sin(\varphi) < 0$, but now $0 < m = 1 - 1/I < 1$. We first fix $\theta = 3\pi/2$ and search for I such that

$$\begin{aligned} \frac{3\pi}{2} - I\tau^*(I, 3\pi/2) &= 0 \\ \frac{3\pi}{2} - (I-1)\tau^*(I, 3\pi/2) &= \pi. \end{aligned}$$

We obtain $I = 3/2$, so $\theta - I\tau_1^*(I, \theta) \in (0, \pi)$ for any $I \geq 3/2$ and $\theta \in (\pi, \theta_+ = 3\pi/2)$. Consequently, $\sin(\theta - I\tau_1^*(I, \theta)) > 0$ and $\dot{I} > 0$. For the values of $I \in (1, 3/2)$ we change the strategy. We look for θ_* such that

$$\begin{aligned} \theta - I\tau^*(I, \theta) &= 0 \\ \theta - (I-1)\tau^*(I, \theta) &= \pi. \end{aligned}$$

We have $\theta_* = \pi I$ and $\theta - I\tau_1^*(I, \theta_*) \in (0, \pi)$ for any $I \in (1, 3/2)$ and $\theta \in (\pi, \theta_*)$, so $\dot{I} > 0$. Note that $\theta_* < 3\pi/2$ and we can define $\theta_+ := \theta_*$.

Observe that for $I = 1$ the crests are vertical, and for $I = 0$, $\theta = \theta - I\tau_1^*(I, \theta)$, and $\dot{I} > 0$ for $\theta \in (\pi, 3\pi/2)$. Consider now the case of vertical crests ($|\alpha(I)\mu| > 1$).

- a) For $I < 0$, $\sin \eta_1(I, \sigma) \sin \sigma = -\mu\alpha(I) \sin^2 \sigma \leq 0$ and $m > 1$. We fix $\theta = 3\pi/2$ and look for I such that

$$\begin{aligned} 3\pi/2 - I\tau^* &= \pi \\ 3\pi/2 - (I-1)\tau^*(I, 3\pi/2) &= 0. \end{aligned}$$

We obtain $I = -1/2$ and therefore, $\sin(\theta - (I-1)\tau_1^*(I, \theta)) > 0$ for $I \in (-\infty, -1/2)$ and $\theta \in (\pi, 3\pi/2)$. Consequently, $\dot{I} > 0$ from (6.41). For $I \in (-1/2, 0)$, we have that $\theta_+ = (1-I)\pi$ satisfies

$$\begin{aligned} \theta - I\tau^*(I, \theta_+) &= \pi \\ \theta_+ - (I-1)\tau^*(I, \theta_+) &= 0. \end{aligned}$$

Therefore, $\sin(\theta - (I-1)\tau_1^*(I, \theta)) > 0$ and $\dot{I} > 0$ for any $\theta \in (\pi, \theta_+)$.

- b) For $0 < I < 1$ $\sin \eta_1(I, \sigma) \sin \sigma \geq 0$ and $m < 0$. $\theta_+ = (I+1)\pi$ satisfies

$$\begin{aligned} \theta - I\tau^*(I, \theta_+) &= \pi \\ \theta_+ - (I-1)\tau^*(I, \theta_+) &= 2\pi. \end{aligned}$$

So, $\sin(\theta - (I-1)\tau_1^*(I, \theta)) > 0$ and $\dot{I} > 0$ for any $\theta \in (\pi, \theta_+)$. Note that $\theta_+ < 3\pi/2$ for $I \in (0, 1/2)$.

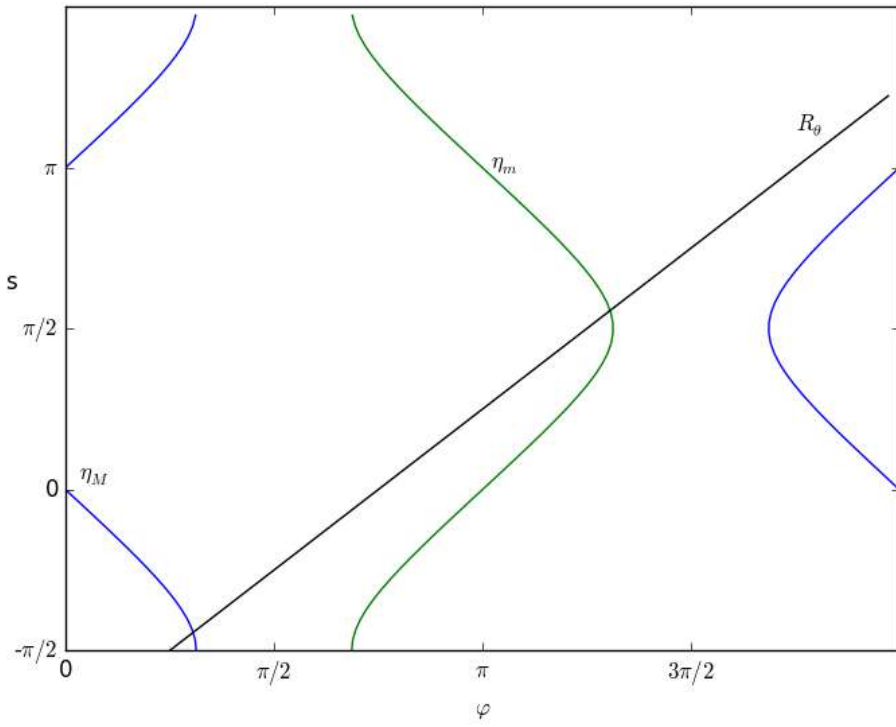


Figure 6.15: vertical crests of $\mathcal{L}^*$ for $\mu = 1.5$ and $I = 1$.

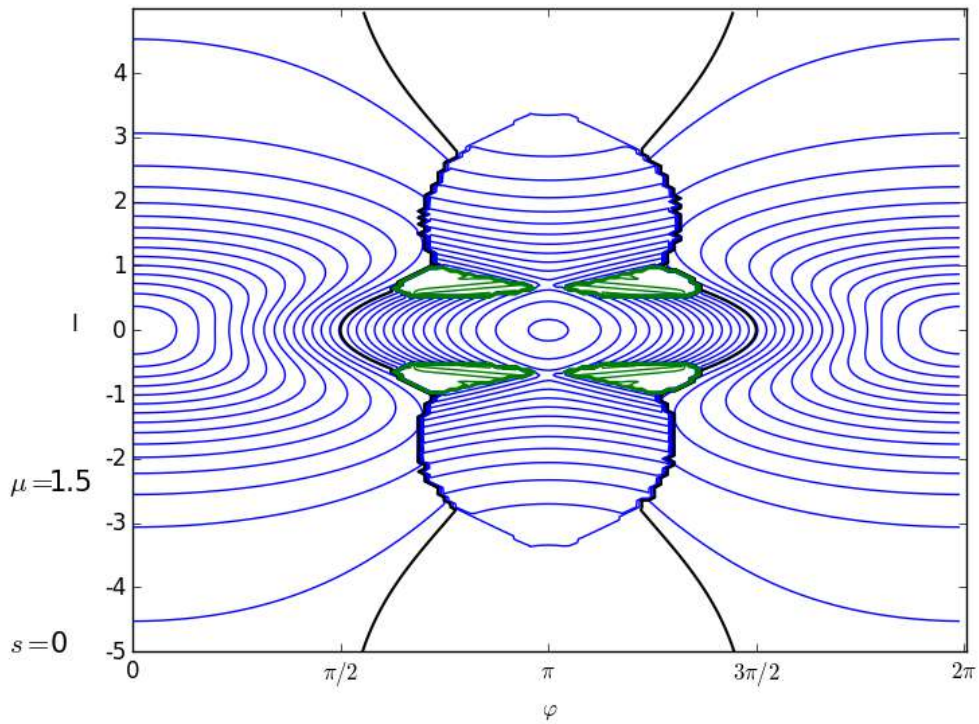


Figure 6.16: The level curves of $\mathcal{L}_M^*(I, \theta)$, $\mu = 1.5$. In green, the region where the scattering map S_M is not defined.

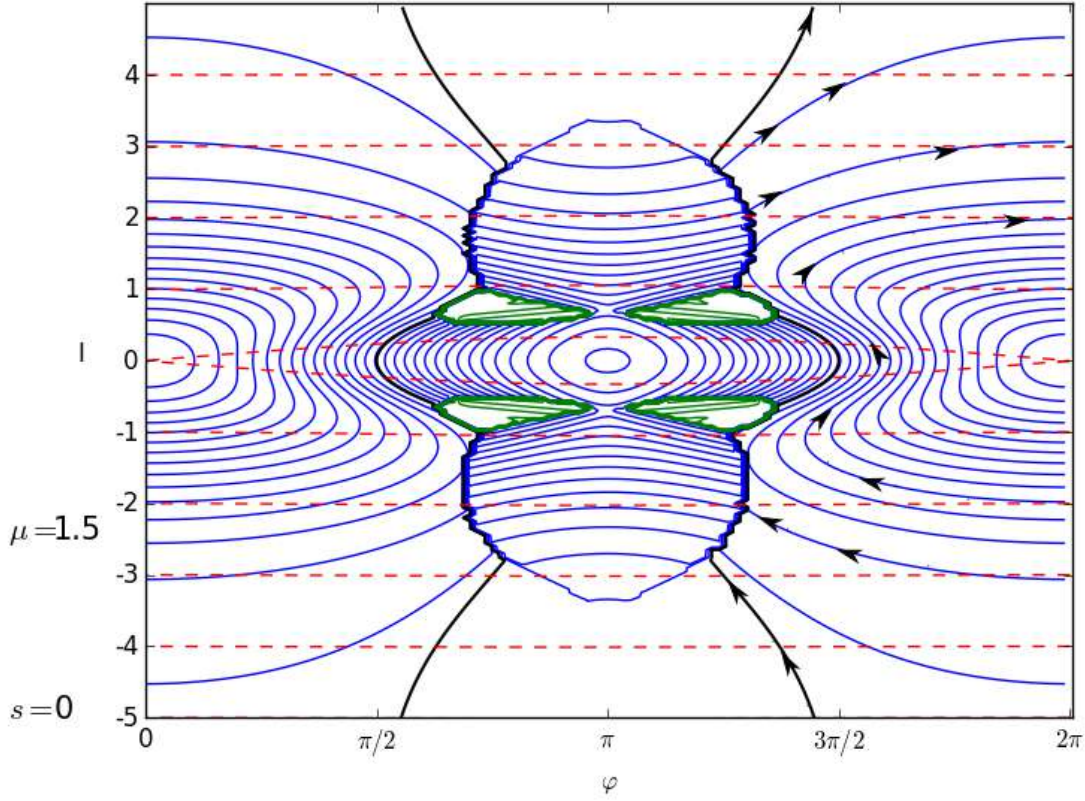


Figure 6.17: In red: Inner map, blue: Scattering map, black: Highways

c) Finally, for $I > 1$, $\sin \eta_1(I, \sigma) \sin \sigma \leq 0$. We have that $\theta - (I - 1)\tau_1^*(I, \theta) \in (\pi, 2\pi)$, so $\sin(\theta - (I - 1)\tau_1^*(I, \theta)) < 0$ and $\dot{I} > 0$ for any $\theta \in (\pi, 3\pi/2)$.

For $I = 0$ the crests are horizontal. For $I = 1$, $\theta = \theta - (I - 1)\tau_1^*(I, \theta)$, so $\dot{I} > 0$ for $\theta \in (\pi, 2\pi)$. □

6.8 $3 + 1/2$ degrees of freedom

6.8.1 A model

We now consider an *a priori* unstable Hamiltonian system with $3 + 1/2$ degrees of freedom (d.o.f.) introduced in [DGS24]

$$H_\varepsilon(p, q, I, \varphi, s) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + h(I) + \varepsilon f(q) g(\varphi, s), \quad (6.43)$$

with $(p, q, I, \varphi, s) \in \mathbb{R} \times \mathbb{T} \times \mathbb{R}^2 \times \mathbb{T}^2 \times \mathbb{T}$, where

$$\begin{aligned} h(I) &= h(I_1, I_2) = \Omega_1 I_1^2/2 + \Omega_2 I_2^2/2, \\ f(q) &= \cos q, \\ g(\varphi, s) &= g(\varphi_1, \varphi_2, s) = a_1 \cos \varphi_1 + a_2 \cos \varphi_2 + a_3 \cos s. \end{aligned} \quad (6.44)$$

Combining again iterates of the *inner* and the *outer* dynamics associated to the 5D-*Normally Hyperbolic Invariant Manifold* (NHIM) $\tilde{\Lambda} = \{q = 0, p = 0\}$, to build a diffusing *pseudo-orbit*, and applying shadowing results, we prove the existence of a diffusing orbit of the system. More precisely, we are able to prove the following theorem on global instability for the following set of parameters:

$$a_1 a_2 a_3 \neq 0 \quad \text{and} \quad |a_1/a_3| + |a_2/a_3| < 0.625. \quad (6.45)$$

Theorem 6.7 ([DGS24]). *Consider the Hamiltonian (6.43)+(6.44). Assume $a_1 a_2 a_3 \neq 0$ and $|a_1/a_3| + |a_2/a_3| < 0.625$. Then, for every $0 < \delta < 1$ and $R > 0$, there exists $\varepsilon_0 = \varepsilon_0(\delta, R) > 0$ such that for every I_+, I_- satisfying $|I_\pm| < R$, there exists an orbit $\tilde{x}(t)$ and $T > 0$, such that*

$$|I(0) - I_-| \leq \delta \quad \text{and} \quad |I(T) - I_+| \leq \delta.$$

6.8.2 Unperturbed case

For $\varepsilon = 0$, Hamiltonian (6.43)+(6.44) becomes

$$H_0(p, q, I, \varphi, s) = \pm \left(\frac{p^2}{2} + \cos q - 1 \right) + \frac{\Omega_1 I_1^2}{2} + \frac{\Omega_2 I_2^2}{2},$$

with associated equations

$$\begin{aligned} \dot{q} &= p & \dot{p} &= \sin q \\ \dot{\varphi}_1 &= \Omega_1 I_1 =: \omega_1 & \dot{I}_1 &= 0 \\ \dot{\varphi}_2 &= \Omega_2 I_2 =: \omega_2 & \dot{I}_2 &= 0 \\ \dot{s} &= 1, \end{aligned}$$

This system consists of one pendulum plus a 2 d.o.f rotor. From the equations above, I_1 and I_2 are constants of motion, and the flow has the form

$$\Phi_t(p, q, I, \varphi) = (p(t), q(t), I, \varphi + t\omega),$$

where $\omega = (\omega_1, \omega_2) := (\Omega_1 I_1, \Omega_2 I_2)$. To include the frequency of the time, we also will use the frequency vector $\tilde{\omega} = (\omega_1, \omega_2, 1)$.

Observe that $(p_0, q_0) = (0, 0)$ is a saddle point on the plane (p, q) with unstable and stable invariant curves. These invariant curves coincide and separate the behavior of orbits and, for this reason, are called *separatrices*. In addition, they can be parametrized by

$$(p_0(t), q_0(t)) = \left(\frac{\pm 2}{\cosh t}, 4 \arctan e^{\pm t} \right). \quad (6.46)$$

For any $I \in \mathbb{R}^2$, $\mathcal{T}_I = \{(0, 0, I, \varphi, s); \varphi, s \in \mathbb{T}^3\}$ is an invariant torus under the flow of the system with the frequency $\omega = (\Omega_1 I_1, \Omega_2 I_2)$ and is called a *whiskered torus*. For each whiskered torus, we have associated coincident stable and unstable manifolds called *whiskers*, which we denote by

$$W^0 \mathcal{T} = \left\{ (p_0(\tau), q_0(\tau), I, \varphi, s) : \tau \in \mathbb{R}, (\varphi, s) \in \mathbb{T}^2 \right\}.$$

The union of all whiskered tori $\mathcal{T}$

$$\tilde{\Lambda} = \{(0, 0, I, \varphi, s) : (I, \varphi, s) \in \mathbb{R} \times \mathbb{T}^3\} \quad (6.47)$$

is a 5D-*Normally Hyperbolic Invariant Manifold* (NHIM) with 6D-coincident stable and unstable invariant manifolds given by

$$W^0 \tilde{\Lambda} = \{(p_0(\tau), q_0(\tau), I, \varphi, s) : \tau \in \mathbb{R}, (I, \varphi, s) \in \mathbb{R}^2 \times \mathbb{T}^3\}.$$

For $\varepsilon \neq 0$, there exists a NHIM $\tilde{\Lambda}_\varepsilon$, which in our system, due to the fact that $f(q) = \cos q$ in (6.43), coincides with the NHIM $\tilde{\Lambda}$. Nevertheless, its stable manifold $W^s(\tilde{\Lambda}_\varepsilon)$ and unstable manifold $W^u(\tilde{\Lambda}_\varepsilon)$ no longer coincide, that is, the separatrices split.

6.8.3 Inner dynamics

The inner dynamics is derived from the restriction of the Hamiltonian (6.43) to $\tilde{\Lambda}$ given in (6.47), that is,

$$K_\varepsilon(I, \varphi, s) = \sum_{k=1}^2 \frac{\Omega_k I_k^2}{2} + \varepsilon \left(\sum_{k=1}^2 a_k \cos \varphi_k + a_3 \cos s \right)$$

and its associated equations are

$$\begin{aligned} \dot{\varphi}_1 &= \omega_1 = \Omega_1 I_1 & \dot{I}_1 &= \varepsilon a_1 \sin \varphi_1 \\ \dot{\varphi}_2 &= \omega_2 = \Omega_2 I_2 & \dot{I}_2 &= \varepsilon a_2 \sin \varphi_2 \\ \dot{s} &= 1. \end{aligned} \tag{6.48}$$

Note that the inner dynamics is integrable, with first integrals

$$\begin{aligned} F_1(I_1, \varphi_1) &= \frac{\Omega_1 I_1^2}{2} + \varepsilon a_1 (\cos \varphi_1 - 1), \\ F_2(I_2, \varphi_2) &= \frac{\Omega_2 I_2^2}{2} + \varepsilon a_2 (\cos \varphi_2 - 1), \end{aligned}$$

in involution. The inner dynamics is described in Fig. 6.18, so there are two resonances, one centered at $I_1 = 0$ and other at $I_2 = 0$.

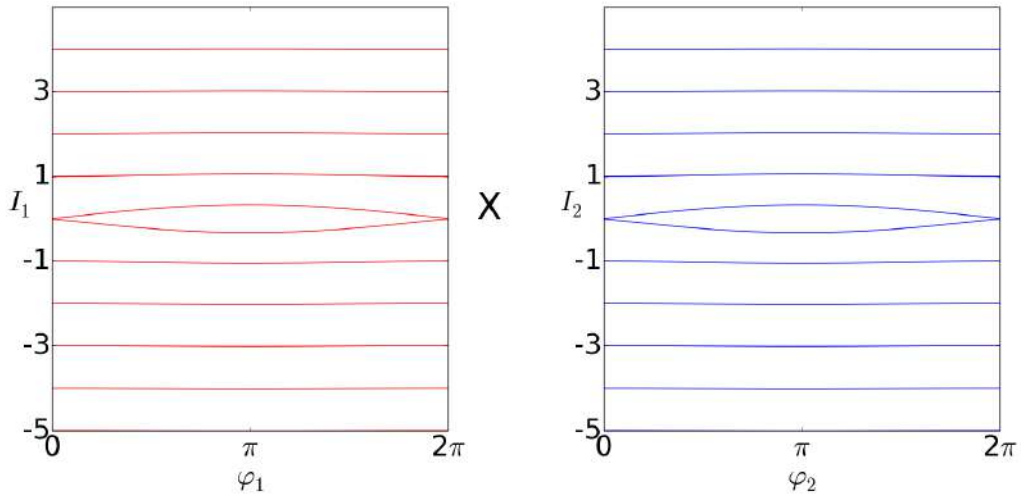


Figure 6.18: Inner dynamics

Remark 6.18. When ε is small enough, the level curves of F_1 and F_2 are almost *flat* or *horizontal* in the action $I = (I_1, I_2)$, i.e., the values of I_1 and I_2 remain almost constant, see Fig. 6.18. Since there is a continuous foliation of invariant tori, a genuine ‘large gap problem’ [DLS06a] does not appear.

Remark 6.19. There is a double resonance at $I_1 = I_2 = 0$. The study of dynamics close to double resonances is a challenging problem and is out of the scope of this work. Since, in our case, the double resonance is just the point $I = (0, 0)$, we will avoid it when necessary.

6.8.4 The Melnikov potential and the scattering map

The *Melnikov potential* of Hamiltonian (6.43) is defined as

$$\mathcal{L}(I, \varphi, s) := \int_{-\infty}^{+\infty} (f(q_0(\rho)) - f(0)) g(\varphi + \rho\omega, s + \rho; 0) d\rho,$$

and takes the form

$$\mathcal{L}(I, \varphi, s) = A_1 \cos \varphi_1 + A_2 \cos \varphi_2 + A_3 \cos s, \tag{6.49}$$

where

$$A_i := A(\tilde{\omega}_i, a_i) = \frac{2\pi\tilde{\omega}_i a_i}{\sinh(\pi\tilde{\omega}_i/2)}, \quad i = 1, 2, 3 \tag{6.50}$$

and $\tilde{\omega} = (\omega_1, \omega_2, 1)$, for $\omega_i \neq 0$, and $A_i = 4a_i$ for $\omega_i = 0$.

Given $(I, \varphi, s) \in [-I_1^*, I_1^*] \times [-I_1^*, I_1^*] \times \mathbb{T}^3$, any non-degenerate critical point $\tau^* = \tau^*(I, \varphi, s)$ of

$$\tau \in \mathbb{R} \longmapsto \mathcal{L}(I, \varphi - \tau\omega, s - \tau) \in \mathbb{R}, \quad (6.51)$$

where $\omega = (\omega_1, \omega_2) = (\Omega_1 I_1, \Omega_2 I_2)$ gives rise, for $0 < \varepsilon$ small enough, to a unique transverse homoclinic point $\tilde{z}$ to $\tilde{\Lambda}_\varepsilon$ of Hamiltonian (6.43), which is ε -close to the point $\tilde{z}^*(I, \varphi, s) = (p_0(\tau^*), q_0(\tau^*), I, \varphi, s) \in W^0(\tilde{\Lambda})$:

$$\tilde{z} = \tilde{z}(I, \varphi, s) = (p_0(\tau^*) + O(\varepsilon), q_0(\tau^*) + O(\varepsilon), I, \varphi, s) \text{ and } \tilde{z} \in W^u(\tilde{\Lambda}_\varepsilon) \pitchfork W^s(\tilde{\Lambda}_\varepsilon).$$

Once a function $\tau^*(I, \varphi, s)$ is chosen, by the geometric properties of the scattering map, [DLS08, DH09, DH11], the scattering map $S = S_{\tau^*}$ has the explicit form

$$S(I, \varphi, s) = \left(I + \varepsilon \nabla_\varphi L^* + \mathcal{O}(\varepsilon^2), \varphi - \varepsilon \nabla_I L^* + \mathcal{O}(\varepsilon^2), s \right),$$

where

$$L^* = L^*(I, \varphi, s) = \mathcal{L}(I, \varphi - \tau^*(I, \varphi, s)\omega, s - \tau^*(I, \varphi, s)). \quad (6.52)$$

Note that the variable s is fixed under the scattering map. As a consequence, introducing the variable

$$\theta = \varphi - s\omega, \quad (6.53)$$

we can define the *reduced Poincaré function* as

$$\mathcal{L}^*(I, \theta) := L^*(I, \varphi - s\omega, 0) = L^*(I, \varphi, s). \quad (6.54)$$

In these variables (I, θ) the scattering map has the simple form

$$\mathcal{S}(I, \theta) = \left(I + \varepsilon \frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) + \mathcal{O}(\varepsilon^2), \theta - \varepsilon \frac{\partial \mathcal{L}^*}{\partial I}(I, \theta) + \mathcal{O}(\varepsilon^2) \right). \quad (6.55)$$

So, up to $\mathcal{O}(\varepsilon^2)$ terms, $\mathcal{S}(I, \theta)$ is the $-\varepsilon$ times flow of the *autonomous* Hamiltonian $\mathcal{L}^*(I, \theta)$. In particular, a finite number of iterates under the scattering map follow the level curves of $\mathcal{L}^*$ up to $\mathcal{O}(\varepsilon^2)$.

It is easy to see [DH11, DS18] that the reduced Poincaré function $\mathcal{L}^*(I, \theta)$ in (6.54) is equivalent to

$$\mathcal{L}^*(I, \theta) = \mathcal{L}(I, \theta - \tau^*(I, \theta)\omega, -\tau^*(I, \theta)),$$

where

$$\tau^*(I, \theta) = \tau^*(I, \varphi, s) - s. \quad (6.56)$$

Therefore, from (6.49) the reduced Poincaré function $\mathcal{L}^*(I, \theta)$ can be explicitly expressed as

$$\begin{aligned} \mathcal{L}^*(I, \theta) &= \sum_{k=1}^2 A_k \cos(\theta_k - \omega_k \tau^*(I, \theta)) \\ &\quad + A_3 \cos(-\tau^*(I, \theta)). \end{aligned} \quad (6.57)$$

From now on, both $\tau^*(I, \varphi, s)$ and $\tau^*(I, \theta)$ will be used at our convenience. It is important to note that, as the variable s is fixed for $\mathcal{S}(I, \theta)$, it plays the rôle of a parameter, which for simplicity [DS17] will be taken $s = 0$.

Remark: The reduced Poincaré function $\mathcal{L}^*(I, \theta)$ can be defined but the associated Hamiltonian vector field *is no longer integrable*.

6.8.5 Crests and NHIM lines

We have seen that the function τ^* plays a key role in our study. Therefore, we are interested in finding the critical points $\tau^* = \tau^*(I, \varphi, s)$ of function (6.51) or, for our concrete case (6.49), τ^* solution of

$$\frac{\partial \mathcal{L}}{\partial \tau}(I, \varphi - \omega\tau, s - \tau) = \nabla_{(\varphi, s)} \mathcal{L}(I, \varphi - \omega\tau, s - \tau) \cdot \tilde{\omega} = 0. \quad (6.58)$$

This equation can be seen from two equivalent geometrical viewpoints. The first one is that to find $\tau^* = \tau^*(I, \varphi, s)$ satisfying (6.58) for any $(I, \varphi, s) \in [-I_1^*, I_1^*] \times [-I_2^*, I_2^*] \times \mathbb{T}^3$ is the same as looking for the extrema of $\mathcal{L}$ on the *NHIM line*

$$R(I, \varphi, s) = \{ (I, \varphi - \tau\omega, s - \tau) : \tau \in \mathbb{R} \}. \quad (6.59)$$

The other point of view is that fixing (I, φ, s) , a solution τ^* of (6.58) is equivalent to finding intersections between a NHIMline (6.59) and a set of points determined by the equation $\nabla_{(\varphi, s)} \mathcal{L}(I, \varphi, s) \cdot \tilde{\omega} = 0$.

Remark 6.20. Note that $R(I, \varphi, s)$ on $\{I\} \times \mathbb{T}^3$ is either a closed line when $\omega \in \mathbb{Q}^2$, or densely fills a torus of dimension 2 or 3.

Remark 6.21. By taking θ as defined in (6.53) and $s = 0$, we can rewrite $R(I, \varphi, s)$ on variables (I, θ) , that is, $R(I, \varphi, s)$ is equivalent to

$$R(I, \theta) = \{(I, \theta - \tau\omega, -\tau) : \tau \in \mathbb{R}\}. \quad (6.60)$$

Definition 4. [DH11] A crest or ridge $\mathcal{C}(I)$ is the set of points $\{(I, \varphi, s), (\varphi, s) \in \mathbb{T}^3\}$ such that

$$\frac{\partial \mathcal{L}}{\partial \tau}(I, \varphi - \tau\omega, s - \tau)|_{\tau=0} = 0,$$

or equivalently,

$$\nabla_{(\varphi, s)} \mathcal{L}(I, \varphi, s) \cdot \tilde{\omega} = 0. \quad (6.61)$$

Fixing I , Eq. (6.61) defines, at least locally, a surface in the variables $(\varphi_1, \varphi_2, s) \in \mathbb{T}^3$, that we want to characterize.

From the expression (6.49) of the Melnikov Potential $\mathcal{L}(I, \varphi, s)$, Eq. (6.61) can be rewritten as

$$\alpha(\omega_1)\mu_1 \sin \varphi_1 + \alpha(\omega_2)\mu_2 \sin \varphi_2 + \sin s = 0 \quad (6.62)$$

where, for $i = 1, 2$,

$$\mu_i = \frac{a_i}{a_3} \quad \text{and} \quad \alpha(\omega_i) = (\omega_i)^2 \frac{\sinh(\pi/2)}{\sinh(\omega_i \pi/2)}. \quad (6.63)$$

Observe that α is well defined for any value of ω_i . For any fixed I , to understand the intersection between NHIMlines $R(I, \cdot)$ and the crest $\mathcal{C}(I)$, we first need to study how the surfaces contained in the crest look like for different values of $\mu_i = a_i/a_3$ and ω_i , for $i = 1, 2$.

Remark 6.22. We wish to emphasize the similarity between Eq. (6.62) of the crest with the equation of the crests studied for 2+1/2 d.o.f. [DS17, DS18]

Eq. (6.62) is just a linear equation for the variables $\sin \varphi_1$, $\sin \varphi_2$ and $\sin s$. To parametrize the crest, we want to isolate one of these variables with respect to the other two.

We begin with the case

$$\text{a) } |\alpha(\omega_1)\mu_1 \sin \varphi_1 + \alpha(\omega_2)\mu_2 \sin \varphi_2| \leq 1, \quad (6.64)$$

where we can write s as a function of φ_1 and φ_2 for any $(\varphi_1, \varphi_2) \in \mathbb{T}^2$, more precisely, we have the two functions

$$s = \begin{cases} \xi_{\mathcal{M}}(I, \varphi) := \arcsin(\alpha(\omega_1)\mu_1 \sin \varphi_1 + \alpha(\omega_2)\mu_2 \sin \varphi_2) \mod 2\pi \\ \xi_{\mathcal{m}}(I, \varphi) := -\arcsin(\alpha(\omega_1)\mu_1 \sin \varphi_1 + \alpha(\omega_2)\mu_2 \sin \varphi_2) + \pi \mod 2\pi. \end{cases}$$

Then the crest $\mathcal{C}(I)$ is formed by two surfaces $\mathcal{C}_{\mathcal{M}}(I)$, $\mathcal{C}_{\mathcal{m}}(I)$ which are simply the *global graphics* in the space $(\varphi_1, \varphi_2, s)$ of the functions $\xi_{\mathcal{M}}(I, \varphi)$, $\xi_{\mathcal{m}}(I, \varphi)$, defined for all $\varphi \in \mathbb{T}^2$. According to the notation used for 2+1/2 d.o.f. [DS17, DS18], the crest $\mathcal{C}(I)$ is called a *horizontal crest*; see Fig. 6.19. From the expression of the function $\alpha(\omega_i)$ given in (6.63), we have $|\alpha(\omega_i)| < 1.03$. This implies

$$|\alpha(\omega_1)\mu_1 \sin \varphi_1 + \alpha(\omega_2)\mu_2 \sin \varphi_2| < 1.03(|\mu_1| + |\mu_2|).$$

Therefore, if

$$|\mu_1| + |\mu_2| < 1/1.03,$$

the two surfaces of the crests $\mathcal{C}(I)$ are horizontal for any value of I_1 and I_2 .

If condition (6.64) is not satisfied, s cannot be written as a global function of φ_1 and φ_2 in (6.62), and then two more possibilities arise: b) we can write φ_i as a global function of φ_j and s , or c) we cannot write any variable φ_1 , φ_2 and s as a global function of the other two and, therefore, the projection of the crest $\mathcal{C}(I)$ on each plane (φ_1, φ_2) , (φ_1, s) and (φ_2, s) , has “holes”.

Case b) is only possible if

$$\left| \frac{\alpha(\omega_j)\mu_j}{\alpha(\omega_i)\mu_i} \sin \varphi_j + \frac{\sin s}{\alpha(\omega_i)\mu_i} \right| \leq 1, \quad (6.65)$$

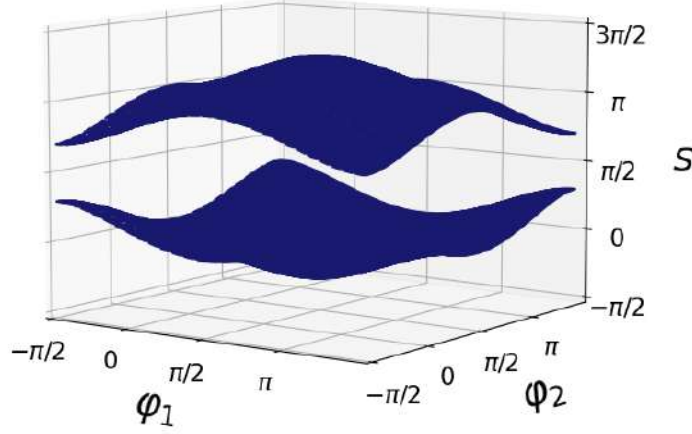


Figure 6.19: *Horizontal Crest* $\mathcal{C}(I)$ formed by two surfaces: $\mu_1 = \mu_2 = 0.4$ and $\omega_1 = \omega_2 = 1$. We plotted $\varphi_1, \varphi_2, s \in [-\pi/2, 3\pi/2)$ for a better illustration.

for $i, j = 1, 2$ and $i \neq j$. Then, the crest $\mathcal{C}(I)$ is formed by two vertical surfaces $\mathcal{C}_M(I)$ and $\mathcal{C}_m(I)$ that can be parameterized by

$$\varphi_i = \begin{cases} \eta_M(I, \varphi_j, s) := \arcsin \left(\frac{1}{\alpha(\omega_i)\mu_i} (\sin s - \alpha(\omega_j)\mu_j \sin \varphi_j) \right) \bmod 2\pi \\ \eta_m(I, \varphi_j, s) := -\arcsin \left(\frac{1}{\alpha(\omega_i)\mu_i} (\sin s - \alpha(\omega_j)\mu_j \sin \varphi_j) \right) + \pi \bmod 2\pi. \end{cases}$$

In this case, $\mathcal{C}(I)$ is called a *vertical crest*; see Fig. 6.20.

Case c) only occurs if Eq. (6.64) and (6.65) do not hold. Then the crest $\mathcal{C}(I)$ is given by a unique surface; see Fig. 6.21. Note that the horizontal and vertical crests $\mathcal{C}(I)$ are formed by two disjoint surfaces that can be parameterized separately $\mathcal{C}_M(I)$ and $\mathcal{C}_m(I)$, and $\mathcal{C}(I) = \mathcal{C}_M(I) \cup \mathcal{C}_m(I)$. In case c), $\mathcal{C}(I)$ is called an *unseparated crest*.

It is worth noting that to express φ_i as a global function of φ_j and s , $|\mu_i|$ is needed to be greater than $1/1.03$. Indeed, assume that there exists an I such that $\varphi_i := \varphi_i(\varphi_j, s)$. From condition (6.61), we have

$$\sin \varphi_i = - \left(\frac{A_j \omega_j \sin \varphi_j}{A_i \omega_i} + \frac{A_3 \sin s}{A_i \omega_i} \right),$$

for any $(\varphi_j, s) \in \mathbb{T}^2$ satisfying (6.65). In particular, for $\varphi_j = 0$ and $s = \pm\pi/2$, so

$$\left| \frac{A_3}{A_i \omega_i} \right| \leq 1, \quad \text{or equivalently} \quad \left| \frac{1}{\alpha(\omega_i)\mu_i} \right| \leq 1.$$

Therefore, we obtain the following.

$$\frac{1}{1.03} < \left| \frac{1}{\alpha(\omega_i)} \right| \leq |\mu_i|.$$

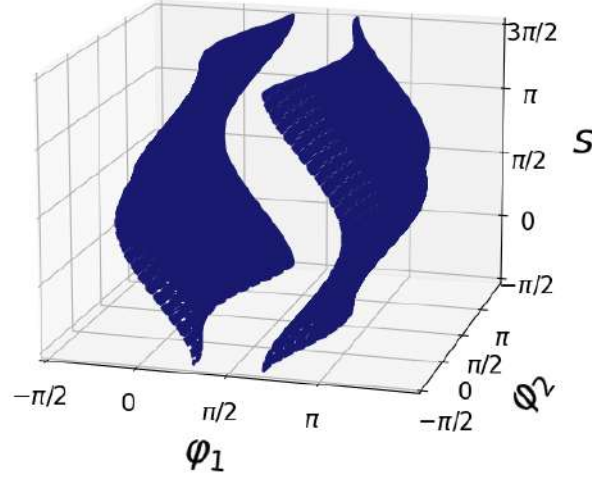


Figure 6.20: Vertical Crest $\mathcal{C}(I)$: $\mu_1 = 1.7$, $\mu_2 = 0.4$ and $\omega_1 = \omega_2 = 1$. We plotted $\varphi_1, \varphi_2, s \in [-\pi/2, 3\pi/2)$ for a better illustration.

As a consequence, if $|\mu_1| + |\mu_2| > 1/1.03$, but $|\mu_1|, |\mu_2| < 1/1.03$, there are no vertical crests, that is, there are only horizontal or unseparated crests.

We now summarize all these calculations.

Proposition 6.8. *For a fixed value of I , if condition (6.64) holds, $\mathcal{C}(I)$ is a horizontal crest formed by two disjoint horizontal global surfaces. Otherwise, we have two cases:*

- a) *If $|\mu_1| > 1/1.03$ or $|\mu_2| > 1/1.03$, $\mathcal{C}(I)$ is a vertical crest formed by two disjoint vertical global surfaces.*
- b) *If $|\mu_1| + |\mu_2| > 1/1.03$ and $|\mu_1|, |\mu_2| < 1/1.03$, $\mathcal{C}(I)$ is an unseparated crest.*

Moreover, if $|\mu_1| + |\mu_2| < 1/1.03$, then (6.64) is satisfied and $\mathcal{C}(I)$ is a horizontal crest formed by two disjoint horizontal global surfaces.

Remark 6.23. The values of μ_1, μ_2 providing equalities are bifurcation values for which the two surfaces intersect tangentially.

Remark 6.24. The notation $\mathcal{C}_M(I)$ and $\mathcal{C}_m(I)$ come from the fact that $(0, 0, 0) \in \mathcal{C}_M(I)$ and $(\pi, \pi, \pi) \in \mathcal{C}_m(I)$, and $(0, 0, 0)$ and (π, π, π) are, respectively, a maximum and a minimum point of the Melnikov potential $\mathcal{L}(I, \varphi, s)$ given by (6.49), for $a_1, a_2, a_3 > 0$.

Tangency condition

The tangency between the NHIM lines $R(I, \varphi, s)$ and the crest $\mathcal{C}(I)$ is an obstacle to the existence of a global scattering map [DS17, DS18]. Since we only deal with global scattering maps, we need to avoid such tangencies. We now make a study about the conditions of their existence.

The crests $\mathcal{C}(I)$ form a family of surfaces, so there exists a tangency between $\mathcal{C}(I)$ and $R(I, \varphi, s)$ if a tangent vector of the straight line $R(I, \varphi, s)$ lies on the tangent bundle of one of these surfaces.

A tangent vector of $R(I, \varphi, s)$ at any point is $-\tilde{\omega}$. Consider the function $F_I : \mathbb{T}^3 \mapsto \mathbb{R}$,

$$F_I(\varphi, s) = \alpha(\omega_1)\mu_1 \sin \varphi_1 + \alpha(\omega_2)\mu_2 \sin \varphi_2 + \sin s.$$

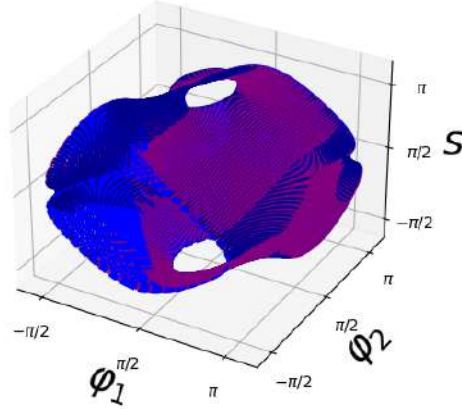


Figure 6.21: *Unseparated Crest* $\mathcal{C}(I)$: $\mu_1 = 0.8$, $\mu_2 = 0.4$ and $\omega_1 = \omega_2 = 1$. We plotted $\varphi_1, \varphi_2, s \in [-\pi/2, 3\pi/2)$ for a better illustration.

We note that the crest $\mathcal{C}(I)$ is defined from (6.62) as the set of $(\varphi, s) \in \mathbb{T}^3$ such that $F_I(\varphi, s) = 0$. Fixing a point $\Psi = (\varphi, s)$ in $\mathcal{C}(I)$, the normal vector of $\mathcal{C}(I)$ at the point Ψ is

$$\nabla F_I(\Psi) = (\alpha(\omega_1)\mu_1 \cos \varphi_1, \alpha(\omega_2)\mu_2 \cos \varphi_2, \cos s).$$

The tangent vector $-\tilde{\omega}$ lies on the tangent space of the crest at the point Ψ if and only if $\nabla F(\Psi) \cdot \tilde{\omega} = 0$. This condition is equivalent to

$$\alpha(\omega_1)\omega_1\mu_1 \cos \varphi_1 + \alpha(\omega_2)\omega_2\mu_2 \cos \varphi_2 + \cos s = 0. \quad (6.66)$$

From (6.62) and (6.66), there is a tangency between a horizontal crest $\mathcal{C}(I)$ and a NHIMline $R(I, \varphi, s)$ for φ_1 and φ_2 satisfying

$$\left(\sum_{k=1}^2 \omega_k \alpha(\omega_k) \mu_k \cos \varphi_k \right)^2 + \left(\sum_{k=1}^2 \alpha(\omega_k) \mu_k \sin \varphi_k \right)^2 = 1.$$

Denote by

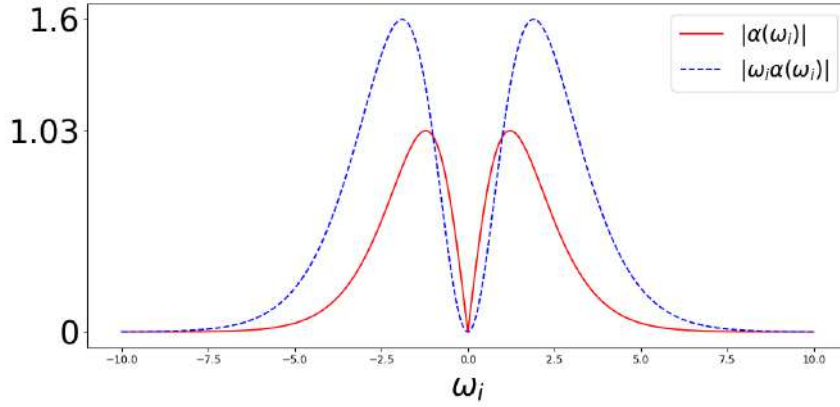
$$f_I(\varphi) = \left(\omega_1 \alpha(\omega_1) \mu_1 \cos \varphi_1 + \omega_2 \alpha(\omega_2) \mu_2 \cos \varphi_2 \right)^2 + \left(\alpha(\omega_1) \mu_1 \sin \varphi_1 + \alpha(\omega_2) \mu_2 \sin \varphi_2 \right)^2.$$

Note that for values of μ_1 and μ_2 such that $f_I(\varphi) < 1$ there is no tangency. As commented above, $|\alpha(\omega_i)| < 1.03$. From (6.63), we obtain $|\omega_i \alpha(\omega_i)| < 1.6$, see Fig. 6.22. This implies

$$\begin{aligned} f_I(\varphi) &< (1.6)^2 (|\mu_1 \cos \varphi_1| + |\mu_2 \cos \varphi_2|)^2 \\ &\quad + (1.03)^2 (|\mu_1 \sin \varphi_1| + |\mu_2 \sin \varphi_2|)^2 \\ &< 1.6^2 |\mu_1|^2 + 1.6^2 |\mu_2|^2 \\ &\quad + 2 |\mu_1| |\mu_2| \left(1.6^2 |\cos \varphi_1| |\cos \varphi_2| \right. \\ &\quad \left. + 1.03^2 |\sin \varphi_1| |\sin \varphi_2| \right) \\ &< 1.6^2 (|\mu_1| + |\mu_2|)^2. \end{aligned}$$

Therefore it is enough to require $|\mu_1| + |\mu_2| < 1/1.6 = 0.625$ to ensure $f_I(\varphi) < 1$ for any value of I . It is easy to verify that if $|\mu_1| + |\mu_2| > 1/1.6$ there exist I and φ such that $f_I(\varphi) > 1$.

We now collect all these properties in the following proposition.

Figure 6.22: Graph of $|\alpha|$ and $|\omega_i \alpha|$.

Proposition 6.9. *For any I , consider the crest $\mathcal{C}(I)$ defined in (4) and the NHIMlines $R(I, \varphi, s)$ defined in (6.59).*

- a) *For $|\mu_1| + |\mu_2| < 0.625$ the crest $\mathcal{C}(I)$ is formed by two horizontal global surfaces and the intersections between any surface and any NHIMline are transversal.*
- b) *For $0.625 \leq |\mu_1| + |\mu_2| \leq 1/1.03$ the crest $\mathcal{C}(I)$ is still formed by two horizontal global surfaces, but for some values of I there are NHIMlines that are tangent to the surfaces.*
- c) *For $1/1.03 < |\mu_1| + |\mu_2|$ and $|\mu_1|, |\mu_2| \leq 1/1.03$, the crest $\mathcal{C}(I)$ is either formed by two global horizontal surfaces or is unseparated, and for some values of I there are NHIMlines that are tangent to the crest.*
- d) *For $1/1.03 < |\mu_1|$ or $1/1.03 < |\mu_2|$, the crest $\mathcal{C}(I)$ is either formed by two horizontal global surfaces, either formed by two vertical global ones, or it is unseparated, and for some values of I there are NHIMlines that are tangent to the crest.*

Here we will consider only case a), that is, $|\mu_1| + |\mu_2| < 0.625$ which is contained in hypothesis (6.45) of Theorem 1, because in this way the crest is formed by two surfaces and the NHIMlines are transverse to them.

We have assumed until now that $s \in \mathbb{T}$. This implies that $\mathcal{C}(I) = \mathcal{C}_M(I) \cup \mathcal{C}_m(I)$ and $R(I, \varphi, s)$ intersects infinitely many times $\mathcal{C}_M(I)$ and $\mathcal{C}_m(I)$. We will restrict our analysis to a finite number of intersections to obtain our results. Taking $s \in \mathbb{R}$, the crest $\mathcal{C}(I)$ is no longer formed by two horizontal surfaces, but it is an infinitely countable family of horizontal surfaces, that is, $\mathcal{C}(I) = \bigcup_{j \in \mathbb{Z}} \mathcal{C}_j(I)$, where $\mathcal{C}_j(I)$ can be parametrized by

$$\xi_j(I, \varphi) = -\arcsin \left(\sum_{k=1}^2 \mu_k \alpha(\omega_k) \sin \varphi_k \right) + 2\pi j, \quad (6.67)$$

if j is even, otherwise

$$\xi_j(I, \varphi) = \arcsin \left(\sum_{k=1}^2 \mu_k \alpha(\omega_k) \sin \varphi_k \right) + \pi + 2\pi j. \quad (6.68)$$

Remark 6.25. Note that if $s \in \mathbb{T}$, $\mathcal{C}_j \equiv \mathcal{C}_M$ for all even j . Analogously, $\mathcal{C}_j \equiv \mathcal{C}_m$ for all odd j .

Therefore, we immediately have the following corollary from Prop. 6.9:

Corollary 6.1. *Consider the crest $\mathcal{C}(I)$ defined in (4) and the NHIMlines $R(I, \varphi, s)$ defined in (6.59) for $s \in \mathbb{R}$. For $|\mu_1| + |\mu_2| < 0.625$ the crest $\mathcal{C}(I)$ is formed by infinitely countable horizontal surfaces $\mathcal{C}_j(I)$, $j \in \mathbb{Z}$, that is, $\mathcal{C}(I) = \bigcup_{j \in \mathbb{Z}} \mathcal{C}_j(I)$, and the intersections between any surface $\mathcal{C}_j(I)$ and any NHIMline $R(I, \varphi, s)$ are transversal.*

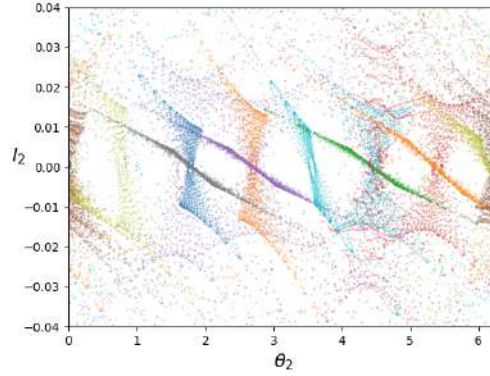


Figure 6.23: Dynamics of the Poincaré map the section $I_1 = 0$ at the energy level $\mathcal{L}^*(0, 0, 5\pi/4, 5\pi/4)$. Initial conditions are taken at the section $\{(I_1, I_2, \theta_2) = (0, 0, [5\pi/4 - 0.2, 5\pi/4 + 0.2])\}$ for $\mu_1 = 0.2$ and $\mu_2 = 0.3$. Each color represents a different orbit of the Poincaré map.

After this construction, each line $R(I, \varphi, s)$ intersects each $\mathcal{C}_j(I)$ at a unique point. We denote by τ_j^* the value of τ such that $R(I, \varphi, s)$ intersects $\mathcal{C}_j(I)$. Following the same philosophy, we denote $\mathcal{L}_j^*(I, \theta) = \mathcal{L}(I, \varphi - \tau_j^* \omega, s - \tau_j^*)$ and $\mathcal{S}_j$ the scattering map associated to $\mathcal{C}_j$, that is,

$$\mathcal{S}_j(I, \theta)^T = (I, \theta)^T + \varepsilon J \nabla \mathcal{L}_j^*(I, \theta)^T + \mathcal{O}(\varepsilon^2),$$

where $J = \begin{pmatrix} 0 & \text{Id}_2 \\ -\text{Id}_2 & 0 \end{pmatrix}$ is the 4×4 symplectic matrix.

Corollary 6.2. *Under the same conditions of Corollary 6.1, the scattering map $\mathcal{S}_j(I, \theta)$ associated to $\mathcal{C}_j$ is globally defined, i.e., it is well defined for any $(I, \theta) \in \mathbb{R}^2 \times \mathbb{T}^2$.*

Proof. The existence of $\tau_j^*(I, \theta)$ for all $(I, \theta) \in \mathbb{R}^2 \times \mathbb{T}^2$ holds by the fact that the slope of $R(I, \varphi, s)$ is $\tilde{\omega} = (\omega_1, \omega_2, 1)$ and the surfaces $\mathcal{C}_j(I)$ are horizontal and there is no tangency between $R(I, \varphi, s)$ and $\mathcal{C}_j(I)$. $\square$

Remark 6.26. In practice, it is enough to deal with $\mathcal{S}_0$ and $\mathcal{S}_1$, which are also called primary scattering maps[DS17, DS18]. Indeed, we will only explicitly use $\mathcal{S}_0$.

6.8.6 Transversality between the Inner and scattering flows

To perform diffusion through a scattering map, that is, to find trajectories of Hamiltonian system (6.43)+(6.44) where the action I changes significantly, we would like to prove that an orbit of the scattering map is not confined in an orbit of the inner dynamics, since the value of I is almost constant under the action of the inner map.

Recall that the scattering map is the ε -time flow of the Hamiltonian $-\mathcal{L}_j^*(I, \theta)$ up to order $\mathcal{O}(\varepsilon^2)$. Then, from a geometrical point of view, looking at the flow associated to the reduced Poincaré function $\mathcal{L}_j^*$ will be very useful.

Definition 5. *The flow $\phi_t^{-\mathcal{L}_j^*}$ of the Hamiltonian $-\mathcal{L}_j^*$ given by the equations*

$$\dot{I} = \frac{\partial \mathcal{L}_j^*}{\partial \theta}(I, \theta) \quad \text{and} \quad \dot{\theta} = -\frac{\partial \mathcal{L}_j^*}{\partial I}(I, \theta) \quad (6.69)$$

is called the scattering flow associated to $\mathcal{L}_j^$.*

The scattering flow is 4-dimensional and autonomous and exhibits rich dynamics. In Figure 6.23 we show a simulation of the Poincaré map onto a hyperplane given by $I_1 = \text{constant}$, where non-integrability is clearly manifested.

From (6.57), the above Hamiltonian equations take the form, for $i = 1, 2$,

$$\begin{aligned} \dot{I}_i &= -A_i \sin(\theta_i - \omega_i \tau_j^*) \\ \dot{\theta}_i &= -\Omega_i \left(\frac{dA_i}{d\omega_i} \cos(\theta_i - \omega_i \tau_j^*) + \tau_j^* A_i \sin(\theta_i - \omega_i \tau_j^*) \right). \end{aligned} \quad (6.70)$$

Remark 6.27. Take an initial point (I_0, θ_0) . After a large number k of iterates of scattering map $\mathcal{S}_j$, $(I_k, \theta_k) = \mathcal{S}_j^k(I_0, \theta_0)$ is expected to accumulate an error with respect to the scattering flow $\phi_t(I_0, \theta)$ at time $t = k\varepsilon$, as the flow is just an approximation of the scattering orbit. However, this error can be controlled by also using the inner dynamics in order to keep the iterations of $\mathcal{S}_j$ close to the scattering flow. A complete description of this mechanism and an analysis of this accumulated was done for 2+1/2 d.o.f. in [DS17] as described in section 6.1

Lemma 6.10. *The scattering flow with equations (6.70) has only four equilibrium points: $(0, 0, 0, 0)$, $(0, 0, 0, \pi)$, $(0, 0, \pi, 0)$ and $(0, 0, \pi, \pi)$.*

Proof. It is an immediate consequence of (6.70) and the form of A_i , given in (6.50), and their derivatives. $\square$

We can now state the following result.

Proposition 6.11. *Consider Hamiltonian (6.43)+(6.44). For $|\mu_1| + |\mu_2| < 0.625$ and I not ε -close to $(0, 0)$, there is no common orbit of the inner flow and the scattering flow.*

Proof. From (6.48), the first integrals on variables (I_i, θ_i) are given by

$$F_i = \frac{\Omega_i I_i^2}{2} + \varepsilon a_i \cos \theta_i, \quad i = \{1, 2\}. \quad (6.71)$$

The transversality of any invariant set of the inner flow and the scattering flow holds if the gradient of the level surfaces of F_1 and F_2 are not parallel to the gradient of the level surfaces of $\mathcal{L}^*$, or equivalently,

$$\{F_i, -\mathcal{L}_j^*\}(\phi_t^{-\mathcal{L}_j^*}(I^0, \theta^0)) \neq 0, \quad i = \{1, 2\}, \quad (6.72)$$

where $\{, \}$ is the Poisson bracket and $\phi_t^{-\mathcal{L}_j^*}(I^0, \theta^0)$ is the scattering flow associated to $-\mathcal{L}_j^*$. Note that

$$\begin{aligned} \{F_i, -\mathcal{L}_j^*\} &= -\frac{\partial F_i}{\partial \theta_i} \frac{\partial \mathcal{L}_j^*}{\partial I_i} + \frac{\partial F_i}{\partial I_i} \frac{\partial \mathcal{L}_j^*}{\partial \theta_i} \\ &= \varepsilon a_i \Omega_i \sin \theta_i \left(\frac{dA_i}{d\omega_i} \cos(\theta_i - \omega_i \tau_j^*) + \tau_j^* A_i \sin(\theta_i - \omega_i \tau_j^*) \right) \\ &\quad - \omega_i A_i \sin(\theta_i - \omega_i \tau_j^*) \end{aligned}$$

Suppose that (6.72) does not hold.

In the case that $|I_i^0| \gg \varepsilon$, for $i = 1, 2$, the dominant part is $-\omega_i A_i \sin(\theta_i - \omega_i \tau_j^*)$. So, $\{F_i, -\mathcal{L}_j^*\} = 0$ only if $\sin(\theta_i - \omega_i \tau_j^*) = 0$, for $i = 1, 2$. This implies that, from (6.70), I_i is constant, for $i = 1, 2$. As F_i and I_i are constant, θ_i is also constant, $i = 1, 2$. Then, we can conclude that (I, θ) is an equilibrium point of $\mathcal{L}_j^*$. From Lemma 6.10, $I = (0, 0)$, a contradiction.

Now, consider the case that $|I_i| \gg \varepsilon$ and $I_l \approx \varepsilon$, for $i \neq l$. As we have seen before, I_i and θ_i are constant. This implies that we can reduce the scattering flow two to a 2D flow. The transversality relies on the same argument for the 2+1/2 d.o.f. case. [DH11, DS17] $\square$

Corollary 6.3. *The same proposition is valid for the scattering map, since the scattering map is the scattering flow plus a term of order $\mathcal{O}(\varepsilon^2)$ for ε small enough.*

6.8.7 Construction of diffusing paths

We are interested in finding a finite drift in the 2-dimensional variable I . In general, we expect to obtain an increment in the value of I by iterating the scattering map. Therefore, the points where the action variable I does not change under the action of the scattering map are useless for our mechanism. From Lemma 6.10 and Prop. 6.11, there are four points to avoid: $(0, 0, 0, 0)$, $(0, 0, \pi, 0)$, $(0, 0, 0, \pi)$ and $(0, 0, \pi, \pi)$ since they are equilibrium points of all scattering flows and inner dynamics.

As we are assuming μ_1, μ_2 such that $|\mu_1| + |\mu_2| < 0.625$, we find that all surfaces $C_j(I)$ are horizontal for any value of I and are transversally intersected by $R(I, \varphi, s)$, see Corollary 6.1. Therefore, $\tau_j^*(I, \theta)$ is always defined, see the proof of Corollary 6.2, and we can introduce a new variable:

$$\psi_j := \theta - \tau_j^*(I, \theta)\omega. \quad (6.73)$$

By (6.62), (6.67) and (6.68)

$$s - \tau_j^*(I\varphi, s) = \xi_j(I, \varphi - \tau_j^*(I, \varphi, s)\omega)$$

By (6.53) and (6.56)

$$-\tau_j^*(I, \theta) = \xi_j(I, \theta - \tau_j^*(I, \theta)\omega).$$

This immediately implies that ψ has a well-defined inverse function

$$\theta = \psi - \xi_j(I, \psi_j)\omega.$$

This variable will be helpful in the proof of the following theorem.

6.9 Global Instability

Theorem 6.7. *Consider the Hamiltonian (6.43)+(6.44). Assume $a_1 a_2 a_3 \neq 0$ and $|a_1/a_3| + |a_2/a_3| < 0.625$. Then, for every $0 < \delta < 1$ and $R > 0$, there exists $\varepsilon_0 = \varepsilon_0(\delta, R) > 0$ such that for every I_+, I_- satisfying $|I_{\pm}| < R$, there exists an orbit $\tilde{x}(t)$ and $T > 0$, such that*

$$\begin{aligned} |I(\tilde{x}(0)) - I_-| &\leq C\delta \\ |I(\tilde{x}(T)) - I_+| &\leq C\delta \end{aligned}$$

Proof. Actually, we are going to prove that given I_-, I_+ and a curve $\gamma : [0, t_f] \rightarrow \mathbb{R}^2$, such that $\gamma(0) = I_-$ and $\gamma(t_f) = I_+$, there exists an orbit $\tilde{x}(t)$ of the Hamiltonian system given by (6.43)+(6.44) satisfying

$$|I(\tilde{x}(t)) - \gamma(\alpha(t))| \leq C\delta, \quad t \in [0, t_f]. \quad (6.74)$$

Our strategy will be to use iterations of the inner and scattering maps to construct a pseudo-orbit δ -close to γ . Later, we will apply shadowing lemmas to ensure the existence of a real diffusing orbit in which condition (6.74) is satisfied.

Consider first the case that γ is a horizontal segment in the plane (I_1, I_2) , so that $I_{-2} = I_{+2}$, where $v_2 = \partial_{\theta_2} \mathcal{L}^*(I, \theta)$ does not vanish. Given $\delta < l(\gamma)$, where $l(\gamma)$ is the length of γ , we define $N := \left\lfloor \frac{l(\gamma)}{\delta} \right\rfloor$ and take the finite open cover of the image of the curve γ given by

$$\bigcup_{i=0}^N B_\delta(\gamma(t_i)),$$

where $B_\delta(\gamma(t_i)) = \{p \in \mathbb{R}^2 : \|\gamma(t_i) - p\|_\infty < \delta\}$ and $t_0 = 0$.

Let $I^i \in B_\delta(\gamma(t_i)) \setminus B_\delta(\gamma(t_{i+1}))$. Applying the scattering map, we want to obtain a $I^j \in B_\delta(\gamma(t_{i+1}))$. From now on, we denote by I^k the values of I obtained by the k th iteration under the scattering map $\mathcal{S}$. We should ensure $I^k \in B_\delta(\gamma(t_i)) \cup B_\delta(\gamma(t_{i+1}))$ for $k \in \{1, \dots, j\}$. Recall that the scattering map can be written as

$$\mathcal{S}(I, \theta)^T = (I, \theta)^T + \varepsilon J \nabla \mathcal{L}^*(I, \theta)^T + \mathcal{O}(\varepsilon^2),$$

where J is the symplectic matrix, and the term $\mathcal{O}(\varepsilon^2)$ can be bounded by $\varepsilon^2 M$, for some constant M depending just on R . Therefore, defining the vector $u^i = \gamma(t_{i+1}) - I^i$, we have to obtain a θ^* such that

$$u_j^i \partial_{\theta_j} \mathcal{L}^*(I^i, \theta^*) > 0, \quad \text{for } j = \{1, 2\}, \quad (6.75)$$

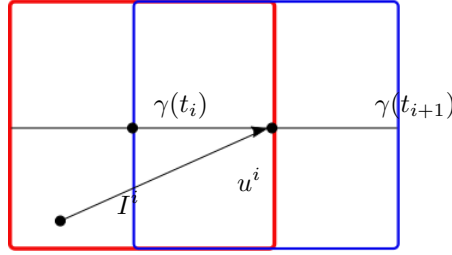
where $\partial_{\theta_j} \mathcal{L}^*(I, \theta) = -A_j \sin(\theta_j - \omega_j \tau^*(I, \theta))$ with A_j defined in (6.50), see Fig. 6.24. Assuming $a_1, a_2 > 0$, (6.75) is satisfied if and only if $\theta^* - \tau^*(I^i, \theta^*)\omega^i \in (\pi, 2\pi)^2$.

If for initial values (I^i, θ^i) , $\theta^i - \tau^*(I^i, \theta^i)\omega_i \notin (\pi, 2\pi)^2$, we need to use inner dynamics to displace θ^i to a point θ^* such that

$$\psi^* := \theta^* - \tau^*(I^i, \tau^*)\omega^i \in (\pi, 2\pi)^2.$$

The inner dynamics is very simple, and we can assume that it is approximately horizontal for finite time[DS17], i.e., it is described by the equations

$$\dot{I}_j = 0 \quad \text{and} \quad \dot{\varphi}_j = \omega_j, \quad j = 1, 2.$$

Figure 6.24: $\partial B_\delta(\gamma(t_i))$ in red and $\partial B_\delta(\gamma(t_{i+1}))$ in blue.

Therefore, $\varphi(t) = \omega t + \varphi(0)$. Then, the existence of θ^* is equivalent to the existence of t^* satisfying

$$\theta(t^*) - \tau^*(I^i, \theta(t^*))\omega^i \in (\pi, 2\pi)^2,$$

where $\theta(t) = \theta^i + t\omega^i$. Define

$$\psi(t) = \theta^i(t) - \tau^*(I^i, \theta^i(t))\omega^i.$$

Assume $\omega_1^i \geq \omega_2^i$ without loss of generality, and as we can choose the initial point with a δ -error, we can take $I_1^i, I_2^i \neq 0$. We can write

$$\psi_2 = \frac{\omega_2^i}{\omega_1^i} \psi_1 + \psi_0, \quad \psi_0 := \theta_2^i - \omega_2^i \theta_1^i / \omega_1^i. \quad (6.76)$$

For $\omega_2^i/\omega_1^i \in \mathbb{R} \setminus \mathbb{Q}$, $(\psi_1, \psi_2(\psi_1))$ is dense in $\mathbb{T}^2$, then there exists a t^* such that $(\psi_1(t^*), \psi_2(t^*)) \in (\pi, 2\pi)^2$.

For $\omega_2^i/\omega_1^i = p/q \in \mathbb{Q}$, consider $qp > 0$, the other case is analogous. This implies $0 < p/q \leq 1$.

We fix $\psi_1 = 2\pi l$, $l \in \mathbb{Z}$. For these values of ψ_1, ψ_2 in (6.76) can be rewritten as

$$\psi_2(l) = r_l(\psi_0) = 2\pi \left(\frac{p}{q} \right) l + \psi_0.$$

Note that ψ_2 is equivalent to a rotation of ψ_0 by the angle $2\pi p/q$ on S^1 . As $r_l(\psi_0)$ is a q -periodic function, an orbit $\mathcal{O} = \{\psi_0, \dots, r_{q-1}(\psi_0)\}$ is an equidistant cover of S^1 . Therefore, if $q \neq 1$ or $\psi_0 \neq \pi$, there exists $l' \in \{0, \dots, q-1\}$ such that $r_{l'}(\psi_0) \in (\pi, 2\pi)$. This immediately implies that $(\psi_1, \psi_2(\psi_1))$ intersects $(\pi, 2\pi)^2$.

For $q = 1$ and $\psi_0 = \pi$, then $\omega_1^i = \omega_2^i$ and it is easy to verify that $(\psi_1, \psi_2(\psi_1))$ does not intersect $(\pi, 2\pi)^2$. Therefore, in this specific case, the inner dynamics is not enough for our purpose. So, here our strategy is slightly different. We will use the scattering map in a similar way to the inner map: to change the values of θ while the value of I remains almost fixed.

First, we apply the inner dynamics up to $\psi_1 = 0$. From (6.76), this implies $\psi_2 = \pi$. For these values, we have $I = 0$. From Prop. 6.11, when we apply the scattering map on this point, its image is on another torus of the inner dynamics. As the values of the variable I remain fixed up to $\mathcal{O}(\varepsilon^2)$, we can consider that these values are within $B_\delta(\gamma(t_i))$. Out of this problematic torus, we can apply the algorithm developed previously.

Now we want to prove that I^k is δ -close to the curve γ for any $k \in \{1, \dots, j\}$. We have

$$I^k = I^{k-1} + \varepsilon \partial_\theta \mathcal{L}^*(I^{k-1}, \theta^{k-1}) + \mathcal{O}(\varepsilon^2). \quad (6.77)$$

So, I^k is δ -close to γ if the following condition is satisfied.

$$|I_2^k - \gamma_2(t_{i+1})| \leq \delta.$$

If we assume $I_2^{k-1} \leq \gamma_2(t_{i+1})$, we only need to verify $I_2^k \leq \gamma_2(t_{i+1}) + \delta$.

From (6.77) and if we consider only the terms of the first order, the condition is equivalent to

$$\varepsilon < \frac{\gamma_2(t_i) - I_2^k + \delta}{v_2^k - \varepsilon M}.$$

Note that $\gamma_2(t_i) - I_2^k < \delta$, then the numerator is positive. In addition, $v_2^k \geq m_2(\gamma)$, the minimum value of $|v_2|$ along the curve γ , so it is enough to require $\varepsilon < m_2(\gamma)/(2M)$, as well as

$$\varepsilon < 2 \frac{\gamma_2(t_i) - I_2^k + \delta}{m_2(\gamma)}. \quad (6.78)$$

Define $\varepsilon_i = \sup \left\{ \varepsilon : \varepsilon < \frac{\gamma_2(t_i) - I_2^i + \delta}{m_2(\gamma)} \right\}$, we obtain that for any $0 < \varepsilon \leq \varepsilon_i$, I^k is δ -close to γ .

For $u_2 \leq 0$, (6.78) takes the form

$$\varepsilon < 2 \frac{I_2^k - \gamma_2(t_i) + \delta}{m_2(\gamma)}.$$

Now we wish to obtain a similar result for any iterate of a scattering map. Introducing $m = \min_{|I| \leq R} v$, the result is true for $\varepsilon < 1/(2M)$ and

$$\varepsilon < \frac{2\delta}{m}.$$

That is, if we take $\varepsilon_0 = \min\{\frac{1}{2m}, \frac{2\delta}{m}\}$, for any $\varepsilon < \varepsilon_0$ we obtain a pseudo-orbit δ -close to γ .

For vertical lines, the same result can be stated *mutatis mutandis*.

The above argument holds for any γ that is δ -distant from the equilibrium point of scattering flow, see Lemma 6.10. If such condition it is not satisfied, it can be approximated by γ' that has a distance $\mathcal{O}(\delta/2)$ from γ close to those points.

For a more general case, that is, C^1 -curve $\gamma : [0, t^*] \rightarrow \mathbb{R}^2$ such that $\gamma(0) = I_-$, $\gamma(t^*) = I_+$, we take a staircase curve γ_{step} , a combination of horizontal and vertical lines, in such a way that γ_{step} is a good enough approximation of γ , where ‘good enough’ we mean, the result holds for γ applying the above results (for horizontal and vertical lines) for γ_{step} .

We can now apply shadowing techniques well adapted to NHIM [FM00, FM03, GLMS20], due to the fact that the inner dynamics is simple enough to satisfy the required hypothesis of these references, to ensure the existence of a diffusion trajectory. $\square$

6.9.1 Highways

The existence of a special invariant set of $-\mathcal{L}_0^*$, called *Highway*, was very useful for the study of the case with $2+1/2$ d.o.f.[DS17]. Iterations of a scattering map along a Highway were enough to obtain a large drift on the action variable I . Moreover, we estimated the time of diffusion of these orbits. We want to detect a similar invariant set for our $3+1/2$ model with the same goal in mind.

We define a Highway as an invariant set $\mathcal{H} = \{(I, \Theta(I))\}$ of the Hamiltonian given by the reduced Poincaré function $\mathcal{L}_0^*(I, \theta)$ which is contained in the level energy $\mathcal{L}_0^*(I, \theta) = A_3$. Therefore, it is a Lagrangian manifold, that is, $\Theta(I)$ is a gradient function, so there exists a function $F(I)$ such that $\Theta(I) = \nabla F(I)$. As Θ is a gradient function, it must satisfy the following condition.

$$\frac{\partial \Theta_1}{\partial I_2} = \frac{\partial \Theta_2}{\partial I_1}.$$

This condition is equivalent to

$$\frac{\partial^2 F}{\partial I_2 \partial I_1} = \frac{\partial^2 F}{\partial I_1 \partial I_2}.$$

Remark 6.28. We take the energy level $\mathcal{L}_0^*(I, \theta) = A_3$ because we have from (6.57) that

$$\lim_{(I_1, I_2) \rightarrow (\pm\infty, \pm\infty)} \mathcal{L}_0^*(I, \theta) = A_3.$$

In addition, $\mathcal{L}_0^*(0, 0, \pm\pi/2, \pm\pi/2) = A_3$. Therefore, the level surface $\mathcal{L}_0^*(I, \theta) = A_3$ is the unique connection possible of the origin of the plane (I_1, I_2) to arbitrarily large values of $|I_1|$ and $|I_2|$.

We start by proving the local existence of Highways for $I_1, I_2 \gg 0$.

Proposition 6.12 (Local existence of Highways). *Consider the Hamiltonian (6.43)+(6.44). Assume $a_1 a_2 a_3 \neq 0$ and $|a_1/a_3| + |a_2/a_3| < 0.625$. For $|I_1|$ and $|I_2|$ close to infinity, the function F takes the*

asymptotic form

$$\begin{aligned}
F(I) = & \frac{\pi}{2} (\pm I_1 \pm I_2) - \sum_{i=1}^2 \frac{2a_i \sinh(\pi/2)}{\pi^4 \Omega_i} \left(\pi^3 |\omega_i|^3 \right. \\
& \left. + 6\pi^2 \omega_i^2 + 24\pi |\omega_i| + 48 \right) e^{-\pi |\omega_i|/2} \\
& + \mathcal{O}(\omega_1^2 \omega_2^2 e^{-\pi(|\omega_1|+|\omega_2|)/2}),
\end{aligned} \tag{6.79}$$

Proof. Assume a candidate for a function $F(I)$ given by (6.79), such that $\Theta = \nabla F(I)$. We have four possible choices for the sign of the first order term of $F(I)$. To fix ideas, we choose $\frac{\pi}{2} (-I_1 - I_2)$ that is equivalent to $\frac{3\pi}{2} (I_1 + I_2)$. $\Theta(I)$ has to satisfy the energy level condition for Highways in the reduced Poincaré function

$$\begin{aligned}
& \sum_{k=1}^2 A_k \cos(\Theta_k - \omega_k \tau^*(I, \Theta)) \\
& + A_3 (\cos(-\tau^*(I, \Theta)) - 1) = 0,
\end{aligned} \tag{6.80}$$

and $\tau^*(I, \Theta)$ has to satisfy the equation of the crest

$$\begin{aligned}
& \sum_{k=1}^2 \omega_k A_k \sin(\Theta_k - \omega_k \tau^*(I, \Theta)) \\
& + A_3 \sin(-\tau^*(I, \Theta)) = 0.
\end{aligned} \tag{6.81}$$

We want to write their version for I_1 and I_2 close to infinity. Using (6.79) we notice that $\Theta_i = \Theta_i(I)$ takes the form

$$\Theta_i = \frac{3\pi}{2} - a_i \sinh(\pi/2) \omega_i^3 e^{\frac{-\pi \omega_i}{2}} + \mathcal{O}\left(\omega_1^2 \omega_2^2 e^{\frac{-\pi(\omega_1 + \omega_2)}{2}}\right).$$

This implies

$$\begin{aligned}
\cos(\Theta_i - \omega_i \tau^*) &= -a_i \sinh(\pi/2) \omega_i^3 e^{\frac{-\pi \omega_i}{2}} - \omega_i \tau_\infty^* \\
&+ \mathcal{O}\left(\omega_1^2 \omega_2^2 e^{\frac{-\pi(\omega_1 + \omega_2)}{2}}\right)
\end{aligned}$$

and

$$\sin(\Theta_i - \omega_i \tau^*) = -1 + \mathcal{O}(\omega_i^6 e^{-\pi \omega_i}),$$

In addition,

$$\begin{aligned}
\cos(-\tau^*(I, \Theta)) &= 1 - \frac{\tau_\infty^{*2}}{2} + \mathcal{O}(\tau_\infty^{*4}), \\
\sin(-\tau^*) &= -\tau_\infty^* + \mathcal{O}(\tau_\infty^*),
\end{aligned}$$

where τ_∞^* is an asymptotic approximation of τ^* that we will estimate in the following. First, we notice that functions A_1 and A_2 can be approximated by

$$\begin{aligned}
A_i &= 4\pi a_i \omega_i e^{\frac{-\pi \omega_i}{2}} \left(1 + e^{-2\pi \omega_i} + \dots \right) \\
&= 4\pi a_i \omega_i e^{\frac{-\pi \omega_i}{2}} + \mathcal{O}\left(\omega_i e^{\frac{-5\pi \omega_i}{2}}\right).
\end{aligned}$$

From (6.62), the function $\tau^*(I, \Theta)$ satisfies

$$-\tau^*(I, \Theta) = -\arcsin \left(\sum_{k=1}^2 \frac{A_k \omega_k}{A_3} \sin(\Theta_k - \omega_k \tau^*(I, \Theta)) \right),$$

and therefore,

$$\tau_\infty^* = \sum_{i=1}^2 -2a_i \sinh(\pi/2) \omega_i^2 e^{\frac{-\pi \omega_i}{2}} + \mathcal{O}\left(\omega_i e^{\frac{-5\pi \omega_i}{2}}\right).$$

Applying these estimates in Eq. (6.80) we obtain that the left-hand side of Eq. (6.80) satisfies

$$\begin{aligned} & \sum_{i=1}^2 \left\{ 4\pi a_i \omega_i e^{-\pi \omega_1/2} \left[-a_i \sinh(\pi/2) \omega_i^3 e^{-\pi \omega_i/2} \right. \right. \\ & \quad \left. \left. - \omega_i \left(\sum_{k=1}^2 2a_k \sinh(\pi/2) \omega_k^2 e^{-\pi \omega_k/2} \right) \right] \right\} \\ & - \frac{A_3}{2} \left(\sum_{i=1}^2 2a_i \sinh(\pi/2) \omega_i^2 e^{-\pi \omega_i/2} \right)^2 \\ & + \mathcal{O}(\omega_1^2 \omega_2^2 e^{-\pi(\omega_1+\omega_2)/2}) = \mathcal{O}(\omega_1^2 \omega_2^2 e^{-\pi(\omega_1+\omega_2)/2}). \end{aligned}$$

In the same way, by applying in Eq. (6.81) the estimates obtained, we have that the left-hand side of Eq. (6.81) satisfies

$$\begin{aligned} & - \sum_{i=1}^2 4\pi a_i \omega_i^2 e^{-\frac{\pi \omega_i}{2}} + A_3 \left(\sum_{i=1}^2 2a_i \sinh(\pi/2) \omega_i^2 e^{-\frac{\pi \omega_i}{2}} \right) \\ & + \mathcal{O}(\omega_1^2 \omega_2^2 e^{-\pi(\omega_1+\omega_2)/2}) = \mathcal{O}(\omega_1^2 \omega_2^2 e^{-\pi(\omega_1+\omega_2)/2}). \end{aligned}$$

Therefore, up to the order $\mathcal{O}(\omega_1^2 \omega_2^2 e^{-\pi(\omega_1+\omega_2)/2})$, the equation of the crest and the energy level of the reduced Poincaré function are satisfied. $\square$

So far, we could ensure the existence of Highways for some specific values of I . However, in the exceptional case $a_1 = a_2$, $\Omega_1 = \Omega_2$, we can completely describe them and thus we can easily construct an explicit diffusing pseudo-orbit.

Proposition 6.13 (Global explicit expression of Highways in a special case). *Consider the Hamiltonian (6.43)+(6.44) and $a_1 = a_2$ satisfying $2|a/a_3| < 0.625$ and $\Omega_1 = \Omega_2$. Let $\phi_t^{-\mathcal{L}_0^*}(I^0, \Theta(I^0))$ be a scattering flow on a Highway such that $I_1^0 = I_2^0$ and $\theta_1^0 = \theta_2^0$. Then, $I_1(t) = I_2(t) = \bar{I}(t)$ and $\theta_1(t) = \theta_2(t) = \bar{\theta}(t)$ for all $t \in \mathbb{R}$ and can be described by*

$$\bar{\theta}_h(\bar{I}) = \begin{cases} \arccos\left(\frac{(1-f(\bar{I}))A_3}{A}\right) + \bar{\omega} \arccos(f(\bar{I})); \\ \arccos\left(\frac{(1-f(\bar{I}))A_3}{A}\right) - \bar{\omega} \arccos(f(\bar{I})); \end{cases}$$

for $\bar{I} \leq 0$ and $\bar{I} > 0$, respectively, or

$$\bar{\theta}_H(\bar{I}) = \begin{cases} -\arccos\left(\frac{(1-f(\bar{I}))A_3}{A}\right) - \bar{\omega} \arccos(f(\bar{I})); \\ -\arccos\left(\frac{(1-f(\bar{I}))A_3}{A}\right) + \bar{\omega} \arccos(f(\bar{I})); \end{cases},$$

for $\bar{I} \leq 0$ and $\bar{I} > 0$, respectively, where $A := 2A_1 = 2A_2$ and

$$f(\bar{I}) := \begin{cases} 1 - \frac{A}{2A_3^2}, & \bar{\omega} = \pm 1 \\ \frac{\bar{\omega}^2 A_3 - \sqrt{A_3^2 + (\bar{\omega}^2 - 1)\bar{\omega}^2 A^2}}{(\bar{\omega}^2 - 1)A_3} & \bar{\omega} \neq \pm 1. \end{cases}$$

Proof. Consider the scattering flow $\phi_t^{-\mathcal{L}_0^*}(I^0, \theta^0)$ defined by the differential equations in (6.70). Assuming $\Omega_1 = \Omega_2 =: \Omega$ and $a_1 = a_2 =: a$ and taking the initial conditions satisfying $I(0) = I^0$ and $\theta(0) = \theta^0$ where $I_1^0 = I_2^0$ and $\theta_1^0 = \theta_2^0$, the solution $(I(t), \theta(t))$ of (6.70) satisfies $\theta_1(t) = \theta_2(t) =: \bar{\theta}(t)$ and $I_1(t) = I_2(t) =: \bar{I}(t)$ for all t .

If the flow $\phi_t^{-\mathcal{L}_0^*}(I^0, \theta^0)$ lies on a Highway, it has to satisfy two equations: the equation of the crests given in (6.61) and

$$\mathcal{L}_0^*(I, \theta) = A_3.$$

These equations can be rewritten as

$$\begin{aligned} A \cos(\bar{\theta} - \bar{\omega} \tau^*(\bar{I}, \bar{\theta})) + A_3 \cos(-\tau^*(\bar{I}, \bar{\theta})) &= A_3 \\ \bar{\omega} A \sin(\bar{\theta} - \bar{\omega} \tau^*(\bar{I}, \bar{\theta})) + A_3 \sin(-\tau^*(\bar{I}, \bar{\theta})) &= 0, \end{aligned} \tag{6.82}$$

where $\bar{\omega} := \omega_1 = \omega_2$ and $A := A(\bar{\omega}) = 4\pi\bar{\omega}a / \sinh(\pi\bar{\omega}/2)$ for $\bar{\omega} \neq 0$ and $A = 8a$.

Multiplying by $\bar{\omega}$ the first equation in (6.82) we obtain

$$\begin{aligned}\bar{\omega}A \cos(\bar{\theta} - \bar{\omega}\tau^*(\bar{I}, \bar{\theta})) &= -\bar{\omega}A_3 (\cos(-\tau^*(\bar{I}, \bar{\theta})) - 1) \\ \bar{\omega}A \sin(\bar{\theta} - \bar{\omega}\tau^*(\bar{I}, \bar{\theta})) &= -A_3 \sin(-\tau^*(\bar{I}, \bar{\theta})).\end{aligned}$$

We sum these two equations squared and we obtain

$$\bar{\omega}^2 A^2 = \left[\bar{\omega}A_3 (\cos(-\tau^*(\bar{I}, \bar{\theta})) - 1) \right]^2 + A^2 \sin^2(-\tau^*(\bar{I}, \bar{\theta})).$$

After some arithmetical manipulations, we obtain the following equation of second degree in the variable $\cos(-\tau^*(\bar{I}, \bar{\theta}))$

$$(\bar{\omega}^2 - 1)A_3^2 \cos^2(-\tau^*(\bar{I}, \bar{\theta})) - 2\bar{\omega}^2 A_3^2 \cos(-\tau^*(\bar{I}, \bar{\theta})) + A_3^2(\bar{\omega}^2 + 1) - \bar{\omega}^2 A^2 = 0.$$

For $\bar{\omega} = \pm 1$, we have

$$\cos(-\tau^*(\bar{I}, \bar{\theta})) = 1 - \frac{A}{2A_3^2}.$$

Otherwise,

$$\cos(-\tau^*(\bar{I}, \bar{\theta})) = \frac{2\bar{\omega}^2 A_3^2 \pm \sqrt{4\bar{\omega}^4 A_3^4 - 4(\bar{\omega}^2 - 1)A_3^2 [A_3^2(\bar{\omega}^2 + 1) - \bar{\omega}^2 A^2]}}{2(\bar{\omega}^2 - 1)A_3^2}.$$

After more arithmetical manipulation and considering $-1 \leq \cos(-\tau^*(\bar{I}, \bar{\theta})) \leq 1$, we have

$$\cos(-\tau^*(\bar{I}, \bar{\theta})) = \frac{\bar{\omega}^2 A_3 - \sqrt{A_3^2 + (\bar{\omega}^2 - 1)\bar{\omega}^2 A^2}}{(\bar{\omega}^2 - 1)A_3}.$$

To simplify the notation, we define

$$f(\bar{I}) := \begin{cases} 1 - \frac{A}{2A_3^2}, & \bar{\omega} = \pm 1 \\ \frac{\bar{\omega}^2 A_3 - \sqrt{A_3^2 + (\bar{\omega}^2 - 1)\bar{\omega}^2 A^2}}{(\bar{\omega}^2 - 1)A_3} & \bar{\omega} \neq \pm 1. \end{cases}$$

And therefore,

$$\Rightarrow -\tau^*(\bar{I}, \bar{\theta}) = \pm \arccos(f(\bar{I})).$$

We have two Highways. This explains why we have found two different values for the function τ^* . Then we can rewrite the first equation of (6.82) as follows.

$$A \cos(\bar{\theta} \pm \bar{\omega} \arccos(f(\bar{I}))) + A_3 f(\bar{I}) = A_3$$

This immediately implies

$$\bar{\theta} = \pm \arccos\left(\frac{A_3(1 - f(\bar{I}))}{A}\right) \mp \bar{\omega} \arccos(f(\bar{I})).$$

From the four possibilities, by comparing with numerical results, we obtain that the Highways are described by

$$\bar{\theta}_h(\bar{I}) = \begin{cases} \arccos\left(\frac{A_3(1 - f(\bar{I}))}{A}\right) + \bar{\omega} \arccos(f(\bar{I})); \\ \arccos\left(\frac{A_3(1 - f(\bar{I}))}{A}\right) - \bar{\omega} \arccos(f(\bar{I})); \end{cases}$$

for $\bar{I} \leq 0$ and $\bar{I} > 0$, respectively, and

$$\bar{\theta}_H(\bar{I}) = \begin{cases} -\arccos\left(\frac{A_3(1 - f(\bar{I}))}{A}\right) - \bar{\omega} \arccos(f(\bar{I})), ; \\ -\arccos\left(\frac{A_3(1 - f(\bar{I}))}{A}\right) + \bar{\omega} \arccos(f(\bar{I})); \end{cases}$$

for $\bar{I} \leq 0$ and $\bar{I} > 0$, respectively. □

Remark 6.29. A very similar result was proved for 2+1/2 d.o.f.[GS18].

Note that since an orbit on a Highway has the form $(I, \Theta(I))$, we have

$$\dot{\Theta} = D\Theta(I)\dot{I}.$$

Therefore, $\dot{I} = 0$ implies $\dot{\Theta} = 0$. Thus, an equilibrium point in the plane (I_1, I_2) is related to an equilibrium point of the scattering flow. From Prop. 6.10, we know that the scattering flow has only four equilibrium points. However, none of them lie on a Highway since $\mathcal{L}_0^*(\mathbf{p}) \neq A_3$, $\mathbf{p} = (0, 0, 0, 0)$, $(0, 0, \pi, \pi)$, $(0, 0, \pi, 0)$ and $(0, 0, 0, \pi)$. We can conclude that there are no equilibrium points for Highways on (I_1, I_2) .

Theorem 6.14 (Global Existence of Highways). *Assume $a_1 a_2 a_3 \neq 0$ and $|a_1/a_3| + |a_2/a_3| < 0.625$ in Hamiltonian (6.43)+(6.44). Inside a Highway there are no orbits that are contained in a compact set on the plane (I_1, I_2) . In particular, given any $0 < c < C$, there exists an orbit of the scattering flow $\phi_t^{-\mathcal{L}_i^*}(I, \theta)$ on a Highway and a time t^* such that*

$$|I(t_0)| < c \quad \text{and} \quad |I(t^*)| > C.$$

Proof. Suppose by contradiction that there is an orbit $(\gamma, \Theta(\gamma))$ on a Highway that is contained in a compact set on the plane (I_1, I_2) . This implies that its ω -limit set $w(\gamma)$ on this plane is nonempty. Since there are no equilibrium points on (I_1, I_2) , $w(\gamma)$ is formed by regular points. From the Poincaré-Bendixson theorem, γ is a periodic orbit. However, this immediately implies an equilibrium point in the interior of γ , a contradiction. Observing that $(0, 0, \pm\pi/2, \pm\pi/2)$ belongs to a Highway, the theorem is proved for any $c > 0$. $\square$

As an immediate consequence, we can ensure that the orbits are diffusing along a Highway.

Corollary 6.4. *Assume $a_1 a_2 a_3 \neq 0$ and $|a_1/a_3| + |a_2/a_3| < 0.625$ in Hamiltonian (6.43)+(6.44). Given any $0 < c_j < C_j$, $j = 1, 2$, there is at least an orbit $(I^i, \theta^i)_{0 \leq i < N}$ of the scattering map $\mathcal{S}_0$ such that*

$$|I_j^0| < c_j \quad \text{and} \quad |I_j^N| > C_j, \quad j = 1, 2.$$

The following result shows that the orbits on a Highway do not wander along the plane (I_1, I_2) . Indeed, they have an explicit asymptotic behavior, as we can see in Fig. 6.25.

Proposition 6.15. *Assume $a_1 a_2 a_3 \neq 0$ and $|a_1/a_3| + |a_2/a_3| < 0.625$ in Hamiltonian (6.43)+(6.44). Let $(I^h, \Theta(I^h))$ be a Highway. For $I_2, I_1 \gg 1$, we have*

$$I_2^h = \frac{\Omega_1}{\Omega_2} I_1^h - \frac{2}{\pi \Omega_2} \log \left(\frac{\Omega_1 a_1}{\Omega_2 a_2} \right) + \mathcal{O}(1/\omega_1),$$

and for $I_2, I_1 \ll -1$,

$$I_2^h = \frac{\Omega_1}{\Omega_2} I_1^h + \frac{2}{\pi \Omega_2} \log \left(\frac{\Omega_1 a_1}{\Omega_2 a_2} \right) + \mathcal{O}(1/\omega_1),$$

Proof. Since $\dot{I}_i = -A_i \sin(\theta_i - \omega_i \tau^*)$ and $\omega_i = \Omega_i I_i$, we have

$$\frac{d\omega_2}{d\omega_1} = \frac{\Omega_2 A_2 \sin(\theta_2 - \omega_2 \tau^*)}{\Omega_1 A_1 \sin(\theta_1 - \omega_1 \tau^*)}.$$

For $I_1, I_2 \gg 1$, the above equation becomes

$$\begin{aligned} \frac{d\omega_2}{d\omega_1} &= \frac{4\pi a_2 \Omega_2 \omega_2 \exp(-\pi\omega_2/2) + \mathcal{O}(w_2 \exp(-5\pi\omega_2/2))}{4\pi a_1 \Omega_1 \omega_1 \exp(-\pi\omega_1/2) + \mathcal{O}(w_1 \exp(-5\pi\omega_1/2))} \\ &= \frac{a_2 \Omega_2 \omega_2 \exp(-\pi\omega_2/2) + \mathcal{O}(w_2 \exp(-5\pi\omega_2/2))}{a_1 \Omega_1 \omega_1 \exp(-\pi\omega_1/2) + \mathcal{O}(w_1 \exp(-5\pi\omega_1/2))}, \end{aligned}$$

so that separating variables, we get

$$\begin{aligned} \frac{1}{a_2 \Omega_2} \int \frac{\exp(\pi\omega_2/2) d\omega_2}{\omega_2} + \mathcal{O} \left(\frac{\exp\left(\frac{5\pi\omega_2}{2}\right)}{\omega_2^2} \right) &= \\ \frac{1}{a_1 \Omega_1} \int \frac{\exp(\pi\omega_1/2) d\omega_1}{\omega_1} + \mathcal{O} \left(\frac{\exp\left(\frac{5\pi\omega_1}{2}\right)}{\omega_1^2} \right), & \end{aligned}$$

which can be also written as

$$\frac{\exp(\pi\omega_2/2)}{a_2\Omega_2\pi\omega_2} + \mathcal{O}(\omega_2^{-2}\exp(\pi\omega_2/2)) = \frac{\exp(\pi\omega_1/2)}{a_1\Omega_1\pi\omega_1} + \mathcal{O}(\omega_1^{-2}\exp(\pi\omega_1/2)) + c_0. \quad (6.83)$$

Assume that ω_2 takes the form $\omega_2 = \omega_1 + g(\omega_1)$. Plugging this formula into Eq. (6.83), we obtain

$$\frac{\exp(\pi g(\omega_1)/2)}{a_2\Omega_2(\omega_1 + g(\omega_1))} + \mathcal{O}\left(\frac{\exp(\pi g(\omega_1)/2)}{(\omega_1 + g(\omega_1))^2}\right) = \frac{1}{a_1\Omega_1\omega_1} + \frac{c_0}{\exp(\pi\omega_1/2)} + \mathcal{O}(\omega_1^{-2}).$$

As we assume that ω_1 is large, the term with ω_1^{-2} dominates the term with $\exp(-\pi\omega_1)$. Therefore,

$$\exp(\pi g(\omega_1)/2) = \left(\frac{a_2\Omega_2}{a_1\Omega_1}\right) \left(1 + \frac{g(\omega_1)}{\omega_1}\right) + \mathcal{O}(\omega_1^{-1}). \quad (6.84)$$

By solving Eq. (6.84), the function g takes the following form.

$$g(\omega_1) = \frac{-2}{\pi} W_n \left(\frac{-\pi a_1 \Omega_1 \omega_1}{2 a_2 \Omega_2} \exp(-\pi\omega_1/2) \right) - \omega_1 + \mathcal{O}(\omega_1^{-1}),$$

where $n \in \mathbb{Z}$ and W_n is the Lambert W function[CGH⁺96]. The Lambert W function can be written both around $z = 0$ and $z \rightarrow \infty$ as[CGH⁺96]

$$W_n(z) = \text{Log}(z) - \log \text{Log}(z) + \sum_{n=0}^{\infty} \sum_{m=1}^{\infty} c_{nm} (\log \text{Log}(z))^m (\text{Log}(z))^{-n-m}, \quad (6.85)$$

where the coefficients c_{nm} can be found using the Lagrange Inverse Theorem, $\text{Log}(z)$ is the complex logarithm for any no-principal branch, and $\log(z)$ is the complex logarithm for the principal branch. As we are working with real numbers, Eq. (6.85) implies that the function g is

$$g(\omega_1) = \frac{-2}{\pi} \left(\log \left(\frac{\pi}{2} \left| \frac{a_1 \Omega_1}{a_2 \Omega_2} \right| \omega_1 \exp \left(-\frac{\pi\omega_1}{2} \right) \right) - \log \left| \log \left(\frac{\pi}{2} \left| \frac{a_1 \Omega_1}{a_2 \Omega_2} \right| \omega_1 \exp \left(-\frac{\pi\omega_1}{2} \right) \right) \right| + \mathcal{O} \right) - \omega_1 + \mathcal{O},$$

where $\mathcal{O} = \mathcal{O}(1/\omega_1)$. After some algebraic manipulations, the function g becomes

$$g(\omega_1) = \frac{-2}{\pi} \left(\log \left(\frac{\pi}{2} \left| \frac{a_1 \Omega_1 \omega_1}{a_2 \Omega_2} \right| \right) - \log \left| \left(\log \left(\frac{\pi}{2} \left| \frac{a_1 \Omega_1 \omega_1}{a_2 \Omega_2} \right| \right) - \pi\omega_1/2 \right) \right| \right) + \mathcal{O} \left(\frac{1}{\omega} \right).$$

We conclude that

$$\lim_{\omega_1 \rightarrow \infty} g(\omega_1) = \frac{2}{\pi} \log \left(\left| \frac{a_2 \Omega_2}{a_1 \Omega_1} \right| \right) + \mathcal{O} \left(\frac{1}{\omega} \right).$$

For $\omega_2, \omega_1 \ll -1$ is analogous.

□

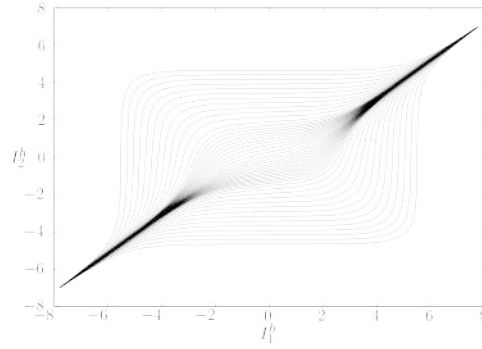


Figure 6.25: Dynamics inside the Highway. Parameter values are $a_1 = 0.3$, $a_2 = 0.1$, $a_3 = 1$ and $\Omega_1 = \Omega_2 = 1$.

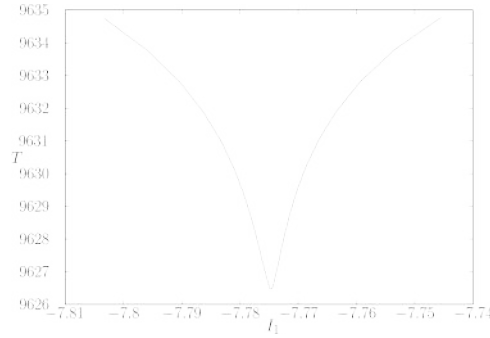


Figure 6.26: Times taken by trajectories in Fig. 6.25 to reach the section $I_2 = 7$ from section $I_2 = -7$.

In Figure 6.25, we simulate the dynamics of the scattering flow restricted to a Highway. This simulation is carried out by taking initial conditions along the sections given by $I_2 = 7$ and $I_2 = -7$ (varying I_1) and integrating backward and forward (respectively) so that the trajectories match at $I_2 = 0$. The initial angles θ_1 and θ_2 are taken by Equation (6.79). Note that for large values of I , the dynamics inside the Highway is given by the straight lines given in Prop. 6.15.

In Figure 6.26 we show the times taken by these trajectories to travel from section $I_2 = -7$ to section $I_2 = 7$. We can see that some orbits are faster than others; however, the difference in time is not quite significant.

Remark 6.30. Fig.6.25 was made in C++ by numerical integration of (28). The numerical method used is Runge-Kutta-Fehlberg (RKF78) with automatic step size control.

6.9.2 The time of diffusion

We have two different types of time to estimate: the time of the scattering flow associated to the Hamiltonian $-\mathcal{L}_0^*(I, \theta)$ and the time along the homoclinic manifold to the NHIM $\tilde{\Lambda}$. We will estimate this time only for orbits close to a Highway $(I, \Theta(I))$. Recall that along the Highways, for large I we can write I_2 asymptotically as a function of I_1 , that is, there exists a function f such that $I_2 = f(I_1)$. Therefore, a diffusion from I_1^0 to I_1^f , both in J , immediately implies a diffusion from $I_2(I_1^0)$ to $I_2(I_1^f)$. This implies that we only need to study the time for the flow related to the differential equation for I_1 .

The time of diffusion of an orbit close to a pseudoorbit built via iterates of scattering maps is estimated to be:

$$T_d = N_s T_h + C_s T_i,$$

where:

- N_s is the total number of iterates under scattering map. It is estimated by T_s/ε , where T_s is the time that the scattering flow spends going through ΔI . This comes from the fact that the scattering map jumps $\mathcal{O}(\varepsilon)$ along the level surfaces of $\mathcal{L}_0^*(I, \theta)$.

- T_h is the time under the flow along the homoclinic invariant manifolds of $\tilde{\Lambda}_\varepsilon$. This is the time spent by each application of the scattering map following the concrete homoclinic orbit to $\tilde{\Lambda}_\varepsilon$.
- C_s is the number of times that we need to apply the inner map to control the accumulated error, see Remark 6.27.
- T_i is the time under the inner map. This time appears if we use the inner map between iterates of the scattering map (it is sometimes called ergodization time).

We can refer to $N_s T_h$ as the time under scattering maps or simply *outer time*, and to $C_s T_i$ as the time under the inner map, or simply *inner time*. In the following theorem, we will prove that the outer time is much larger than the inner time: $N_s T_h \gg C_s T_i$, for orbits close to Highways. Hence, we prove that $T_d \approx N_s T_h$.

Theorem 6.16. *The time of diffusion T_d close to a Highway of Hamiltonian (6.43)+(6.44) with $|a_1/a_3| + |a_2/a_3| < 0.625$ between I_1^0 and I_1^f satisfies the following asymptotic expression.*

$$T_d = \frac{T_s}{\varepsilon} \left[2 \log \left(\frac{C}{\varepsilon} \right) + \mathcal{O}(\varepsilon^b) \right], \quad (6.86)$$

for $\varepsilon \rightarrow 0$, where $0 < b < 1$, with

$$T_s = \frac{1}{2\pi a_1 \Omega_1} \int_{\omega_0}^{\omega_f} \frac{-\sinh(\pi\omega_1/2)d\omega_1}{\omega_1 \sin(\theta_1 - \omega_1 \tau^*)}, \quad (6.87)$$

where $\omega_0 = \Omega_1 I_1^0$ and $\omega_f = \Omega_1 I_1^f$, and

$$C = 16 \left(|a_1| + \sum_{k=1}^2 \frac{2|a_3 \mu_k| \sinh(\pi/2) |\mu_1|}{\pi [1 - 1.466(|\mu_1| + |\mu_2|)]} M(\omega_k) \right).$$

where $\alpha(\omega_i)$ was given in (6.63), $\mu_i = a_i/a_3$ and $M(\omega_i) = \max_{I_i \in [I_i^0, I_i^f]} |\omega_i - \alpha(\omega_i)|$.

Proof. We estimate the time of diffusion to be

$$T_d \approx T_s T_h / \varepsilon,$$

where T_s is the time under the scattering flow on the Highway and T_h is the time along the homoclinic manifolds to $\tilde{\Lambda}$. We begin by studying T_s .

The differential equation for I_1 is given by

$$\frac{dI_1}{dt} = -A_1 \sin(\theta_1 - \omega_1 \tau^*),$$

where $\theta_1 = \Theta_1(I_1)$ and $\tau^* = \tau^*(I_1)$. Then, we have

$$T_s = \frac{1}{2\pi a_1 \Omega_1} \int_{\omega_0}^{\omega_f} \frac{-\sinh(\pi\omega_1/2)d\omega_1}{\omega_1 \sin(\theta_1 - \omega_1 \tau^*)},$$

where $\omega_0 = \Omega_1 I_1^0$ and $\omega_f = \Omega_1 I_1^f$.

A point $(p_\varepsilon(\tau), q_\varepsilon(\tau)) \in \bar{B}_\delta(0) \cap W_\varepsilon^{s,u}(0)$ lies on the perturbed separatrices on the plane (p, q) and is given by $(p_\varepsilon(\tau), q_\varepsilon(\tau)) = (p_0(\tau), q_0(\tau)) + \mathcal{O}(\varepsilon)$, where $(p_0(\tau), q_0(\tau)) = (2/\cosh \tau, 4 \arctan e^\tau)$. The point $(p_0(\tau), q_0(\tau))$ can be asymptotically approximated by

$$\begin{aligned} p_0(\tau) &= \frac{4}{e^{|\tau|}} \left(1 + \mathcal{O}(e^{-2|\tau|}) \right) \quad \text{and} \\ q_0(\tau) &= \mp \frac{4}{e^{|\tau|}} \left(1 + \mathcal{O}(e^{-2|\tau|}) \right) \quad \text{mod } 2\pi. \end{aligned}$$

Taking into account the starting and ending points on $\partial B_\delta(0, 0)$ and $\tau_f = -\tau_i$, we have

$$\frac{4\sqrt{2}}{e^u} \left(1 + \mathcal{O}(e^{-2u}) \right) = \delta.$$

where $u = |\tau_i|, |\tau_f|$. Therefore,

$$u = \log \left[\frac{4\sqrt{2}}{\delta} \left(1 + \mathcal{O}(\delta^2) \right) \right] = \log \left(\frac{4\sqrt{2}}{\delta} \right) + \mathcal{O}(\delta^2).$$

Then, the time along the homoclinic manifolds can be given by

$$T_h = 2 \log \left(\frac{4\sqrt{2}}{\delta} \right) + \mathcal{O}(\delta^2) + \mathcal{O}(\varepsilon), \quad (6.88)$$

where δ is the distance between the NHIM and the piece of the invariant manifold that we are using to calculate the time. Then, we have to estimate the value of δ , since it must be small enough to preserve the scattering map.

Recall that from $p^2/2 + \cos q - 1 = 0$ the Melnikov potential given in (6.49), can be written as

$$\begin{aligned} \mathcal{L}(I, \varphi, s) = & \int_{-\infty}^{+\infty} \frac{p^2(\sigma)}{2} \left(\sum_{k=1}^2 a_k \cos(\varphi_k + \omega_k \sigma) \right. \\ & \left. + a_3 \cos(s + \sigma) \right) d\sigma. \end{aligned}$$

This implies that the reduced Poincaré function (6.54) is

$$\begin{aligned} \mathcal{L}_0^*(I, \theta) = & \frac{1}{2} \int_{-\infty}^{+\infty} p^2(\sigma) \left(a_1 \cos(\theta_1 - \omega_1 \tau^* + \omega_1 \sigma) \right. \\ & \left. + a_2 \cos(\theta_2 - \omega_2 \tau^* + \omega_2 \sigma) + a_3 \cos(-\tau^* + \sigma) \right) d\sigma. \end{aligned}$$

As we are considering just a piece of the homoclinic invariant manifold δ -close to $\tilde{\Lambda}$, we are going to approximate the above integration by integrating for a finite interval of time $[t_0, t_f]$ in such a way that we have

$$\left| \frac{\partial \mathcal{L}_0^*}{\partial \theta_1} - \left(\frac{\partial \mathcal{L}_0^*}{\partial \theta_1} \right)_\delta \right| < \varepsilon, \quad (6.89)$$

where

$$\begin{aligned} \left(\frac{\partial \mathcal{L}_0^*}{\partial \theta_1} \right)_\delta = & \frac{1}{2} \int_{t_0}^{t_f} \frac{\partial}{\partial \theta_1} p^2(\sigma) \left(a_1 \cos(\theta_1 - \omega_1 \tau^* + \omega_1 \sigma) \right. \\ & \left. + a_2 \cos(\theta_2 - \omega_2 \tau^* + \omega_2 \sigma) + a_3 \cos(-\tau^* + \sigma) \right) d\sigma. \end{aligned}$$

To simplify the calculations, we assume $t_0 = -t_f$. Then, we have

$$\begin{aligned} \left| \frac{\partial \mathcal{L}_0^*}{\partial \theta_1} - \left(\frac{\partial \mathcal{L}_0^*}{\partial \theta_1} \right)_\delta \right| = & \left| \int_{t_f}^{+\infty} p^2(\sigma) \left[-a_1 \left(1 - \omega_1 \frac{\partial \tau^*}{\partial \theta_1} \right) \sin(\theta_1 - \omega_1 \tau^* + \omega_1 \sigma) + \right. \right. \\ & \left. \left. a_2 \omega_2 \frac{\partial \tau^*}{\partial \theta_1} \sin(\theta_2 - \omega_2 \tau^* + \omega_2 \sigma) + a_3 \frac{\partial \tau^*}{\partial \theta_1} \sin(-\tau^* + \sigma) \right] d\sigma \right| \end{aligned}$$

Using the equation of the crest given in (6.62) and the Triangular inequality

$$\begin{aligned} \left| \frac{\partial \mathcal{L}_0^*}{\partial \theta_1} - \left(\frac{\partial \mathcal{L}_0^*}{\partial \theta_1} \right)_\delta \right| \leq & |a_1| \int_{t_f}^{+\infty} p^2(\sigma) d\sigma \\ & + \sum_{k=1}^2 |a_3 \mu_k| \int_{t_f}^{+\infty} p^2(\sigma) \left| \frac{\partial \tau^*}{\partial \theta_1} \right| |\omega_k - \alpha(\omega_k)| d\sigma \\ \leq & \int_{t_f}^{+\infty} p^2(\sigma) d\sigma (|a_1| \\ & + \sum_{k=1}^2 |a_3 \mu_k| \left| \frac{\partial \tau^*}{\partial \theta_1} \right| \max_{I_k \in [I_k^0, I_k^1]} |\omega_k - \alpha(\omega_k)|) d\sigma. \end{aligned} \quad (6.90)$$

As $(I, \Theta(I))$ is on a Highway and from the equation of the crest, we have

$$\frac{\partial \tau^*}{\partial \theta_1} = \frac{\alpha(\omega_1) \mu_1 \cos(\theta_1 - \omega_1 \tau^*)}{1 + \sum_{k=1}^2 (\omega_k^2 - 1) \frac{A_k}{A_3} \cos(\theta_k - \omega_k \tau^*)}$$

Applying the fact that we are assuming $|\mu_1| + |\mu_2| < 0.625$,

$$\left| \frac{\partial \tau^*}{\partial \theta_1} \right| \leq \frac{2 \sinh(\pi/2) |\mu_1|}{\pi [1 - 1.466(|\mu_1| + |\mu_2|)]}.$$

In addition, we have $p(\sigma) = 4e^{-|\sigma|} (1 + \mathcal{O}(e^{-2|\sigma|}))$. Therefore, inequality (6.90) can be rewritten as

$$\left| \frac{\partial \mathcal{L}_0^*}{\partial \theta_1} - \left(\frac{\partial \mathcal{L}_0^*}{\partial \theta_1} \right)_\delta \right| \leq C e^{-t_f} + \mathcal{O}(e^{-3t_f}),$$

where

$$C = 16 \left(|a_1| + \sum_{k=1}^2 \frac{2 |a_3 \mu_k| \sinh(\pi/2) |\mu_1|}{\pi [1 - 1.466(|\mu_1| + |\mu_2|)]} M(\omega_k) \right), \quad (6.91)$$

with $M(\omega_i) = \max_{I_i \in [I_i^0, I_i^f]} |\omega_i - \alpha(\omega_i)|$. So, by using the expression of T_h given in (6.88), we have

$$\left| \frac{\partial \mathcal{L}_0^*}{\partial \theta_1} - \left(\frac{\partial \mathcal{L}_0^*}{\partial \theta_1} \right)_\delta \right| \leq \frac{C \delta (1 + \mathcal{O}(\delta^2))}{4\sqrt{2}},$$

To satisfy Eq. (6.89), we have to take a δ satisfying

$$\delta = \frac{4\varepsilon\sqrt{2}}{C} (1 + \mathcal{O}(\varepsilon^2)).$$

Therefore, by inserting this value of δ , time T_h can be expressed as

$$T_h = 2 \log \left(\frac{C}{\varepsilon} \right) + \mathcal{O}(\varepsilon),$$

where C is given by (6.91).

Note that this time is only related to the outer time under the scattering map. However, the inner map plays a role in the diffusion dynamics, and in principle the inner time should be taken into account. As in the case of 2+1/2 d.o.f, this is not true [DS17], since the inner time is much shorter than the outer, so it can be neglected.

We want to estimate the diffusion time for an orbit close to a Highway. Then, let (I^h, θ^h) be a point on a Highway, take a point $(I^h, \theta^h) + \Delta(I, \theta)$, with $\|\Delta(I, \theta)\|$ small enough. From Grönwall's inequality, we have

$$\left\| \phi_t^{-\mathcal{L}_0^*}((I^h, \theta^h) + \Delta(I, \theta)) - \phi_t^{-\mathcal{L}_0^*}((I^h, \theta^h)) \right\| \leq \left\| \Delta(I, \theta) \right\| e^{K|t-t_0|}$$

where $K = \max_{s \in [t_0, t]} \left\| \text{Hess}(\phi_s^{-\mathcal{L}_0^*}((I^h, \theta^h))) \right\|$ and Hess is the Hessian matrix of $-\mathcal{L}_0^*$, and $\phi_t^{-\mathcal{L}_0^*}$ is the scattering flow. To ensure that this orbit is close to the Highway we will take $\|\Delta(I, \theta)\|$ and $|t - t_0|$ small, Then, $\|\Delta(I, \theta)\| = \varepsilon^a$ and $|t - t_0| = \varepsilon^c$ where c is taken in such a way $e^{K|t-t_0|} = \mathcal{O}(1)$. After this interval of time, we apply the inner map to reach a point closer to the Highway. The time by this application of the inner map is estimated by applying the following theorem.

Theorem 6.17 (Minkowski's theorem [Sie89]). *For $Q > 0$ and the linear operator $L : \mathbb{R}^m \rightarrow \mathbb{R}^n$ there exists a solution $(0, 0) \neq (x, y) \in \mathbb{Z}^m \times \mathbb{Z}^n$ for the inequalities $\|x\|_\infty \leq Q$, $\|Lx - y\|_\infty \leq Q^{-\frac{m}{n}}$.*

We consider that the inner dynamics is constant on the variable $I = (I_1, I_2)$, then we have to estimate t such that $\|\varphi + t\omega - \varphi \bmod 2\pi\| \leq \varepsilon^a$. By considering a time 2π - periodic, this equation can be written as

$$2\pi \|l\omega - k\| \leq \varepsilon^a, \quad l \in \mathbb{N} \text{ and } k \in \mathbb{Z}^2.$$

From Theorem 6.17, the time t satisfies $|t| \leq 2\pi\varepsilon^{-2a}$. Therefore, we see that the time related to the inner dynamics T_i satisfies

$$|T_i| \leq \frac{T_s}{\varepsilon^{1+c}} \left(2\pi\varepsilon^{-2a} \right).$$

Observe that this time T_i is comparable to the time under the scattering map if $\log \varepsilon^{-1}$ is comparable to ε^{-c-2a} . But, taking $1 \gg -c \geq 2a > 0$ we obtain $\log \varepsilon^{-1} \gg \varepsilon^{-c-2a}$.

We can now conclude that the diffusion time T_d takes the form (6.86), where $b = -c - 2a$. $\square$

Remark 6.31. We emphasize that the estimation of time obtained in the above theorem is very similar to the estimation for the diffusing time for $2+1/2$ d.o.f. [DS17] and agrees with the estimation of ‘optimal’ diffusing time [BBB03b, CG03b, Tre04]. The main novelty here is that the constants T_s and C are explicitly given for diffusion orbits close to a Highway. Note that T_s depends on τ^* , which does not have an analytical expression. However, it can be easily computed using numerical methods.

Chapter 7

(Planar) elliptic restricted three body problem (ER3BP)

7.1 The problem

The (planar) elliptic restricted three body problem (*ER3BP*) describes the motion q of a massless particle (a *comet*) under the gravitational field of two massive bodies (the *primaries*, say the *Sun* and *Jupiter*) with mass ratio μ revolving around their center of mass on *elliptic* orbits with eccentricity ϵ_J .

Typical models are the Sun–Jupiter–asteroid or comet: $\epsilon_J = 0.048$ and Sun–Earth–Moon systems: $\epsilon_J = 0.016$.

We search for trajectories of motion which show a *large* variation of the angular momentum $G = q \times \dot{q}$, so we search for *global instability* (“diffusion” is the term usually used) in the angular momentum of this problem.

7.2 The Main Result

Theorem 7.1 (The Main Result [DKRS19]). *There exist two constants $C > 0$, $c > 0$ and $\mu^* = \mu^*(C, c) > 0$ such that for any $0 < \epsilon_J < c/C$ and $0 < \mu < \mu^*$, and for any two values of the angular momentum in the region $C \leq G_1^* < G_2^* \leq c/\epsilon_J$, there exists a trajectory of the ER3BP such that $G(0) < G_1^*$, $G(T) > G_2^*$ for some $T > 0$.*

If $\epsilon_J = 0$, the primaries revolve along *circular* orbits, and such diffusion is *not* possible, since the (planar) restricted circular three body problem (R3BP) is governed by an autonomous Hamiltonian with 2 degrees-of-freedom.

This is not the case for the ER3BP, which is a $2+1/2$ degrees-of-freedom Hamiltonian system with time-periodic Hamiltonian.

7.3 Previous results

7.3.1 Restricted 3 BP

There are related results about oscillatory motions and diffusion for several Restricted Three Body Problems:

- Euler libration points: [LMS85, CZ11, DGR13, DGR16]
- Collisions: [Bol06]
- The (parabolic) infinity: [LS80, Xia93, Xia94, Mos01, Moe07, MP94, MS14b, GMS16, CGM⁺22]
- Mean motion resonances: [FGKR16]
- Aubry-Mather theory: [GK11]

7.4 Setting of the problem

7.4.1 The equations

The motion of the massless particle q (comet) is described by

$$\frac{d^2 q}{dt^2} = (1 - \mu) \frac{q_S - q}{|q_S - q|^3} + \mu \frac{q_J - q}{|q_J - q|^3}$$

where $1 - \mu$ is the mass of the primary (Sun) at q_S and μ the mass of the primary (Jupiter) at q_J .

Introducing $p = dq/dt$, this is a 2+1/2 degree-of-freedom Hamiltonian system with time-periodic Hamiltonian

$$H_\mu(q, p, t; \epsilon_J) = \frac{p^2}{2} - U_\mu(q, t; \epsilon_J)$$

with self-potential

$$U_\mu(q, t; \epsilon_J) = \frac{1 - \mu}{|q - q_S(t, \epsilon_J)|} + \frac{\mu}{|q - q_J(t, \epsilon_J)|}$$

The parameters are $0 < \mu, \epsilon_J < 1$ small.

7.4.2 Two body problem: Sun-comet

When $\mu = 0$, there is no Jupiter in the equation of motion and the Sun is fixed at the origin: $q_S = 0$.

The Sun q_S and the comet q form a two-body problem with the Hamiltonian $H_0(q, p, t; \epsilon_J) = H_0(q, p) = \frac{p^2}{2} - \frac{1}{|q|} = \frac{p^2}{2} - U_0(q)$.

The two-body problem is integrable, and there is no dependence on the eccentricity ϵ_J or the time t .

7.4.3 Equations of the primaries

$$q_S = q_S(t, \epsilon_J) = \mu r(\cos f, \sin f)$$

$$q_J = q_J(t, \epsilon_J) = -(1 - \mu)r(\cos f, \sin f)$$

with

$$r = r(t; \epsilon_J) = \frac{1 - \epsilon_J^2}{1 + \epsilon_J \cos f}, \quad \frac{df}{dt} = \frac{(1 + \epsilon_J \cos f)^2}{(1 - \epsilon_J^2)^{3/2}},$$

where $f = f(t; \epsilon_J)$ is the *true anomaly*. If $q = \rho(\cos \alpha, \sin \alpha)$,

$$\begin{aligned} |q - q_S|^2 &= \rho^2 - 2\mu r \rho \cos(\alpha - f) + \mu^2 r^2, \\ |q - q_J|^2 &= \rho^2 + 2(1 - \mu)r \rho \cos(\alpha - f) + (1 - \mu)^2 r^2. \end{aligned}$$

Remark Also

$$r = r(t; \epsilon_J) = 1 - \epsilon_J \cos E, \quad t = E - \epsilon_J \sin E,$$

where E is the *eccentric anomaly*.

7.4.4 Polar coordinates

Performing a standard polar-canonical change of variables $(q, p) \mapsto (\rho, \alpha, P_\rho, P_\alpha)$

$$q = (\rho \cos \alpha, \rho \sin \alpha), \quad p = \left(P_\rho \cos \alpha - \frac{P_\alpha}{\rho} \sin \alpha, P_\rho \sin \alpha + \frac{P_\alpha}{\rho} \cos \alpha \right)$$

the Hamiltonian becomes

$$H_\mu^*(\rho, \alpha, P_\rho, P_\alpha, t; \epsilon_J) = \frac{P_\rho^2}{2} + \frac{P_\alpha^2}{2\rho^2} - U_\mu^*(\rho, \alpha, t; \epsilon_J)$$

with a self-potential U_μ^*

$$U_\mu^*(\rho, \alpha, t; \epsilon_J) = U_\mu(\rho \cos \alpha, \rho \sin \alpha, t; \epsilon_J) = \frac{1}{\rho} + O(\mu).$$

From now on we will write

$$G = P_\alpha, \quad y = P_\rho,$$

so that Hamiltonian (7.4.4) becomes

$$H_\mu^*(\rho, \alpha, y, G, t; \epsilon_J) = \frac{y^2}{2} + \frac{G^2}{2\rho^2} - U_\mu^*(\rho, \alpha, t; \epsilon_J).$$

Remark 7.1. In the (planar) circular case $\epsilon_J = 0$ (R3BP), $r = 1$ and $f = t$, and $|q - q_S|, |q - q_J|$ depend on the time t and the angle α just through their difference $\alpha - t$. As a consequence, $U_\mu^*(\rho, \alpha, t; 0)$ as well as $H_\mu^*(\rho, \alpha, y, G, t; 0)$ depend also on t and α just through the same difference $\alpha - t$, the sinodic angle. This implies that the Jacobi constant $H^* + G$ is a first integral of the system.

7.4.5 McGehee coordinates

Through McGehee non-canonical change of variables, for $x > 0$,

$$\rho = \frac{2}{x^2}$$

the infinity $\rho = \infty$ is sent to the origin $x = 0$ and the equations become

$$\begin{aligned} \frac{dx}{dt} &= -\frac{1}{4}x^3y & \frac{dy}{dt} &= \frac{1}{8}G^2x^6 - \frac{x^3}{4}\frac{\partial \mathcal{U}_\mu}{\partial x} \\ \frac{d\alpha}{dt} &= \frac{1}{4}x^4G & \frac{dG}{dt} &= \frac{\partial \mathcal{U}_\mu}{\partial \alpha}, \end{aligned}$$

where the self-potential $\mathcal{U}_\mu$ is given now by

$$\mathcal{U}_\mu(x, \alpha, t; \epsilon_J) = U_\mu^*(2/x^2, \alpha, t; \epsilon_J) = \frac{x^2}{2} \left(\frac{1-\mu}{\sigma_S} + \frac{\mu}{\sigma_J} \right)$$

with

$$\begin{aligned} |q - q_S|^2 &= \sigma_S^2 = 1 - \mu r x^2 \cos(\alpha - f) + \frac{1}{4}\mu^2 r^2 x^4, \\ |q - q_J|^2 &= \sigma_J^2 = 1 + (1 - \mu) r x^2 \cos(\alpha - f) + \frac{1}{4}(1 - \mu)^2 r^2 x^4. \end{aligned}$$

It is important to notice that the true anomaly f is present in these equations, so that the equation for f should be added to have the complete description of the dynamics.

7.4.6 The b^3 -symplectic structure

Under McGehee change of variables $\rho = 2/x^2$ for $x > 0$,

$$d\rho \wedge dy + d\alpha \wedge dG \quad \text{is transformed to} \quad \omega = -\frac{4}{x^3} dx \wedge dy + d\alpha \wedge dG$$

which is a b^3 -symplectic form, the new Hamiltonian reads as

$$\mathcal{H}_\mu(x, \alpha, y, G, t; \epsilon_J) = \frac{y^2}{2} + \frac{x^4 G^2}{8} - \mathcal{U}_\mu(x, \alpha, t; \epsilon_J),$$

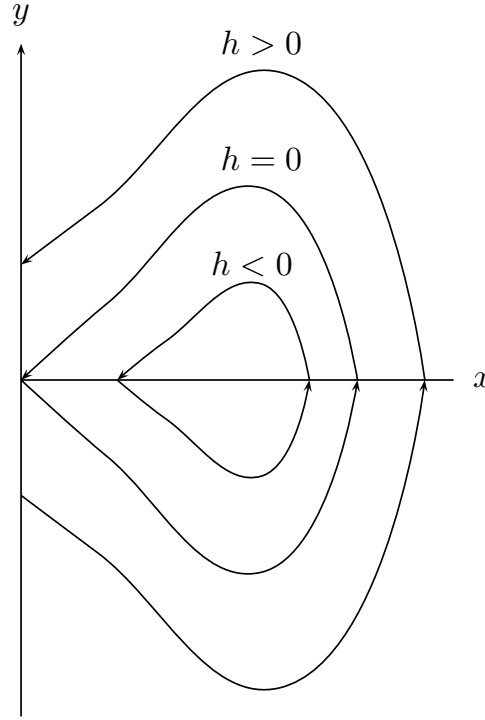
and the the Hamiltonian equations become

$$\begin{aligned} \frac{dx}{dt} &= -\frac{x^3}{4} \left(\frac{\partial \mathcal{H}_\mu}{\partial y} \right) & \frac{dy}{dt} &= -\frac{x^3}{4} \left(-\frac{\partial \mathcal{H}_\mu}{\partial x} \right) \\ \frac{d\alpha}{dt} &= \frac{\partial \mathcal{H}_\mu}{\partial G} & \frac{dG}{dt} &= -\frac{\partial \mathcal{H}_\mu}{\partial \alpha}. \end{aligned}$$

which can be written as $dz/dt = \{z, \mathcal{H}_\mu\}$ in terms of the Poisson bracket

$$\{f, g\} = -\frac{x^3}{4} \left(\frac{\partial f}{\partial x} \frac{\partial g}{\partial y} - \frac{\partial f}{\partial y} \frac{\partial g}{\partial x} \right) + \frac{\partial f}{\partial \alpha} \frac{\partial g}{\partial G} - \frac{\partial f}{\partial G} \frac{\partial g}{\partial \alpha}.$$

- Some sources of b^m -symplectic structures can be found in [Sco16, KMS16, GMW18, GMW19].
- Other examples can be found in [GMS16, DKM17, BDM⁺19].
- New examples in [BFM20, BFM24, GMP25].

Figure 7.1: Level curves of $\mathcal{H}_0$ in the $(x \geq 0, y)$ plane, for fixed $G > 0$

7.5 The Kepler problem ($\mu = 0$)

7.5.1 The (parabolic) infinity manifold

For $\mu = 0$ and $G > 0$, Hamiltonian $\mathcal{H}_0$ becomes Duffing Hamiltonian:

$$\mathcal{H}_0(x, y, G) = \frac{y^2}{2} + \frac{x^4 G^2}{8} - \mathcal{U}_0(x) = \frac{y^2}{2} + \frac{x^4 G^2}{8} - \frac{x^2}{2}$$

$\mathcal{H}_0$ is autonomous and independent of ϵ_J and α . Its associated equations are

$$\begin{aligned} \frac{dx}{dt} &= -\frac{1}{4}x^3y & \frac{dy}{dt} &= \frac{1}{8}G^2x^6 - \frac{1}{4}x^4 \\ \frac{d\alpha}{dt} &= \frac{1}{4}x^4G & \frac{dG}{dt} &= 0 \end{aligned}$$

The angular momentum G is a conserved quantity, $G > 0$ from now on. The phase space $(x, \alpha, y, G) \in \mathbb{R}_{\geq 0} \times \mathbb{T} \times \mathbb{R} \times \mathbb{R}_+$ includes the set of equilibrium points

$$\mathcal{E}_\infty = \{z = (x = 0, \alpha, y, G) \in \mathbb{R}_{\geq 0} \times \mathbb{T} \times \mathbb{R} \times \mathbb{R}_+\}.$$

For any fixed $\alpha \in \mathbb{T}, G \in \mathbb{R}$,

$$\Lambda_{\alpha, G} = \{(0, \alpha, 0, G)\}$$

is a parabolic equilibrium point, which is topologically equivalent to a saddle point, since it possesses stable and unstable 1D-invariant manifolds. The union of such points is the 2D-(symplectic) manifold of equilibrium points

$$\Lambda_\infty = \bigcup_{\alpha, G} \Lambda_{\alpha, G}.$$

which is the (parabolic) infinity manifold for the Kepler problem.

As we will deal with a time-periodic Hamiltonian, it is natural to work in the *extended* phase space

$$\tilde{z} = (z, s) = (x, \alpha, y, G, s) \in \mathbb{R}_{\geq 0} \times \mathbb{T} \times \mathbb{R} \times \mathbb{R}_+ \times \mathbb{T}$$

just by writing s instead of t in the Hamiltonian and adding the equation

$$\frac{ds}{dt} = 1$$

The extended versions of the invariant sets $\Lambda_{\alpha,G}$, Λ_∞ for the Kepler problem are the 2π -periodic orbits with motion $ds/dt = 1$

$$\tilde{\Lambda}_{\alpha,G} = \{\tilde{z} = (0, \alpha, 0, G, s), s \in \mathbb{T}\},$$

and the 3D-invariant manifold (the “parabolic” *infinity manifold*)

$$\tilde{\Lambda}_\infty = \bigcup_{\alpha,G} \tilde{\Lambda}_{\alpha,G} = \{(0, \alpha, 0, G, s), (\alpha, G, s) \in \mathbb{T} \times \mathbb{R}_+ \times \mathbb{T}\} \simeq \mathbb{T} \times \mathbb{R}_+ \times \mathbb{T},$$

which is *topologically equivalent to a normally hyperbolic invariant manifold* (TNHIM).

Parameterizing the points in $\tilde{\Lambda}_\infty$ by

$$\tilde{\mathbf{x}}_0 = \tilde{\mathbf{x}}_0(\alpha, G, s) = (\mathbf{x}_0(\alpha, G), s) = (0, \alpha, 0, G, s) \in \tilde{\Lambda}_\infty \simeq \mathbb{T} \times \mathbb{R}_+ \times \mathbb{T}$$

the inner dynamics on $\tilde{\Lambda}_\infty$ is trivial, since it is given by the dynamics on each periodic orbit $\tilde{\Lambda}_{\alpha,G}$:

$$\tilde{\phi}_{t,0}(\tilde{\mathbf{x}}_0) = (0, \alpha, 0, G, s+t) = (\mathbf{x}_0(\alpha, G), s+t) = \tilde{\mathbf{x}}_0(\alpha, G, s+t),$$

where we denote by $\tilde{\phi}_{t,\mu}$ the flow of our system in the extended phase space.

7.5.2 The separatrix

The equilibrium points $\Lambda_{\alpha,G}$ have stable and unstable 1D-invariant manifolds which coincide:

$$\begin{aligned} \gamma_{\alpha,G} &= W^u(\Lambda_{\alpha,G}) = W^s(\Lambda_{\alpha,G}) \\ &= \left\{ z = (x, \hat{\alpha}, y, G), \mathcal{H}_0(x, y, G) = 0, \hat{\alpha} = \alpha - G \int_{\mathcal{H}_0=0} \frac{x}{y} dx \right\}, \end{aligned}$$

whereas the 2D-manifold of equilibrium points Λ_∞ has stable and unstable 3D-invariant manifolds which coincide and are given by

$$\gamma = W^u(\Lambda_\infty) = W^s(\Lambda_\infty) = \{z = (x, \alpha, y, G), \mathcal{H}_0(x, y, G) = 0\}.$$

In the extended phase space, the surface

$$\begin{aligned} \tilde{\gamma}_{\alpha,G} &= W^u(\tilde{\Lambda}_{\alpha,G}) = W^s(\tilde{\Lambda}_{\alpha,G}) \\ &= \left\{ \tilde{z} = (x, \hat{\alpha}, y, G, s), s \in \mathbb{T}, \mathcal{H}_0(x, y, G) = 0, \hat{\alpha} = \alpha - G \int_{\mathcal{H}_0=0} \frac{x}{y} dx \right\} \end{aligned}$$

is a 2D-homoclinic manifold to the periodic orbit $\tilde{\Lambda}_{\alpha,G}$. The 4D-stable and unstable manifolds of the infinity manifold $\tilde{\Lambda}_\infty$ coincide along the 4D-homoclinic invariant manifold (the *separatrix*), which is just the union of the homoclinic surfaces $\tilde{\gamma}_{\alpha,G}$:

$$\begin{aligned} \tilde{\gamma} &= W^u(\tilde{\Lambda}_\infty) = W^s(\tilde{\Lambda}_\infty) = \bigcup_{\alpha,G} \tilde{\gamma}_{\alpha,G} \\ &= \{ \tilde{z} = (x, \alpha, y, G, s), (\alpha, G, s) \in \mathbb{T} \times \mathbb{R}_+ \times \mathbb{T}, \mathcal{H}_0(x, \alpha, y, G) = 0 \} \end{aligned}$$

7.5.3 Separatrix parameterization

The homoclinic solutions to the periodic orbit $\tilde{\Lambda}_{\alpha,G}$ are given by

$$\begin{aligned} x_h(t; G) &= \frac{2}{G(1 + \tau^2)^{1/2}} & y_h(t; G) &= \frac{2\tau}{G(1 + \tau^2)} \\ \alpha_h(t; \alpha, G) &= \alpha + \pi + 2 \arctan \tau & G_h(t; G) &= G \\ s_h(t; s) &= s + t & & \end{aligned},$$

where α and G are the 2 free parameters and the relation between t and τ is

$$t = \frac{G^3}{2} \left(\tau + \frac{\tau^3}{3} \right) \quad \text{which is equivalent to} \quad \frac{dt}{d\tau} = \frac{2G}{x^2},$$

Due to the factor $-x^3/4$ in front of the equations, the convergence along the separatrix to the infinity manifold is power-like in τ and t :

$$x_h, y_h, \frac{\alpha - \alpha_h + \pi}{G} \sim \frac{2}{G\tau} \sim \frac{2}{\sqrt[3]{\pm 6t}}, \quad \tau, t \rightarrow \pm\infty.$$

Introducing the notation

$$\tilde{\mathbf{z}}_0 = \tilde{\mathbf{z}}_0(\sigma, \alpha, G, s) = (\mathbf{z}_0(\sigma, \alpha, G), s) = (x_h(\sigma; G), \alpha_h(\sigma; \alpha, G), y_h(\sigma; G), G, s)$$

we can parameterize any homoclinic surface $\tilde{\gamma}_{\alpha, G}$ as

$$\tilde{\gamma}_{\alpha, G} = \{\tilde{\mathbf{z}}_0 = \tilde{\mathbf{z}}_0(\sigma, \alpha, G, s) = (\mathbf{z}_0(\sigma, \alpha, G), s), \sigma \in \mathbb{R}, s \in \mathbb{T}\}.$$

and the 4-dimensional separatrix $\tilde{\gamma} = W(\tilde{\Lambda}_\infty)$ as

$$\tilde{\gamma} = \{\tilde{\mathbf{z}}_0 = \tilde{\mathbf{z}}_0(\sigma, \alpha, G, s) = (\mathbf{z}_0(\sigma, \alpha, G), s), \sigma \in \mathbb{R}, G \in \mathbb{R}_+, (\alpha, s) \in \mathbb{T}^2\}.$$

The motion on $\tilde{\gamma}$ and $\tilde{\Lambda}_\infty$ is given by

$$\begin{aligned} \tilde{\phi}_{t,0}(\tilde{\mathbf{z}}_0) &= \tilde{\mathbf{z}}_0(\sigma + t, \alpha, G, s + t) = (\mathbf{z}_0(\sigma + t, \alpha, G), s + t) \\ \tilde{\phi}_{t,0}(\tilde{\mathbf{x}}_0) &= (0, \alpha, 0, G, s + t) = (\mathbf{x}_0(\alpha, G), s + t) = \tilde{\mathbf{x}}_0(\alpha, G, s + t), \end{aligned}$$

and the following asymptotic formula follows:

$$\tilde{\phi}_{t,0}(\tilde{\mathbf{z}}_0) - \tilde{\phi}_{t,0}(\tilde{\mathbf{x}}_0) = (\mathbf{z}_0(\sigma + t, \alpha, G), s + t) - (\mathbf{x}_0(\alpha, G), s + t) \xrightarrow[t \rightarrow \pm\infty]{} 0.$$

7.5.4 The scattering map

The *scattering map* $\tilde{S}$ describes the homoclinic orbits to the infinity manifold $\tilde{\Lambda}_\infty$ (defined in (7.5.1)) to itself. Given $\tilde{\mathbf{x}}_-, \tilde{\mathbf{x}}_+ \in \tilde{\Lambda}_\infty$, we define

$$\tilde{S}_\mu(\tilde{\mathbf{x}}_-) := \tilde{\mathbf{x}}_+$$

if there exists $\tilde{\mathbf{z}}^* \in W_\mu^u(\tilde{\Lambda}_\infty) \cap W_\mu^s(\tilde{\Lambda}_\infty)$ such that

$$\tilde{\phi}_{t,\mu}(\tilde{\mathbf{z}}^*) - \tilde{\phi}_{t,\mu}(\tilde{\mathbf{x}}_\pm) \longrightarrow 0 \quad \text{for } t \rightarrow \pm\infty.$$

In the case $\mu = 0$ the previous asymptotic relation

$$\tilde{\phi}_{t,0}(\tilde{\mathbf{z}}_0) - \tilde{\phi}_{t,0}(\tilde{\mathbf{x}}_0) = (\mathbf{z}_0(\sigma + t, \alpha, G), s + t) - (\mathbf{x}_0(\alpha, G), s + t) \xrightarrow[t \rightarrow \pm\infty]{} 0.$$

implies $\tilde{S}_0(\tilde{\mathbf{x}}_0) = \tilde{\mathbf{x}}_0$ so that the scattering map $\tilde{S}_0 : \tilde{\Lambda}_\infty \longrightarrow \tilde{\Lambda}_\infty$ is the identity.

7.6 The ER3BP ($\mu > 0$)

7.6.1 $\tilde{\Lambda}_\infty$, $W_\mu^s(\tilde{\Lambda}_\infty)$ and $W_\mu^u(\tilde{\Lambda}_\infty)$

For $\mu > 0$, the set $\mathcal{E}_\infty$ remains invariant as well as infinity manifold $\tilde{\Lambda}_\infty$, which is again a TNHIM, as well as all the periodic orbits $\tilde{\Lambda}_{\alpha, G}$.

The inner dynamics on $\tilde{\Lambda}_\infty$ is the same as in the case $\mu = 0$, so that the parametrization $\tilde{\mathbf{x}}_0$ as well as its trivial dynamics remain the same.

From [McG73, GSMS17] we know that $W_\mu^s(\tilde{\Lambda}_\infty)$ and $W_\mu^u(\tilde{\Lambda}_\infty)$ exist for μ small enough and are 4-dimensional in the extended phase space.

The existence of scattering maps will depend on the transversal intersections between these two manifolds.

7.6.2 The Melnikov potential

Introduce now the *Melnikov potential* $\mathcal{L} : \tilde{\Lambda}_\infty \longrightarrow \mathbb{R}$ [DG00, DLS06a]

$$\mathcal{L}(\alpha, G, s; \epsilon_J) = \int_{-\infty}^{\infty} \Delta \mathcal{U}_0(x_h(t; G), \alpha_h(t; \alpha, G), s + t; \epsilon_J) dt,$$

where $\Delta \mathcal{U}_0$ is defined by

$$\Delta \mathcal{U}_0(x, \alpha, s; \epsilon_J) := \left. \frac{\partial \mathcal{U}_\mu}{\partial \mu} \right|_{\mu=0} (x, \alpha, s; \epsilon_J) = O(x^4) \quad \text{as } x \rightarrow 0.$$

The asymptotics above follows from the asymptotic behavior of the solutions along the separatrix and of the self potential close to the parabolic infinity manifold, and guarantees that this integral is absolutely convergent.

7.6.3 $W_\mu^s(\tilde{\Lambda}_\infty) \cap W_\mu^u(\tilde{\Lambda}_\infty)$

Proposition 7.2 (Transverse homoclinic points to the infinite manifold $\tilde{\Lambda}_\infty$). *Given $(\alpha, G, s) \in \mathbb{T} \times \mathbb{R}^+ \times \mathbb{T}$, assume that the function*

$$\sigma \in \mathbb{R} \longmapsto \mathcal{L}(\alpha, G, s - \sigma; \epsilon_J) \in \mathbb{R}$$

has a non-degenerate critical point $\sigma^ = \sigma^*(\alpha, G, s; \epsilon_J)$. Then, there exists $\mu^* = \mu^*(G, \epsilon_J)$, such that for $0 < \mu < \mu^*$, close to the point $\tilde{\mathbf{z}}_0^* = (\mathbf{z}_0(\sigma^*, \alpha, G), s) \in \tilde{\gamma}$ there exists a locally unique point*

$$\tilde{\mathbf{z}}^* = \tilde{\mathbf{z}}^*(\sigma^*, \alpha, G, s; \epsilon_J, \mu) \in W_\mu^s(\tilde{\Lambda}_\infty) \cap W_\mu^u(\tilde{\Lambda}_\infty)$$

of the form $\tilde{\mathbf{z}}^ = \tilde{\mathbf{z}}_0^* + O(\mu)$, and there exist unique points $\tilde{\mathbf{x}}_\pm = (0, \alpha_\pm, 0, G_\pm, s) = (0, \alpha, 0, G, s) + O(\mu) \in \tilde{\Lambda}_\infty$ such that*

$$\tilde{\phi}_{t,\mu}(\tilde{\mathbf{z}}^*) - \tilde{\phi}_{t,\mu}(\tilde{\mathbf{x}}_\pm) \longrightarrow 0 \quad \text{for } t \rightarrow \pm\infty.$$

Moreover, we have

$$G_+ - G_- = \mu \frac{\partial \mathcal{L}}{\partial \alpha}(\alpha, G, s - \sigma^*(\alpha, G, s; \epsilon_J)) + O(\mu^2).$$

7.6.4 Reduced Poincaré function

Once we have found a critical point $\sigma^* = \sigma^*(\alpha, G, s; \epsilon_J)$ of

$$\sigma \in \mathbb{R} \longmapsto \mathcal{L}(\alpha, G, s - \sigma; \epsilon_J) \in \mathbb{R}$$

on a domain of (α, G, s) , we can define the *reduced Poincaré function* [DLS06a]

$$\mathcal{L}^*(\alpha, G; \epsilon_J) := \mathcal{L}(\alpha, G, s - \sigma^*; \epsilon_J) = \mathcal{L}(\alpha, G, s^*; \epsilon_J)$$

with $s^* = s - \sigma^*$. Note that the reduced Poincaré function does not depend on the s chosen, since by the previous Proposition

$$\frac{\partial}{\partial s} \left(\mathcal{L}(\alpha, G, s - \sigma^*(\alpha, G, s; \epsilon_J); \epsilon_J) \right) \equiv 0.$$

Note also that if the function $\sigma \in \mathbb{R} \longmapsto \mathcal{L}(\alpha, G, s - \sigma; \epsilon_J) \in \mathbb{R}$ has *different non degenerate* critical points there will exist *different* scattering maps.

The next Proposition gives an approximation of the scattering map in the general case $\mu > 0$.

7.6.5 Scattering map

Proposition 7.3 (Expression of the scattering map). *The associated scattering map $(\alpha_+, G_+, s_+) = \tilde{S}_\mu(\alpha, G, s)$ for any non degenerate critical point $\sigma^* = \sigma^*(\alpha, G, s; \epsilon_J)$ of the function $\sigma \in \mathbb{R} \longmapsto \mathcal{L}(\alpha, G, s - \sigma; \epsilon_J) \in \mathbb{R}$ is an exact symplectic map given by*

$$(\alpha, G, s) \longmapsto \left(\alpha - \mu \frac{\partial \mathcal{L}^*}{\partial G}(\alpha, G; \epsilon_J) + O(\mu^2), G + \mu \frac{\partial \mathcal{L}^*}{\partial \alpha}(\alpha, G; \epsilon_J) + O(\mu^2), s \right)$$

where $\mathcal{L}^*$ is the Poincaré reduced function.

Remark: the scattering map $\tilde{S}_\mu$ follows closely the level curves of the Hamiltonians $\mathcal{L}^*$. More precisely, up to $O(\mu^2)$ terms, $\tilde{S}_\mu$ is given by the time $-\mu$ map of the Hamiltonian flow of Hamiltonian $\mathcal{L}^*$. The $O(\mu^2)$ remainder will be negligible as long as

$$|\mu| \ll \left| \frac{\partial \mathcal{L}^*}{\partial G} \right|, \left| \frac{\partial \mathcal{L}^*}{\partial \alpha} \right|.$$

7.6.6 Computation of $\mathcal{L}(\alpha, G, s; \epsilon_J)$

$$\begin{aligned} \mathcal{L}(\alpha, G, s; \epsilon_J) = \int_{-\infty}^{\infty} & \left[\frac{x_h^2}{[4 + x_h^4 r^2 + 4x_h^2 r \cos(\alpha_h - f)]^{1/2}} \right. \\ & \left. + \left(\frac{x_h^2}{2} \right)^2 r \cos(\alpha_h - f) - \frac{x_h^2}{2} \right] dt \end{aligned}$$

where x_h and α_h , solutions on the separatrix, are evaluated at t , whereas r and f , concerning the primaries, are evaluated at $s + t$.

Fourier expanding with respect to angular variables α, s , $\mathcal{L}$ is an even function α, s : $\mathcal{L}(-\alpha, G, -s; \epsilon_J) = \mathcal{L}(\alpha, G, s; \epsilon_J)$, and therefore $\mathcal{L}$ has a Fourier Cosine series with real coefficients $L_{q,k}$:

$$\mathcal{L} = L_{0,0} + 2 \sum_{k \geq 1} L_{0,k} \cos k\alpha + 2 \sum_{q \geq 1} \sum_{k \in \mathbb{Z}} L_{q,k} \cos(qs + k\alpha).$$

Using the method of steepest descent along adequate complex paths, and playing both with the eccentric and the true anomaly, it is possible to compute these Fourier coefficients.

Theorem 7.4 (Computation of the Melnikov potential). *For $G \geq 32$, $\epsilon_J G \leq 1/8$, the Melnikov potential is given by*

$$\mathcal{L}(\alpha, G, s; \epsilon_J) = \mathcal{L}_0(\alpha, G; \epsilon_J) + \mathcal{L}_1(\alpha, G, s; \epsilon_J) + \mathcal{L}_{\geq 2}(\alpha, G, s; \epsilon_J)$$

with

$$\begin{aligned} \mathcal{L}_0(\alpha, G; \epsilon_J) &= L_{0,0} + L_{0,1} \cos \alpha + \mathcal{E}_0(\alpha, G; \epsilon_J) \\ \mathcal{L}_1(\alpha, G, s; \epsilon_J) &= 2L_{1,-1} \cos(s - \alpha) + 2L_{1,-2} \cos(s - 2\alpha) \\ &\quad + 2L_{1,-3} \cos(s - 3\alpha) + \mathcal{E}_1(\alpha, G, s; \epsilon_J), \end{aligned}$$

where $L_{i,j} = L_{i,j}(G; \epsilon_J)$ with $L_{0,0} = \frac{\pi}{2G^3}(1 + E_{0,0})$ and

$$\begin{aligned} L_{0,1} &= -\frac{15\pi\epsilon_J}{8G^5}(1 + E_{0,1}), \quad 2L_{1,-1} = \sqrt{\frac{\pi}{8G}} e^{-G^3/3}(1 + E_{1,-1}) \\ 2L_{1,-2} &= -3\sqrt{2\pi}\epsilon_J G^{3/2} e^{-G^3/3}(1 + E_{1,-2}) \\ 2L_{1,-3} &= \frac{19}{8}\sqrt{2\pi}\epsilon_J^2 G^{5/2} e^{-G^3/3}(1 + E_{1,-3}). \end{aligned}$$

Theorem 7.5 (Continuation of the computation of the Melnikov potential). *The error functions satisfy*

$$\begin{aligned} |E_{0,0}| &\leq 2^{12} G^{-4} + 2^2 49 \epsilon_J^2 \\ |E_{0,1}| &\leq 2^{13} G^{-4} + \epsilon_J^2 \\ |E_{1,-1}| &\leq 2^{21} G^{-1} + 2 49 \epsilon_J^2 \\ |E_{1,-2}| &\leq 2^{17} G^{-1} + \frac{49}{3} \epsilon_J \\ |E_{1,-3}| &\leq 2^{17} G^{-1} + 15 \epsilon_J \\ |\mathcal{E}_0| &\leq 2^{14} \epsilon_J^2 G^{-7} \\ |\mathcal{E}_1| &\leq 2^{18} \epsilon_J e^{-G^3/3} \left[\epsilon_J^2 G^{7/2} + G^{-3/2} \right] \\ |\mathcal{L}_{\geq 2}| &\leq 2^{28} G^{3/2} e^{-2G^3/3} \end{aligned}$$

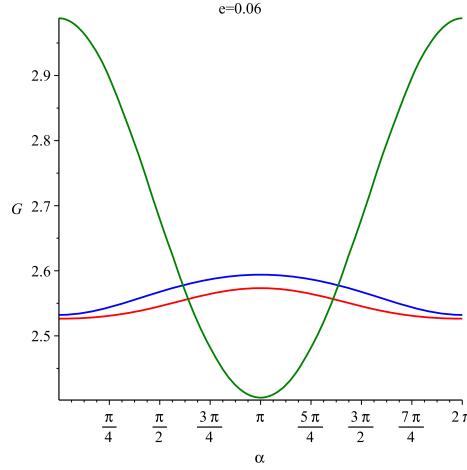


Figure 7.2: Illustration of the level Sets of $\mathcal{L}_+^*$ ($\mathcal{L}_-^*$) in Blue (Red) and $d = 0$ in Green

7.6.7 Critical points of $\mathcal{L}(\alpha, G, \cdot; \epsilon_J)$

$s \mapsto \mathcal{L}(\alpha, G, s; \epsilon_J)$ is indeed a *cosine-like* function, that is, with a non-degenerate maximum (minimum) and no other critical points, so we can find easily its critical points.

Proposition 7.6. *There exists $C > 32$ and $c < 1/8$ such that, for $G \geq C$ and $\epsilon_J G < c$, $s \mapsto \mathcal{L}(\alpha, G, s; \epsilon_J)$ is a cosine-like function, and its two critical points are given by*

$$s_+^* = s_+^*(\alpha, G; \epsilon_J) = \alpha + \theta + \varphi^*, \quad s_-^* = s_-^* = \alpha + \theta + \pi + \varphi^*$$

where $\theta = \theta(\alpha, G; \epsilon_J)$ and $\varphi^* = O(G^{3/2}e^{-G^3/3})$.

By the previous Theorem, for $G > C$ big enough and $G\epsilon_J < c$ small enough, the two critical points of $\mathcal{L}$ in the variable s are well approximated by the two critical points of the function $\mathcal{L}_0 + \mathcal{L}_1$ (in fact of $\mathcal{L}_1$ because $\mathcal{L}_0$ does not depend on s).

7.6.8 Two different scattering maps

We can define two different reduced Poincaré functions

$$\begin{aligned} \mathcal{L}_\pm^*(\alpha, G; \epsilon_J) &= \mathcal{L}(\alpha, G, s_\pm^*; \epsilon_J) \\ &= \mathcal{L}_0(\alpha, G; \epsilon_J) \pm \mathcal{L}_1^*(\alpha, G; \epsilon_J) + \mathcal{E}_\pm(\alpha, G; \epsilon_J). \end{aligned}$$

and two different scattering maps $\tilde{S}_\pm(\alpha, G, s) = (S_\pm(\alpha, G, s), s)$, where

$$S_\pm(\alpha, G, s) = \left(\alpha - \mu \frac{\partial \mathcal{L}_\pm^*}{\partial G}(\alpha, G; \epsilon_J) + O(\mu^2), G + \mu \frac{\partial \mathcal{L}_\pm^*}{\partial \alpha}(\alpha, G; \epsilon_J) + O(\mu^2) \right).$$

which follow closely the level curves of the Hamiltonians $\mathcal{L}_\pm^*$. More precisely, up to $O(\mu^2)$ terms, $S_\pm$ is given by the time $-\mu$ map of the Hamiltonian flow of Hamiltonian $\mathcal{L}_\pm^*$. The $O(\mu^2)$ remainder will be negligible as long as

$$|\mu| \ll \left| \frac{\partial \mathcal{L}_\pm^*}{\partial G} \right|, \left| \frac{\partial \mathcal{L}_\pm^*}{\partial \alpha} \right|,$$

which is true as long as $0 < \mu < \mu^* = e^{-(c/\epsilon_J)^3/3}$.

One has to check that the foliations of $\mathcal{L}_\pm^* = \text{constant}$ are different, since this will imply that the scattering maps $S_\pm$ are different. From

$$\begin{aligned} \{\mathcal{L}_+^*, \mathcal{L}_-^*\} &= \{\mathcal{L}_0 + \mathcal{L}_1^* + \dots, \mathcal{L}_0 - \mathcal{L}_1^* + \dots\} \\ &= -2\{\mathcal{L}_0, \mathcal{L}_1^*\} + \mathcal{E}_3 \end{aligned}$$

one computes

$$\{\mathcal{L}_0, \mathcal{L}_1^*\} = -\frac{15\pi\epsilon_J\mathcal{L}_1^*d\sin\alpha}{8G^3B^2},$$

where $B > 0$ and $d = d(G, \alpha)$. The level curves of $\mathcal{L}_+^*$ and $\mathcal{L}_-^*$ are transversal in the region $G \geq C > 32$ and $\epsilon_J G \leq c < 1/8$, except for the three curves $\alpha = 0$, $\alpha = \pi$ and $d = 0$, which are transversal to any of these level curves of $\mathcal{L}_+^*$ and $\mathcal{L}_-^*$, see Fig. 7.2.

Indeed, this is clear for the lines $\alpha = 0$ and $\alpha = \pi$, and the same happens for the curve $d = 0$ using its complete expression.

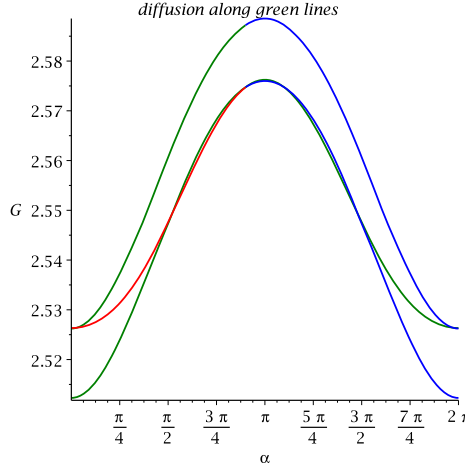


Figure 7.3: Zone of diffusion: Level curves of $\mathcal{L}_+^*$ ($\mathcal{L}_-^*$) in blue (red) and diffusion trajectories in green.

7.6.9 Strategy for diffusion

- Apart from these three curves $\alpha = 0, \pi$ and $d = 0$, at any point in the plane (α, G) the slopes $dG/d\alpha$ of the level curves of $\mathcal{L}_+^*$ and $\mathcal{L}_-^*$ are different.
- We can choose which level curve increases more the value of G (see Fig. 7.3).
- In the same way, we can find trajectories along which the angular momentum performs arbitrary excursions.
- Strictly speaking, this mechanism only produces *pseudo-orbits*, that is, heteroclinic connections between different periodic orbits in the infinity manifold which are commonly known as *transition chains* after Arnold.
- The existence of true orbits relies on shadowing methods [Moe02, Moe07, GL06, GLMS20, GSMS17].

Theorem 7.7 (Main Result again). *Let $G_1^* < G_2^*$ large enough and $\epsilon_J > 0$, $\mu > 0$ small enough. More precisely $C \leq G_1^* < G_2^* \leq c/\epsilon_J$ and $0 < \mu < \mu^* = \frac{c}{C}e^{-(8\epsilon_J)^{-3/3}}$, for $C < 32$ large enough and $c < 1/8$ small enough. Then, for any finite sequence of values $G_i \in (G_1^*, G_2^*)$, $i = 1, \dots, n$, there exists a trajectory of the ER3BP such that $G(T_i) = G_i$, $i = 1, \dots, n$ for some $0 < T_i < T_{i+1}$. In particular, for any two values $G_1 < G_2 \in (G_1^*, G_2^*)$, there exists a trajectory such that $G(0) < G_1$, and $G(T) > G_2$ for some time $T > 0$.*

Chapter 8

Generic global diffusion for analytic a priori unstable systems

8.1 Introduction

For a nearly integrable Hamiltonian

$$H_\epsilon(I, \varphi) = H_0(I) + \epsilon H_1(I, \varphi), \quad (8.1)$$

a large part of the phase space is occupied by invariant KAM tori, making the system remarkably stable. Arnold diffusion is the study of topological instability in the complement of these KAM tori. The instability is created by resonances of the unperturbed frequency $\partial_I H_0(I)$. Indeed, in the first example of Arnold diffusion, Arnold [Arn64] considers the system

$$H_\epsilon = \frac{1}{2}(I_1^2 + I_2^2) + \epsilon(\cos \varphi_1 - 1) + \epsilon\mu(\cos \varphi_1 - 1)f(\varphi_2, t), \quad (8.2)$$

and proves that for suitable f and $0 < \mu \ll \epsilon$, there exists an orbit whose I_2 component change for an arbitrary large distance along the resonance $\{I_1 = 0\}$. Since μ is taken much smaller than ϵ , after a rescaling we may assume $\epsilon = 1$ in (8.2). This type of systems are called *a priori unstable* because the hyperbolic structure that leads to instability exists even at $\mu = 0$. The original problem (8.1) is called *a priori stable*, since the unperturbed system is completely integrable.

We have seen much progress in proving Arnold diffusion holds for *generic* C^r *a priori stable* systems for a *convex* H_0 , while the non-convex case remains wide open. We refer to [DH09, Mat12, Che17, Che19, Mar24, KZ20] for a non-exhaustive list of references. Those results are built on decades of progress on *a priori unstable* systems, see [Ber08, CY04, CY09, DLS06a, DLS08, Tre02, Tre04, BKZ16, GM22] and reference therein.

For real analytic systems, however, generic Arnold diffusion for *a priori stable* systems remain wide open. A large body of literature is dedicated to analytic examples of diffusion (for example [Zha11, KLS14]) and concrete systems like the N-body problems (for example [DKRS19, CFG24]). A related problem is the instability around elliptic fixed points or KAM tori, see [Dou88, FF22, Fay23]. For generic analytic perturbation of *a priori chaotic* systems, we mention the works of Gelfreich-Turaev [GT17] and Clarke-Turaev [CT23]. For *a priori unstable* systems, Delshams-Schaefer [DS17, DS18] studied the diffusion for a finite parameter family of perturbations.

The most relevant work to our results is [CL22] by Chen-de la Llave, who proved that for an *a priori unstable* system of the type

$$H_\epsilon = H_0(p, q, I) + \epsilon h(p, q, I, \varphi, t), \quad H_0(p, q, I) = G(I) + \sum_{i=1}^d \pm \left(\frac{1}{2} p_i^2 + V_i(q_i) \right), \quad (8.3)$$

$$p \in \mathbb{R}^n, q \in \mathbb{T}^n, I \in \mathbb{R}^d, \varphi \in \mathbb{T}^d, t \in \mathbb{T},$$

for a Mañé generic analytic perturbation H_1 (precise definition to be given later), there exists a diffusion orbit $(p, q, I, \varphi)(t)$ and $T > 0$ such that

$$|I(T) - I(0)| > \rho(H_1).$$

The point is that the magnitude of the topological instability does not vanish as $\epsilon \rightarrow 0$.

Our main result is that in a system of type (8.3), for $n = 1$ and $d = 1$, one can achieve *large-scale* diffusion for a Mañé generic analytic perturbation independent of H_1 . Indeed, our main result claims that given *any* $I^- < I^+$, for a Mañé generic analytic potential H_1 , *for all* $\epsilon < \epsilon_0(H_1)$, the system $H_0 + \epsilon H_1$ admits an orbit $(p, q, I, \varphi)(t)$ and $T > 0$ such that

$$I(0) < I^- < I^+ < I(T).$$

We call this large drift of the variable I *global diffusion*, compared to the local-scale diffusion of [CL22]. In particular, it follows from our result that Arnold's Theorem in [Arn64] remains true for a generic analytic perturbation of the type $h(\varphi_1, \varphi_2, t)$ instead of the special perturbation $(\cos \varphi_1 - 1)f(\varphi_2, t)$ chosen by Arnold.

One of our goals is to show generic global instability in a simple way so that it is accessible to a wider audience. To avoid technical complications, we have restricted ourselves to the one-dimensional case both with regard to the pendulum variables p, q , and the action-angle variables I, φ .

On the one hand, following the philosophy that more hyperbolic variables generate more instability paths, we believe that, by appropriately modifying the Melnikov Potential used, the method followed in this work could be applied to the case in which this hyperbolicity is produced by several pendulums, although this would affect the genericity of the unperturbed model.

On the other hand, the introduction of multi-dimensional action variables entails the treatment of several possible instability directions as well as the appearance of resonances, and here the method presented could not be applied directly.

Besides the a-priori unstable system (8.3), it is interesting to consider the *coupled* a priori unstable systems which include also a term coupling I, p . These coupled systems seems more relevant in the study of normal forms in near integrable systems, see, for instance [DG01]. In these coupled a priori unstable systems, the scattering map involves a phase-shift. We will not consider this here. Moreover, since the name a priori unstable has already been used many times in the literature, we have preferred not to include the adjective “uncoupled” throughout the text for the a priori unstable systems we are considering.

Our proof uses the scattering map approach (see [DLS06a, DLS08, GL06, GLMS20]). The diffusion orbit travels close to a normally hyperbolic invariant manifold (NHIM), and the dynamics can be described by the scattering map (homoclinic excursion) and inner map (dynamics restricted to the NHIM). The scattering map can be computed to the first order by means of the Melnikov potential $\mathcal{L}_h(I, \varphi, s)$ introduced in (8.6). Our approach is twofold:

- Generically, for every fixed I the Melnikov potential $\mathcal{L}_h(I, \cdot, \cdot)$ admits a non-degenerate local minimum. These local minima are obtained from local extension of the global minima.
- Near these local minima of the Melnikov potential, we show that there exists a pseudo-orbit of the scattering map and the restricted dynamics to the invariant manifold whose I component is increasing. We call this the “Ascending Ladder”. We then show that there exists a trajectory of the Hamiltonian system which shadows the ascending ladder.

It is important to emphasize that these previous conditions that guarantee genericity are fully verifiable in specific systems from Physics, Engineering or other applied fields, and allow the explicit calculation of the pseudoorbits of the scattering map which are then shadowed by trajectories of the system.

In the approach followed, no quantitative estimates of diffusion time are made nor is there an attempt to optimize them, since our goal is to propose a very general, simple, and constructive diffusion mechanism. In pursuit of simplicity for the reader, this chapter is almost self-contained, except for the theory of scattering maps and the geometric mechanism of diffusion (Proposition 8.2, equation (8.8), and Lemma 8.17), for which specific references are given.

8.2 Formulation of the main result

Consider the Hamiltonian

$$H_\epsilon(p, q, I, \varphi, t) = \frac{1}{2}p^2 + V(q) + G(I) + \epsilon h(p, q, I, \varphi, t), \quad (8.4)$$

where

$$(p, q, I, \varphi, t) \in M := \mathbb{R} \times \mathbb{T} \times \mathbb{R} \times \mathbb{T} \times \mathbb{T}.$$

Assume that

1. V has a non-degenerate global maximum; without loss of generality, suppose it is at $q = 0$.
2. For the Hamiltonian system $\frac{1}{2}p^2 + V(q)$, the stable and unstable manifolds of $(0, 0)$ intersect along a homoclinic trajectory
$$\left\{ (p_0(t), q_0(t)) : t \in \mathbb{R} \right\}. \quad (8.5)$$
3. The frequency map $I \mapsto \omega(I) := G'(I)$ admits the following property: For every interval $(I_1, I_2) \subset [I^-, I^+]$, $\omega((I_1, I_2))$ contains a nontrivial interval. Note that in particular, this is satisfied if $\omega(I)$ never vanishes.

Definition 6. Let $U \subset M$ be an open set. We define its σ -complex neighborhood to be

$$\mathcal{B}_\sigma(U) = \{ \tilde{z} = (p, q, I, \varphi, t) \in \mathbb{C} \times (\mathbb{C}/\mathbb{Z}) \times \mathbb{C} \times (\mathbb{C}/\mathbb{Z}) \times (\mathbb{C}/\mathbb{Z}) : \text{dist}(\tilde{z}, U) < \sigma \}.$$

Let $\mathcal{A}_\sigma(U)$ denote the space of all real analytic functions on U that can be extended to a bounded analytic function on $\mathcal{B}_\sigma(U)$. Equipped with the supremum norm, this is a Banach space. Let

$$Q = \mathbb{T} \times \mathbb{T} \times \mathbb{T}$$

denote the configuration space, i.e., the space of the variables (q, φ, t) . We will also consider the complex strip

$$\mathcal{D}_\sigma = \{(q, \varphi, t) \in (\mathbb{C}/\mathbb{Z}) \times (\mathbb{C}/\mathbb{Z}) \times (\mathbb{C}/\mathbb{Z}) : \|\Re(q, \varphi, t)\| < \sigma\}$$

and the space $\mathcal{P}_\sigma$ of real analytic functions on Q extensible to a bounded function on $\mathcal{D}_\sigma$. Identifying a function $f \in \mathcal{P}_\sigma$ with its trivial extension to $\mathcal{B}_\sigma(M)$, $\mathcal{P}_\sigma \subset \mathcal{B}_\sigma(U)$ for any U .

Theorem 8.1. Let $U \subset M$ be open. Let $I^- < I^+$ be such that

$$\{(p_0(t), q_0(t)) : t \in \mathbb{R}\} \times [I^-, I^+] \times \mathbb{T} \times \mathbb{T} \subset U.$$

Then for any $h \in \mathcal{A}_\sigma(U)$, there exists an open and dense set $\mathcal{G}_h$ of $\mathcal{P}_\sigma$ such that, for any $g \in \mathcal{G}_h$, the following holds for the Hamiltonian system

$$H_\epsilon = \frac{1}{2}p^2 + V(q) + G(I) + \epsilon(h(p, q, I, \varphi, t) + g(q, \varphi, t)).$$

There exists $\epsilon_0(h + g) > 0$ such that for all $\epsilon \in (0, \epsilon_0)$, the system H_ϵ admits a trajectory $(p, q, I, \varphi)(t)$, $t \in [0, T]$, satisfying

$$I(0) < I^-, \quad I(T) > I^+.$$

Remark 8.1. Our theorem says that for the system $\frac{1}{2}p^2 + V(q) + G(I) + \epsilon h$ a diffusion trajectory whose I variable varies over the range $[I^-, I^+]$ always exists after a (possibly arbitrarily small) generic potential perturbation ϵg . This is commonly referred to as *generic in the sense of Mañé* (see [Man92]), which is stronger than genericity in the space $\mathcal{A}_\sigma$. The size of diffusion is independent of the size of the function $G(I)$, which may be relevant to multi-time-scale systems.

Remark 8.2. Let $\mathcal{X}$ be a subspace of the Banach space $\mathcal{A}_\sigma$. We say a subset $\mathcal{G} \subset \mathcal{A}_\sigma$ is generic along transversals $\mathcal{X}$ if for any $h \in \mathcal{A}_\sigma$, the set $\{g \in \mathcal{X} : h + g \in \mathcal{G}\}$ is open and dense in $\mathcal{X}$. The concept of Mañé genericity is then a special case when the transversals are chosen to be the space of all potentials.

8.3 Geometric description of diffusion for a generic perturbation

8.3.1 Scattering map and the geometric construction of diffusion

For $\varepsilon = 0$, Hamiltonian (8.4) becomes

$$\frac{1}{2}p^2 + V(q) + G(I),$$

with associated equations

$$\dot{p} = V'(q), \quad \dot{q} = p, \quad \dot{I} = 0, \quad \dot{\varphi} = \omega(I), \quad \dot{s} = 1,$$

so that I is a constant of motion and the flow based on the homoclinic trajectory (8.5) has the form

$$\Phi_0^t(I, \varphi) = (p_0(t), q_0(t), I, \varphi + t\omega(I)).$$

For any $I \in \mathbb{R}$, $\tilde{\mathcal{T}}_I^0 = \{(0, 0, I, \varphi, s); (\varphi, s) \in \mathbb{T}^2\}$ is an invariant 2D-torus under the flow of the system with frequency $\tilde{\omega}(I) = (\omega(I), 1)$ and is called a *whiskered torus*. For each whiskered torus $\tilde{\mathcal{T}}_I^0$, we have associated coincident stable and unstable 3D-manifolds called *whiskers*, which we denote by

$$W^0 \tilde{\mathcal{T}}_I^0 = \left\{ (p_0(\tau), q_0(\tau), I, \varphi, s) : \tau \in \mathbb{R}, (\varphi, s) \in \mathbb{T}^2 \right\}.$$

The union of all whiskered tori $\tilde{\mathcal{T}}_I^0$

$$\tilde{\Lambda}_0 = \left\{ (0, 0, I, \varphi, s) : (I, \varphi, s) \in \mathbb{R} \times \mathbb{T}^2 \right\}$$

is a 3D-*Normally Hyperbolic Invariant Manifold* (NHIM) with 4D-coincident stable and unstable invariant manifolds, forming a so-called *separatrix*, given by

$$W^0 \tilde{\Lambda}_0 = \{(p_0(\tau), q_0(\tau), I, \varphi, s) : \tau \in \mathbb{R}, (I, \varphi, s) \in \mathbb{R} \times \mathbb{T}^2\}.$$

For $0 < \varepsilon \ll 1$, the NHIM $\tilde{\Lambda}_0$ is preserved to a NHIM $\tilde{\Lambda}_\varepsilon$ [DLS08, Sec. 4.2], and the separatrix $W^0 \tilde{\Lambda}_0$ is locally preserved to the stable manifold $W^s(\tilde{\Lambda}_\varepsilon)$ and unstable manifold $W^u(\tilde{\Lambda}_\varepsilon)$ of $\tilde{\Lambda}_\varepsilon$, which are defined as

$$W^{s,u}(\tilde{\Lambda}_\varepsilon) = \bigcup_{x \in \tilde{\Lambda}_\varepsilon} W_x^{s,u}(\tilde{\Lambda}_\varepsilon), \quad W_x^{s,u}(\tilde{\Lambda}_\varepsilon) = \left\{ z : \text{dist}(\Phi_\varepsilon^t(z), \Phi_\varepsilon^t(x)) \xrightarrow{t \rightarrow \pm\infty} 0 \right\}.$$

In general, these two invariant manifolds no longer coincide, that is, the separatrix splits. The existence of this splitting can be detected by a perturbation argument in terms of the *Melnikov potential*

$$\begin{aligned} \mathcal{L}(I, \varphi, s) = \mathcal{L}_h(I, \varphi, s) := & - \int_{-\infty}^{\infty} [h(p_0(t), q_0(t), \varphi + t\omega(I), I, s + t) \\ & - h(0, 0, \varphi + t\omega(I), I, s + t)] dt. \end{aligned} \quad (8.6)$$

Notice that this integral is absolutely convergent, because the homoclinic trajectory (8.5) converges exponentially fast to $(0, 0)$ as $t \rightarrow \pm\infty$.

Proposition 8.2 ([DLS06a]). *Given $(I, \varphi, s) \in [-I^*, I^*] \times \mathbb{T}^2$, assume that the real function*

$$\tau \in \mathbb{R} \mapsto \mathcal{L}(I, \varphi - \tau\omega(I), s - \tau) \in \mathbb{R} \quad (8.7)$$

has a non-degenerate critical point $\tau^ = \tau^*(I, \varphi, s)$. Then, for $0 < \varepsilon$ small enough, there exists a unique transverse homoclinic point $\tilde{z}_\varepsilon$ to $\tilde{\Lambda}_\varepsilon$ of Hamiltonian (8.4), which is ε -close to the point $\tilde{z}^*(I, \varphi, s) = (p_0(\tau^*), q_0(\tau^*), I, \varphi, s) \in W^0(\tilde{\Lambda})$:*

$$\begin{aligned} \tilde{z}_\varepsilon = \tilde{z}_\varepsilon(I, \varphi, s) &= (p_0(\tau^*) + O(\varepsilon), q_0(\tau^*) + O(\varepsilon), I, \varphi, s) \\ \text{and } \tilde{z}_\varepsilon &\in W^u(\tilde{\Lambda}_\varepsilon) \cap W^s(\tilde{\Lambda}_\varepsilon). \end{aligned}$$

Using this Proposition we can introduce the notion of the *scattering map*, which plays a central rôle in our mechanism for detecting diffusion. Let W be an open set of $[-I^*, I^*] \times \mathbb{T}^2$ such that the invariant manifolds of the NHIM $\tilde{\Lambda}_\varepsilon$ intersect transversely along a homoclinic manifold $\Gamma_\varepsilon = \{\tilde{z}_\varepsilon(I, \varphi, s), (I, \varphi, s) \in W\}$ and for any $\tilde{z}_\varepsilon \in \Gamma_\varepsilon$ there exists a unique $\tilde{x}_\pm = \tilde{x}_{\pm, \varepsilon}(I, \varphi, s) \in \tilde{\Lambda}_\varepsilon$ such that $\tilde{z}_\varepsilon \in W_\varepsilon^s(\tilde{x}_-) \cap W_\varepsilon^u(\tilde{x}_+)$. Let

$$H_\pm = \bigcup \{\tilde{x}_\pm = \tilde{x}_{\pm, \varepsilon}(I, \varphi, s) : (I, \varphi, s) \in W\}.$$

The scattering map associated to Γ_ε is the map

$$\begin{aligned} S_\varepsilon : H_- &\longrightarrow H_+ \\ \tilde{x}_- &\longmapsto S_\varepsilon(\tilde{x}_-) = \tilde{x}_+. \end{aligned}$$

Notice that the domain of definition of the scattering map depends on the homoclinic manifold chosen, but it is a subset of $O(1)$ size in $\tilde{\Lambda}_\varepsilon$ with respect to ε , i.e., it has a non-trivial limit as $\varepsilon \rightarrow 0$. If necessary,

we can even restrict it further to avoid a non trivial monodromy in the definition of the scattering map, see, for instance, the comments in [DLS00]. Therefore, for the characterization of the scattering maps, it is required to select the homoclinic manifold Γ_ϵ , which is determined by the function $\tau^*(I, \varphi, s)$. Once a function $\tau^*(I, \varphi, s)$ is chosen, by the geometric properties of the scattering map, particularly its exactness, see [DLS08], the scattering map $S_\epsilon = S_{\epsilon, \tau^*}$ has the explicit form [DLS06a, eq. (9.9)]

$$S_\epsilon(I, \varphi, s) = \left(I + \epsilon \partial_\varphi L^* + \mathcal{O}(\epsilon^2), \varphi - \epsilon \partial_I L^* + \mathcal{O}(\epsilon^2), s \right), \quad (8.8)$$

where $L^* = L^*(I, \varphi, s)$ is the *Poincaré function* defined by

$$L^*(I, \varphi, s) = \mathcal{L}(I, \varphi - \tau^*(I, \varphi, s) \omega(I), s - \tau^*(I, \varphi, s)). \quad (8.9)$$

Notice that if $\tau^*(I, \varphi, s)$ is a critical point of (8.7), $\tau^*(I, \varphi, s) - \sigma$ is a critical point of

$$\begin{aligned} \tau \in \mathbb{R} &\mapsto \mathcal{L}(I, \varphi - (\tau + \sigma) \omega(I), s - (\tau + \sigma)) \\ &= \mathcal{L}(I, \varphi - \sigma \omega(I) - \tau \omega(I), s - \sigma - \tau) \end{aligned} \quad (8.10)$$

Since $\tau^*(I, \varphi - \sigma \omega(I), s - \sigma)$ is a critical point of the right-hand side of (8.10), by the uniqueness in W we can conclude that

$$\tau^*(I, \varphi - \sigma \omega(I), s - \sigma) = \tau^*(I, \varphi, s) - \sigma.$$

Thus, by (8.9), the Poincaré function L^* satisfies

$$L^*(I, \varphi - \sigma \omega(I), s - \sigma) = L^*(I, \varphi, s), \quad \sigma \in \mathbb{R},$$

and, in particular, for $\sigma = s$,

$$L^*(I, \varphi - s \omega(I), 0) = L^*(I, \varphi, s).$$

In other words, the Poincaré function L^* is invariant under the flow $\dot{\varphi} = \omega(I), \dot{s} = 1$ or, equivalently, is constant along any line in the (φ, s) -plane $\varphi - s \omega(I) = \text{constant}$.

These previous equations are telling us that we can reduce the variables in both the Poincaré function L^* and the time τ^* . Indeed, writing them for $\sigma = s$ and introducing the variable

$$\theta = \varphi - s \omega(I), \quad (8.11)$$

we can define the *reduced Poincaré function* $\mathcal{L}^*$ as well as the reduced time $\bar{\tau}^*$, defined only in the variables (I, θ) , as

$$\begin{aligned} \mathcal{L}^*(I, \theta) &:= L^*(I, \varphi - s \omega(I), 0) = L^*(I, \varphi, s), \\ \bar{\tau}^*(I, \theta) &:= \tau^*(I, \varphi - s \omega(I), 0) = \tau^*(I, \varphi, s) - s. \end{aligned} \quad (8.12)$$

Moreover we also have

$$\mathcal{L}^*(I, \theta) = \mathcal{L}(I, \theta - \bar{\tau}^*(I, \theta) \omega(I), -\bar{\tau}^*(I, \theta)). \quad (8.13)$$

From now on, both $\tau^*(I, \varphi, s)$ and $\bar{\tau}^*(I, \theta)$ will be used at our convenience.

Note that the variable s is fixed under the scattering map (8.8). As a consequence, we can consider, for instance, the section

$$\Lambda_\epsilon = \tilde{\Lambda}_\epsilon \cap \{s = 0\}$$

and the scattering map S_ϵ is well defined on Λ_ϵ .

In the variables (I, θ) introduced in (8.11), the scattering map has the simple form

$$\mathcal{S}_\epsilon(I, \theta) = \mathcal{S}_\epsilon(I, \varphi) = \left(I + \epsilon \frac{\partial \mathcal{L}^*}{\partial \theta}(I, \theta) + \mathcal{O}(\epsilon^2), \theta - \epsilon \frac{\partial \mathcal{L}^*}{\partial I}(I, \theta) + \mathcal{O}(\epsilon^2) \right).$$

So, up to $\mathcal{O}(\epsilon^2)$ terms, $\mathcal{S}_\epsilon(I, \theta)$ is the $-\epsilon$ times flow of *autonomous* Hamiltonian $\mathcal{L}^*(I, \theta)$. In particular, a finite number of iterates under the scattering map follow the level curves of $\mathcal{L}^*$ up to $\mathcal{O}(\epsilon^2)$.

Remark 8.3. $\mathcal{S}_\epsilon$ is close to identity only when there is no phase shift, i.e., thanks to the fact that we are only dealing with an *uncoupled* a priori unstable system. If we introduce a coupling term between p and I in Hamiltonian (8.4), then one might expect that

$$\mathcal{S}_\epsilon(I, \theta) = (I, \theta + \gamma(I)) + \mathcal{O}(\epsilon),$$

where $\gamma(I)$ is the phase shift. In this case $\mathcal{S}_\epsilon$ is no longer close to identity.

We now introduce another map defined on the NHIM Λ_ϵ . Since $\tilde{\Lambda}_\epsilon$ is invariant under the Hamiltonian flow and Λ_ϵ is a global section, there exists a Poincaré map

$$T_\epsilon : \Lambda_\epsilon \rightarrow \Lambda_\epsilon.$$

The map T_ϵ preserves the restriction of the symplectic form to Λ_ϵ , and has the expansion

$$T_\epsilon(I, \varphi) = (I, \varphi + \omega(I)) + \mathcal{O}(\epsilon).$$

We call this map the *inner map*.

In the sequel, we call a measure on a manifold a *smooth measure* if it is given by a non-zero density multiplied by the volume form supported on an open set.

Lemma 8.3. *There exists $\epsilon_0 > 0$ such that for all $0 < \epsilon < \epsilon_0$ the following hold. There exists $\gamma_-, \gamma_+ \subset \Lambda_\epsilon$ that are graphs over the variable θ and invariant under T_ϵ , such that the T_ϵ -invariant subset of Λ_ϵ bounded by γ_- and γ_+ contains*

$$[I^-, I^+] \times \mathbb{T} \cap \Lambda_\epsilon.$$

In particular, the dynamics of T_ϵ on Λ_ϵ preserves a smooth measure whose support contains $[I^-, I^+] \times \mathbb{T} \cap \Lambda_\epsilon$.

We now restrict Λ_ϵ to the compact invariant set between $\gamma_\pm$, which is still called Λ_ϵ .

The following statement is a minor modification of the main result of [GLMS20], and is our main technical tool for construction of diffusion orbits. This result is non-perturbative, so we formulate it for a general Hamiltonian H with a compact invariant NHIM Λ .

Proposition 8.4. *Assume the Hamiltonian H admits a compact NHIM Λ on which multiple scattering maps S_j are defined on open subsets of Λ . Assume that the inner map T preserves a smooth measure on Λ , and each S_j maps positive (Lebesgue) measure sets to positive measure sets and zero measure sets to zero measure sets.*

Let $x_0, \dots, x_{N-1}$ be a pseudo-orbit¹ under the iterate of either the inner map or one of the scattering maps, that is,

$$x_{i+1} = f_i(x_i), \quad 1 \leq i \leq N-1,$$

where f_i is either T or one of the scattering maps S_j . Then for any $\delta > 0$, there exists a trajectory $z : \mathbb{R} \rightarrow M$ of H_ϵ shadowing the pseudo-orbit x_i , i.e., there exists $t_0 < \dots < t_N$ such that

$$\text{dist}(x_i, z(t_i)) < \delta, \quad 0 \leq i \leq N.$$

Theorem 3.7 of [GLMS20] states that if the pseudo-orbit only involves the scattering maps, then the shadowing result holds. However, the proof in [GLMS20] can be adapted to prove Proposition 8.4 with minor changes, see Appendix 8.5.

Remark 8.4. Proposition 8.4 does not provide an estimate of “diffusion time”, i.e., upper bound estimates on t_i . This is due to the lack of return time estimates for the inner dynamics. See Remark 3.15 of [GLMS20].

8.3.2 Conditions on the Melnikov potential

Definition 7. *Define $\mathcal{G}(I^-, I^+)$ to be the set of functions h in the space $\mathcal{A}_\sigma(U)$ introduced in Def. 6 for which the following holds:*

- *There exists intervals (I_j^-, I_j^+) , $j = 1, \dots, k$ such that*

$$I_1^- < \dots < I_k^-, \quad (I_j^-, I_j^+) \cap (I_{j+1}^-, I_{j+1}^+) \neq \emptyset, \quad j = 1, \dots, k-1,$$

and

$$[I^-, I^+] \subset \bigcup_j (I_j^-, I_j^+).$$

¹We use the term pseudo-orbit to stress that it is not an orbit of the Hamiltonian dynamics, even though it is an orbit of the polysystem (i.e. iteration under multiple maps).

- For each j , there exists a smooth mapping

$$(\varphi_j^*, s_j^*) : [I_j^-, I_j^+] \rightarrow \mathbb{T} \times \mathbb{T},$$

such that for each $I \in [I_j^-, I_j^+]$, $(\varphi_j^*, s_j^*)(I)$ is a non-degenerate local minimum of the function

$$\mathcal{L}_h(I, \cdot, \cdot).$$

We will show (Proposition 8.5) that for a generic h , the associated Melnikov potential $\mathcal{L}_h(I, \varphi, s)$ satisfies the conditions in Definition 7. In fact, the local minima (φ_j^*, s_j^*) can be chosen as local extension of the global minima of $\mathcal{L}_h(I, \cdot, \cdot)$. Moreover, in Lemma 8.8 we will see that they generate local minima $\theta_j^*(I)$ of $\mathcal{L}_h^*(I, \cdot)$. In Figure 8.1, we give an illustration of the position of global minima over $\mathbb{T}$ for a typical reduced Poincaré function $\mathcal{L}_h^*(I, \theta)$.

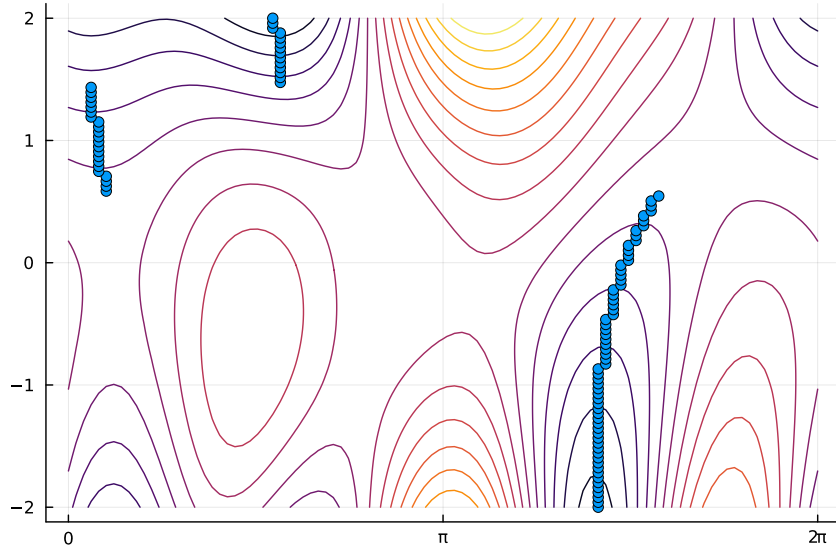


Figure 8.1: The levels curves and global minima of a typical reduced Poincaré function $\mathcal{L}_h^*(I, \theta)$ defined on $\mathbb{R} \times \mathbb{T}$. Note: the vertical coordinate is I and horizontal coordinate is θ .

Proposition 8.5. *For any $h \in \mathcal{A}_\sigma(U)$, there exists an open and dense set $\mathcal{G}_h \subset \mathcal{P}_\sigma$ such that $h + g \in \mathcal{G}(I^-, I^+)$ for all $g \in \mathcal{G}_h$.*

Proposition 8.6. *Suppose $h \in \mathcal{G}(I^-, I^+)$, then there exists $\epsilon_0(h) > 0$ such that for all $\epsilon \in (0, \epsilon_0)$, there exists an orbit $(p, q, I, \varphi)(t)$ of (8.4) and $T > 0$ such that*

$$I(0) < I^- < I^+ < I(T).$$

Proposition 8.5 will be proven later. In the sequel, let us fix $h \in \mathcal{G}(I^-, I^+)$ and prove existence of a diffusion trajectory.

Lemma 8.7. *Suppose $h \in \mathcal{G}(I^-, I^+)$, then there exists neighborhoods $U_j(I)$ of $(\varphi_j^*(I), s_j^*(I))$ for $I \in [I_j^-, I_j^+]$, and functions $\tau_j^*(I, \varphi, s)$*

$$(\varphi, s) \in U_j(I) \mapsto \tau_j^*(I, \varphi, s), \quad \tau_j^*(I, \varphi_j^*(I), s_j^*(I)) = 0,$$

depending smoothly in (φ, s, I) , such that each τ_j^* is a non-degenerate local minimum of

$$\tau \mapsto \mathcal{L}_h(I, \varphi - \tau\omega(I), s - \tau). \quad (8.14)$$

Proof. We need to solve the equation

$$\partial_\tau (\mathcal{L}_h(I, \varphi - \tau\omega(I), s - \tau)) = -(\omega(I) \cdot \partial_\varphi \mathcal{L}_h + \partial_s \mathcal{L}_h)|_{(I, \varphi - \tau\omega(I), s - \tau)} = 0. \quad (8.15)$$

Since $(\varphi_j^*(I), s_j^*(I))$ is a non-degenerate local minimum of $\mathcal{L}_h(I, \cdot, \cdot)$, $\tau = 0$ solves (8.15) at $(\varphi_j^*(I), s_j^*(I))$.

Since $\partial_{(\varphi,s)}^2 \mathcal{L}_h(I, \varphi_j^*(I), s_j^*(I))$ is positive definite, and

$$\begin{aligned} & \partial_\tau \left(-(\omega(I) \cdot \partial_\varphi \mathcal{L}_h + \partial_s \mathcal{L}_h) \Big|_{(I, \varphi - \tau \omega(I), s - \tau)} \right) \\ &= -\partial_\tau \left(\partial_{(\varphi,s)} \mathcal{L}_h \begin{bmatrix} \omega(I) \\ 1 \end{bmatrix} \Big|_{(I, \varphi - \tau \omega(I), s - \tau)} \right) \\ &= [\omega(I) \quad 1] \partial_{(\varphi,s)}^2 \mathcal{L}_h(I, \varphi - \tau \omega(I), s - \tau) \begin{bmatrix} \omega(I) \\ 1 \end{bmatrix}, \end{aligned}$$

we get

$$\partial_\tau^2 \left(\mathcal{L}_h(I, \varphi_j^*(I) - \tau \omega(I), s_j^*(I) - \tau) \right) > 0. \quad (8.16)$$

By the implicit function theorem, there exists a unique $\tau_j^*(I, \varphi, s)$, depending smoothly on (I, φ, s) in a neighborhood of the graph $(I, \varphi_j^*(I), s_j^*(I))$ over the variable I , solving equation (8.15). Moreover, τ_j^* are non-degenerate local minima for the mapping (8.14) due to (8.16). $\square$

In view of this Lemma, on each interval (I_j^-, I_j^+) and for $\theta = \varphi - s \omega(I)$ with $(\varphi, s) \in U_j(I)$, we can now introduce $\bar{\tau}_j^*(I, \theta)$ and $\mathcal{L}_j^*(I, \theta)$ by the same formulas (8.12, 8.13) defining $\bar{\tau}^*(I, \theta)$ and $\mathcal{L}^*(I, \theta)$, simply changing τ^* to τ_j^* . We will also denote

$$\theta_j^*(I) = \varphi_j^*(I) - s_j^* \omega(I).$$

Lemma 8.8. *For each $I \in [I_j^-, I_j^+]$, $\theta_j^*(I)$ is a non-degenerate minimum of $\mathcal{L}_j^*(I, \cdot)$.*

Proof. If $\tau^* = \tau^*(I, \varphi, s)$ is a critical point of (8.14), it satisfies

$$(\omega(I) \partial_\varphi \mathcal{L}_h + \partial_s \mathcal{L}_h) (I, \varphi - \tau^* \omega(I), s - \tau^*) = 0,$$

so that we also have

$$\begin{aligned} & (\omega(I) \partial_\varphi \mathcal{L}_h + \partial_s \mathcal{L}_h) \Big|_{(I, \theta - \bar{\tau}^*(I, \theta) \omega(I), -\bar{\tau}^*(I, \theta))} \\ &= (\omega(I) \partial_\varphi \mathcal{L}_h + \partial_s \mathcal{L}_h) \Big|_{(I, \theta - \tau^*(I, \theta, 0) \omega(I), -\tau^*(I, \theta, 0))} = 0. \end{aligned} \quad (8.17)$$

Denote by id the identity matrix, then differentiating (8.13) we get

$$\begin{aligned} \partial_\theta \mathcal{L}_j^*(I, \theta) &= \partial_\varphi \mathcal{L}_h \left(\text{id} - \partial_\theta \bar{\tau}_j^* \omega(I) - \partial_\theta \bar{\tau}_j^* \partial_s \mathcal{L}_h \right) \Big|_{(I, \theta - \bar{\tau}_j^* \omega(I), -\bar{\tau}_j^*)} \\ &= \left(\partial_\varphi \mathcal{L}_h - \partial_\theta \bar{\tau}_j^* (\omega(I) \partial_\varphi \mathcal{L}_h + \partial_s \mathcal{L}_h) \right) \Big|_{(I, \theta - \bar{\tau}_j^* \omega(I), -\bar{\tau}_j^*)} \\ &= \partial_\varphi \mathcal{L}_h \Big|_{(I, \theta - \bar{\tau}_j^* \omega(I), -\bar{\tau}_j^*)} \end{aligned}$$

by (8.17). Since $\bar{\tau}_j^* = \bar{\tau}_j^*(I, \theta_j^*) = \tau_j^*(I, \varphi_j^*(I), s_j^*(I)) = -s_j^*(I)$ by (8.12), we have that $(I, \theta - \bar{\tau}_j^* \omega(I), -\bar{\tau}_j^*) = (I, \varphi_j^*(I), s_j^*(I))$, and we get that $\theta_j^*(I)$ is a critical point of $\mathcal{L}_j^*(I, \cdot)$. Furthermore, repeating the same calculation, we have

$$\partial_{\theta\theta}^2 \mathcal{L}_j^* = \partial_{\varphi\varphi}^2 \mathcal{L}_h \Big|_{(I, \theta - \bar{\tau}_j^* \omega(I), -\bar{\tau}_j^*)}.$$

Since $\partial_{\varphi\varphi}^2 \mathcal{L}_h$ is positive definite at (φ_j^*, s_j^*) , θ_j^* is a non-degenerate local minimum. $\square$

Lemma 8.9 (Ascending ladder). *There exists $\delta_0 > 0$ such that for every $\delta \in (0, \delta_0)$, there exists a sequence of curves*

$$\gamma_{i,j} \subset [I^-, I^+] \times \mathbb{T} \quad 1 \leq i \leq m_j, 1 \leq j \leq k, l \in \{1, 2\}$$

such that the following holds.

1. *For each i, j , the curve $\gamma_{i,j}$ is a smooth graph over the variable I , i.e.,*

$$\gamma_{i,j} = \{(I, f_{i,j}(I)) : I \in [I_{i,j}^1, I_{i,j}^2]\}.$$

$\gamma_{i,j}$ is a segment of the level curve of $\mathcal{L}_j^$ and the Hamiltonian flow of $\mathcal{L}_j^*$ on $\gamma_{i,j}$ is increasing in the I component.*

3. $I_{m_j, j}^2 = I_{1, j+1}^1$ for all $j = 1, \dots, k-1$.

Let us also denote by $x_{i,j}^1, x_{i,j}^2$ the lower and upper end points of the curves $\gamma_{i,j}$.

Proof. Since $\theta_j^*(I)$ is a non-degenerate local minimum of $\partial_\theta \mathcal{L}_j^*(I, \cdot)$, for every $I \in [I_j^-, I_j^+]$, there exists $\phi(I) > \theta_j^*(I)$, such that

$$\partial_{\theta} \mathcal{L}_j^*(I, \phi(I)) > 0.$$

This means there is a segment $\gamma_j(I)$ of the level curve of $\mathcal{L}_j^*$, on which I is increasing under the Hamiltonian flow of $\mathcal{L}_j^*$. By compactness, there exists a finite collection $\gamma_{i,j}$ of such level curves, $1 \leq i \leq m_j$ such that $\bigcup_i \pi_I(\gamma_{i,j}) \supset [I_j^-, I_j^+]$. One can adjust the collection so that $\pi_I(\gamma_{i,j}) \cap \pi_I(\gamma_{i,j+1}) \neq \emptyset$ and $I_j^- \in \pi_I(\gamma_{1,j})$ and $I_j^+ \in \pi_I(\gamma_{m_j,j})$. It suffices to choose

$$\begin{aligned} I_{i,j}^1 &\in \pi_I(\gamma_{i,j}) \cap \pi_I(\gamma_{i,j-1}), & j \geq 2, \\ I_{i,j}^2 &\in \pi_I(\gamma_{i,j}) \cap \pi_I(\gamma_{i,j+1}), & j \leq m_j + 1, \end{aligned}$$

and $I_{1,j}^1, I_{2,j}^2$ satisfying (2) and (3); then truncate the curves $\gamma_{i,j}$ to the I interval $[I_{i,j}^1, I_{i,j}^2]$.

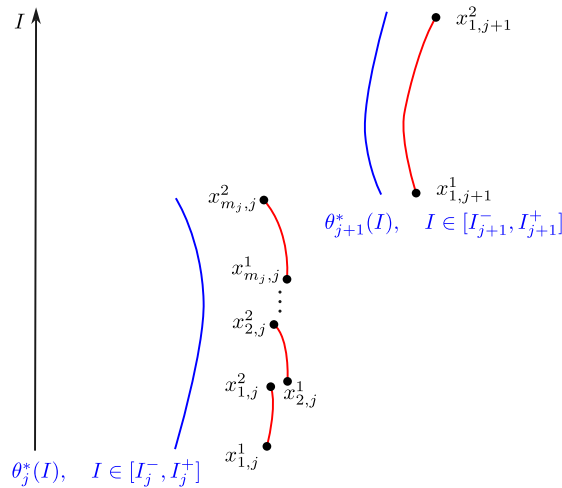


Figure 8.2: The ascending ladder

8.3.3 Constructing the transition chain

Proposition 8.10 (Transition chain). *Let $h \in \mathcal{G}(I^-, I^+)$, and let $\gamma_{i,j}$ be the ascending ladder constructed in Lemma 8.9. Then there is $\delta_1 > 0$ such that for every $\delta \in (0, \delta_1)$, there exists $\epsilon_0 > 0$ depending on h and δ , such that for every $\epsilon \in (0, \epsilon_0)$, there exist*

$$y_{i,j}^l \in [I^-, I^+] \times \mathbb{T}, \quad 1 \leq i \leq m_j, 1 \leq j \leq k, l \in \{1, 2\},$$

and $M_{i,j}, N_{i,j} \in \mathbb{N}$ such that the following hold.

Let $S_{j,\epsilon}$ denote the scattering map associated to $\mathcal{L}_j^*$, and T_ϵ denote the inner dynamics.

1. $S_{j,\epsilon}^{M_{i,j}}(y_{i,j}^1) = y_{i,j}^2.$
2. $T_\epsilon^{N_{i,j}}(y_{i,j}^2) = y_{i+1,j}^1, i = 1, \dots, m_j - 1.$
3. $T_\epsilon^{N_{m_j,j}}(x_{m_j,j}^2) = x_{1,j+1}^1, j = 1, \dots, k - 1.$
4. $|x_{i,j}^l - y_{i,j}^l| < \delta$ for all $i = 1, \dots, m_j, j = 1, \dots, k, l = 1, 2.$

We first prove Proposition 8.6 assuming Proposition 8.10.

Proof of Proposition 8.6. Let $I(\cdot)$ denote the projection $(I, \theta) \mapsto I$. By Lemma 8.9 and Proposition 8.10, there exists a pseudo-orbit $\{y_{i,j}^l\}$ of the maps $S_{j,\epsilon}$ and T_ϵ , such that $I(y_{1,1}^1) < I^-$ and $I(y_{m_k,k}^2) > I^+$. By Proposition 8.4, there exists an orbit $(q, p, I, \varphi)(t)$ of the original Hamiltonian system and $T > 0$ such that

$$I(0) < I^-, \quad I(T) > I^+.$$

□

The remaining section is dedicated to proving Proposition 8.10.

We have the following simple lemma about integrable twist maps.

Lemma 8.11. *Consider the map $T : [I^-, I^+] \times \mathbb{T} \rightarrow \mathbb{R} \times \mathbb{T}$ defined by*

$$T(I, \theta) = (I, \theta + \omega(I)).$$

Assume that for every interval $(I_1, I_2) \subset [I^-, I^+]$, $\omega((I_1, I_2))$ contains a nontrivial interval. Let $T_\epsilon : [I^-, I^+] \times \mathbb{T} \rightarrow \mathbb{R} \times \mathbb{T}$ be a family of maps such that

$$\|T_\epsilon - T\|_{C^1} \leq C\epsilon$$

for an independent constant C .

Then for any two C^1 graphs γ_1, γ_2 over the variable I

$$\gamma_1 = \{(I, f(I)) : I \in (I_1, I_2)\}, \quad \gamma_2 = \{(I, g(I)) : I \in (I_1, I_2)\},$$

$x_1 \in \gamma_1$ and $\delta > 0$, there exists $\epsilon_0 > 0$, $N \in \mathbb{N}$, $x_2 \in \gamma_2$, $\delta' > 0$ depending on x_1 , δ depending only on T and C , and I_1, I_2 , such that for all $\epsilon \in (0, \epsilon_0)$,

$$T_\epsilon^N(B_\delta(x_1)) \supset B_{\delta'}(x_2).$$

Proof. By assumption, $\omega((I_1, I_2))$ contains a nontrivial interval (a, b) . Let $c_1 = \inf_{I \in (I_1, I_2)} (f(I) - g(I))$ and $c_2 = \sup_{I \in (I_1, I_2)} (f(I) - g(I))$, then

$$\{f(I) - g(I) + N\omega(I) : I \in (I_1, I_2)\} \supset (Na + c_2, Nb + c_1). \quad (8.18)$$

Let N be such that $N(b - a) + c_1 - c_2 > 1$, then the set (8.18) projects onto the torus $\mathbb{T}$ in the θ component. This implies

$$T^N(\gamma) = \{f(I) + \omega(I) : I \in (I_1, I_2)\} \cap \gamma_2 \neq \emptyset$$

as subsets of $\mathbb{R} \times \mathbb{T}$. Denote the intersection $x_2 = T^N(x_1)$ where $x_1 \in \gamma_1$, $x_2 \in \gamma_2$.

It follows that there exists $\delta_1 > 0$ depending only on T and N such that

$$T^N(B_\delta(x_1)) \supset B_{\delta_1}(x_2).$$

Moreover, we can choose ϵ_0 small enough such that for all $\|T_\epsilon - T\|_{C^1} < C\epsilon_0$, we have

$$T_\epsilon^N(B_\delta(x_1)) \supset B_{\delta_1/2}(x_2).$$

□

Let $\gamma_{i,j}$, $1 \leq i \leq m_j$, $1 \leq j \leq k$, $l = 1, 2$ be the ascending ladder constructed in Lemma 8.9.

Lemma 8.12. *There exists $\delta_0 > 0$ such that for any $\delta \in (0, \delta_0)$, there exists $\epsilon_0 > 0$ and $C > 1$ depending only on the perturbation h and δ , such that for all $1 \leq i \leq m_j$, $1 \leq j \leq k$, any $x_1, x_2 \in \gamma_{i,j}$ with $\pi_I(x_1) < \pi_I(x_2)$, and $\epsilon < \epsilon_0$ there exists $M \in \mathbb{N}$ depending on $x_1, x_2, \delta, \epsilon$ such that*

$$S_{\epsilon,j}^M(B_\delta(x_1)) \supset B_{\delta/C}(x_2),$$

where $B_r(x)$ denote the ball of radius r at x .

Proof of Lemma 8.12. Let ϕ_j^t denote the Hamiltonian flow defined by the Hamiltonian $\mathcal{L}_j^*$. By construction, there exists $t > 0$ such that

$$\phi_j^t(x_1) = x_2$$

There exists $c > 0$ (depending only on $\mathcal{L}_j$, which depends only on h) and a local flow-box coordinate

$$\chi_{i,j} : (-c, t+c) \times (-c, c) \rightarrow \mathbb{T} \times \mathbb{R}$$

such that $x_1 = \chi_{i,j}(0, 0)$ and

$$\phi^t \circ \chi_{i,j}(s, m) = \chi_{i,j}(s+t, m).$$

In particular, $x_2 = \chi_{i,j}(0, t)$. Let $M = \lfloor t/\epsilon \rfloor$. Since $S_{\epsilon,j} = \phi_{\epsilon,j}^\epsilon + O(\epsilon^2)$, $S_{\epsilon,j}^M = \phi_{\epsilon,j}^{\epsilon t} + O(\epsilon)$,

$$\chi_{i,j}^{-1} \circ S_{\epsilon,j}^M \circ \chi_{i,j}(s, m) = (s+t, m) + O(\epsilon).$$

For any $r \in (0, c)$ and ϵ_0 small enough, we have

$$\chi_{i,j}^{-1} \circ S_{\epsilon,j}^M \circ \chi_{i,j}(B_r(s, m)) \supset B_{r/2}(s+t, m).$$

Let $C_1 = \max \{ \sup \|D\chi_{i,j}\|, \sup \|D\chi^{-1}\| \}$ which depends only on the perturbation h . Then if $C_1\delta \in (0, c)$,

$$\begin{aligned} S_{\epsilon,j}^M(B_\delta(x_1)) &\supset \chi_{i,j} \circ \chi_{i,j}^{-1} \circ S_{\epsilon,j}^M \circ \chi_{i,j}(B_{\delta/C_1}(s, m)) \\ &\supset \chi_{i,j}(B_{\delta/(2C_1)}(s+t, m)) \supset B_{\delta/(2C_1^2)}(x_2). \end{aligned}$$

This conclude the proof of Lemma 8.12. $\square$

Proof of Proposition 8.10. We now construct a sequence of balls

$$B_{\delta_{i,j}^l}(z_{i,j}^l) \subset B_\delta(x_{i,j}^l),$$

and $M_{i,j}, N_{i,j} \in \mathbb{N}$ such that

$$S_{\epsilon,j}^{M_{i,j}}(B_{\delta_{i,j}^1}(z_{i,j}^1)) \supset B_{\delta_{i,j}^2}(z_{i,j}^2), \quad 1 \leq i \leq m_j, \quad 1 \leq j \leq k, \quad (8.19)$$

and

$$T_\epsilon^{N_{i,j}}(B_{\delta_{i,j}^2}(z_{i,j}^2)) \supset B_{\delta_{i^*,j^*}^1}(z_{i^*,j^*}^1),$$

where $(i^*, j^*) = (i+1, j)$ if $i < m_j$ and $(i^*, j^*) = (1, j+1)$ if $i = m_j$ and $j < k$. This implies existence of $y_{i,j}^l \in B_{\delta_{i,j}^l}(z_{i,j}^l)$ satisfying the conclusion of our Proposition.

We choose $\delta_{1,1}^1 = \delta$ and $z_{1,1}^1 = x_{1,1}^1$. Constructing by induction, we assume $\delta_{i,j}^1$ and $z_{i,j}^1$ are already chosen. Choose $z_{i,j}^2 = x_{i,j}^2$ and apply Lemma 8.12 to get existence of $\epsilon_0 > 0$ and $M_{i,j}^\epsilon \in \mathbb{N}$ and $\delta_{i,j}^2$ such that (8.19) holds for all $\epsilon \in (0, \epsilon_0)$.

The curves $\gamma_{i,j}$ and γ_{i^*,j^*} are given by graphs over the variable I

$$\gamma_{i,j} = \{(I, f(I)) : I \in [I_{i,j}^1, I_{i,j}^2]\}, \quad \gamma_{i^*,j^*} = \{(I, g(I)) : I \in [I_{i^*,j^*}^1, I_{i^*,j^*}^2]\},$$

where $I_{i,j}^2 = I_{i^*,j^*}^1$. Extending these curves along the level curves of $\mathcal{L}_j^*$ and $\mathcal{L}_{j^*}^*$, we may assume that the extended curves overlap in I direction for some interval

$$I \in [I_{i,j}^2, I_{i,j}^2 + c].$$

Lemma 8.11 applies to the inner map. By possibly reducing ϵ_0 , there exists $N \in \mathbb{N}$, $z_{i^*,j^*}^1 \in \gamma_{i^*,j^*}$, and $\delta_{i^*,j^*}^1 > 0$ such that for all $\epsilon \in (0, \epsilon_0)$,

$$T^N(B_{\delta_{i,j}^2}(z_{i,j}^2)) \supset B_{\delta_{i^*,j^*}^1}(z_{i^*,j^*}^1).$$

We can continue the construction until all the balls are defined. Note that we need to reduce ϵ_0 up to finitely many times, but it will be well defined at the end of the construction. This concludes the proof of Proposition 8.10. $\square$

8.4 Genericity

We prove Proposition 8.5 in this section. The proof follows a standard parametric transversality argument. In Section 8.4.1, we prove that the map $g \mapsto \mathcal{L}_{h+g}$ satisfies a transversality condition. This transversality allows us to generically avoid certain degeneracies of derivatives.

8.4.1 Transversality of parameters

Denote $x = (I, \varphi, s)$, and $X = \mathbb{R} \times \mathbb{T} \times \mathbb{T}$. The spaces of functions $\mathcal{P}_\sigma$ and $\mathcal{A}_\sigma$ are introduced in Def. 6.

Proposition 8.13. *At every $x \in \mathbb{R} \times \mathbb{T} \times \mathbb{T}$, the mapping*

$$E(g) := g \mapsto \begin{bmatrix} \partial_{(s,\varphi)} \\ \partial_{(s,\varphi)}^2 \\ \partial_{(s,\varphi)}^3 \end{bmatrix} \mathcal{L}_g(x), \quad \mathcal{P}_\sigma \rightarrow \mathbb{R}^{2+3+4} \quad (8.20)$$

is a surjection.

Before the proof, we state some Lemmas.

Lemma 8.14. *The mapping*

$$(x, h) \mapsto \mathcal{L}_h(x), \quad X \times \mathcal{A}_\sigma \rightarrow \mathbb{R}$$

is C^∞ in both x and h . Moreover, for every $l > r \geq 0$, the mapping $h \mapsto \mathcal{L}_h$ is well defined as a mapping $C^l \mapsto C^l$, and there exists a constant $M_r > 0$ such that

$$\|\mathcal{L}_{h_1} - \mathcal{L}_{h_2}\|_{C^r} \leq M_r \|h_1 - h_2\|_{C^{r+1}}.$$

Proof. Recall (8.6):

$$\begin{aligned} \mathcal{L}_h(I, \varphi, s) = & - \int_{-\infty}^{\infty} [h(p_0(t), q_0(t), \varphi + \omega(I)t, I, s + t) \\ & - h(0, 0, \varphi + \omega(I)t, I, s + t)] dt. \end{aligned} \quad (8.21)$$

By assumption $(p_0(t), q_0(t))$ converges exponentially fast to $(0, 0)$ as $t \rightarrow \pm\infty$, the integral (8.21) converges absolutely and uniformly over all $x \in X$, with the estimate

$$\sup_{x \in X} |\mathcal{L}_h(x)| \leq C_r \sup_{x \in X} |\partial_{(q,p)} h| \quad (8.22)$$

for some $C_r > 0$.

Therefore for any multi-index $\alpha \in \mathbb{N}^3$,

$$\partial_x^\alpha \mathcal{L}_h = \mathcal{L}_{\partial_x^\alpha h}.$$

Since h is analytic, $\mathcal{L}_h$ is C^∞ in x . $\mathcal{L}_h$ is C^∞ in h since it is linear in h .

Moreover, using (8.22), we have

$$\|\mathcal{L}_h\|_{C^r} = \sup_{|\alpha| \leq r} \sup_x |\partial_x^\alpha \mathcal{L}_h| \leq \sup_{|\alpha| \leq r} \sup_x |\mathcal{L}_{\partial_x^\alpha h}| \leq M_r \|h\|_{C^{r+1}}$$

for some $M_r > 0$ depending on C_r . □

Given $r \geq 1$, let

$$\Delta_r = \{j, k \in \mathbb{Z} : j, k \geq 0, j + k \leq r\}.$$

Lemma 8.15. *Given $r \geq 1$, $(I_0, s_0, \varphi_0) \in X$, and*

$$\{c_{j,k} \in \mathbb{R} : (j, k) \in \Delta_r\},$$

for every $\delta > 0$, there exists $g \in \mathcal{P}_\sigma$ such that

$$|\partial_\phi^j \partial_s^k \mathcal{L}_g(I_0, s_0, \varphi_0) - c_{j,k}| < \delta, \quad \forall j, k \in \Delta_r.$$

Proof. Let $G_0(\varphi, s)$ be a smooth function that satisfies

$$\partial_\varphi^j \partial_s^k G_0(\varphi_0, s_0) = c_{j,k}, \quad \forall j, k \in \Delta_r.$$

In a neighborhood U of $q_0(0)$ we consider a coordinate change $\phi : U \rightarrow \mathbb{R}^d$ such that $\varphi(q_0(t)) = te_1$ for all t such that $q_0(t) \in U$, where e_1 is the first coordinate vector. Let $a > 0$ be small enough such that $[-a, a]^d \subset \phi(U)$, and given $\delta_1 > 0$ let η_1 be a smooth function supported on $(-a/2, a/2)$ such that

$$\left| \int \eta_1(t) f(t) dt - f(0) \right| < \delta_1 \|f\|_{C^r}$$

for any test function f . Let η be a smooth function such that $\eta(x_1, \dots, x_d) = \eta_1(x_1)$ on $[-a/2, a/2]^d$ and supported on $[-a, a]^d$, then define

$$R_0(q) = \eta \circ \varphi(q).$$

Let $f(t)$ be a smooth test function, we have

$$\left| \int_{-\infty}^{\infty} R_0(q_0(t)) f(t) dt - f(0) \right| = \left| \int_{-\infty}^{\infty} \eta_1(te_1) f(t) dt - f(0) \right| \leq \delta_1 \|f\|_{C^r}.$$

Define $g_0(q, \varphi, t) = R_0(q)G_0(\varphi, s)$, we get

$$\begin{aligned} & |\partial_\varphi^j \partial_s^k \mathcal{L}_g(I_0, \varphi_0, s_0) - c_{j,k}| \\ &= \left| \int_{-\infty}^{\infty} (R(q_0(t)) - R(0)) \partial_\varphi^j \partial_s^k G(\varphi_0 + \omega(I)t, s_0 + t) dt - c_{j,k} \right| \\ &= \left| \int_{-\infty}^{\infty} R(q_0(t)) \partial_\varphi^j \partial_s^k G(\varphi_0 + \omega(I)t, s_0 + t) dt - c_{j,k} \right| \leq \delta_1 C, \end{aligned}$$

where C is a constant that depends only on G . We now choose δ_1 so that $\delta_1 C < \delta/2$.

Since $\mathcal{P}_\sigma$ is dense in $C^{r+1}(\mathbb{T}^3)$, by Lemma 8.14, we can choose $g \in \mathcal{P}_\sigma$ such that

$$\|\mathcal{L}_g - \mathcal{L}_{g_0}\|_{C^r} < \delta/2.$$

This choice of g verifies the claim of our lemma. □

Proof of Proposition 8.13. We can represent the codomain of (8.20) by

$$\{c_{j,k} : j, k \in \Delta_r \setminus \{(0, 0)\}\}.$$

Let $\mathbf{c}_1, \dots, \mathbf{c}_{10}$ be a basis of the above space, then by Lemma 8.15, for any $\delta > 0$, there exists $g_1, \dots, g_{10} \in \mathcal{P}_\sigma$ such that

$$\|E(g_i) - \mathbf{c}_i\|_\infty < \delta$$

for all $1 \leq i \leq 10$. It suffices to choose δ small enough so that $E(g_i)$ still form a basis. □

8.4.2 Generic property of critical points

We proceed to prove Proposition 8.6.

Lemma 8.16. *There exists an open and dense subset $\mathcal{G}(I^-, I^+) \subset \mathcal{P}_\sigma$, such that for all $I \in [I^-, I^+]$ and $g \in \mathcal{G}(I^-, I^+)$, the function*

$$(s, \varphi) \mapsto \mathcal{L}_{h+g}(I, s, \varphi), \quad \mathbb{T}^2 \rightarrow \mathbb{R}$$

does not admit any degenerate local minima or maxima.

Proof. Let $\mathbb{S}^1 = \{v \in \mathbb{R}^2 : \|v\| = 1\}$, consider the mapping

$$F(x, v, g) = \begin{bmatrix} \partial_\varphi \mathcal{L}_{h+g}(x) \\ \partial_s \mathcal{L}_{h+g}(x) \\ \partial_{(s,\varphi)}^2 \mathcal{L}_{h+g}(x) v \\ \partial_{(s,\varphi)}^3 \mathcal{L}_{h+g}(x) [v, v, v] \end{bmatrix}, \quad X \times \mathbb{S}^1 \times \mathcal{P}_\sigma \rightarrow \mathbb{R}^5.$$

Since F is linear in g ,

$$\partial_g F(x_0, v_0, g_0)(\delta g) = F(x_0, v_0, \delta g).$$

By Proposition 8.13, at every $(x_0, v_0, g_0) \in \mathbb{R} \times \mathbb{S}^1 \times \mathcal{P}_\sigma$, there exists a finite dimensional subspace $E \subset \mathcal{P}_\sigma$, such that the mapping

$$\delta g \mapsto \partial_g F(x_0, v_0, g_0)(\delta g) = F(x_0, v_0, \delta g), \quad E \rightarrow \mathbb{R}^5$$

is a surjection. Moreover, by the smoothness of the mapping F in (x_0, v_0, g_0) , the same is true for all (x, v, g) contained in a neighborhood U_{loc} of $(x_0, v_0, g_0) \in X \times \mathbb{S}^1 \times E$. By the implicit function theorem, the set

$$W_{\text{loc}} = \{(x, v, g) : F(x, v, g) = 0\}$$

is a submanifold of codimension 5 in U_{loc} . Let π_g be the projection into the g component, then by Sard's Theorem, the set of regular values $g \in \pi_g(U_{\text{loc}})$, denoted $\mathcal{G}_{\text{loc}}$, is a residual set in U_{loc} . Since $d\pi_g$ has at most co-rank 4, g_1 is a regular value implies $\pi_g^{-1}(g_1) \cap W_{\text{loc}} = \emptyset$, which means $F(x, v, g_1) \neq 0$ for all $g_1 \in \mathcal{G}_{\text{loc}}$ and $(x, v, g_1) \in U_{\text{loc}}$.

Let U_i be a countable covering of the separable space $X \times \mathbb{S}^1 \times \mathcal{P}_\sigma$, we apply the above argument to each U_i to obtain a relatively residual set $\mathcal{G}_i \subset U_i$, such that $F(x, v, g_1) \neq 0$ for all $g_1 \in \mathcal{G}_i$ and $(x, v, g_1) \in U_i$. Then

$$\mathcal{G} = \bigcup_i \mathcal{G}_i$$

is a residual subset of $\mathcal{P}_\sigma$, such that for every $g \in \mathcal{G}$ and $(x, v) \in X \times \mathbb{S}^1$,

$$F(x, v, g) \neq 0.$$

Finally, set

$$\mathcal{G}(I^-, I^+) = \{g : F(x, v, g) \neq 0, \text{ for all } x, v \in [I^-, I^+] \times \mathbb{T} \times \mathbb{T} \times \mathbb{S}^1\},$$

this set is open due to compactness in (x, v) . It is also dense since $\mathcal{G}(I^-, I^+) \supset \mathcal{G}$.

To prove our lemma, let $g \in \mathcal{G}(I^-, I^+)$ and let $x_0 = (I_0, s_0, \varphi_0)$ be a degenerate critical point of $\mathcal{L}_{h+g}$, i.e., $\partial_{(s, \varphi)} \mathcal{L}_{h+g} = 0$ and there exists $v \in \mathbb{S}^1$ such that

$$\partial_{(s, \varphi)}^2 \mathcal{L}_{h+g}(x_0)v = 0.$$

Since $F(x, v, g) \neq 0$, we must have

$$\partial_s^3(s, \varphi) \mathcal{L}_{h+g}(x)[v, v, v] \neq 0.$$

We conclude that the function $t \mapsto \mathcal{L}_{h+g}(x_0 + t(0, v))$ is an open mapping near $t = 0$, hence (s_0, φ_0) cannot be a local minimum or maximum of $\mathcal{L}_{h+g}(I_0, \cdot, \cdot)$. $\square$

Proof of Proposition 8.6. By Lemma 8.16, if $g \in \mathcal{G}(I^-, I^+)$, then for all $I \in [I^-, I^+]$ the function $\mathcal{L}_{h+g}(I, \cdot, \cdot)$ has no degenerate minima or maxima.

Fix $g \in \mathcal{G}(I^-, I^+)$, and let $M_g \subset \mathbb{T} \times \mathbb{T}$ denote the set of all global minima of $\mathcal{L}_{h+g}(I, \cdot, \cdot)$ for some $I \in [I^-, I^+]$. Since all the minima are non-degenerate, they are isolated on each level $\{I\} \times \mathbb{T} \times \mathbb{T}$. Moreover, any non-degenerate local minima can be extended smoothly to a neighborhood of I . We conclude that M_g is contained in a finite family of curves of non-degenerate local minima $\{(I, \varphi_J^*(I), s_J^*(I)) : I \in J\}$ where $J \in \mathcal{J}$ is a finite collection of open intervals, and $\bigcup_{J \in \mathcal{J}} J \supset [I^-, I^+]$. We now select the intervals $[I_j^-, I_j^+]$ inductively as such:

- Let (I_1^-, I_1^+) be any interval in $\mathcal{J}$ what contains I^- .
- If intervals (I_j^-, I_j^+) are selected for $j \leq m$, pick any interval (a, b) in $\mathcal{J}$ that contains I_m^+ . Set $I_{m+1}^- = \max\{a, (I_m^- + I_m^+)/2\}$ and $I_{m+1}^+ = b$.

$\square$

8.5 Appendix: Shadowing pseudo-orbits using Poincaré recurrence

In this section we describe the proof of Proposition 8.4. This Proposition has minor differences from Theorem 3.7 of [GLMS20] by allowing the iterates of inner dynamics. Our assumption on the measure preserving properties of T and S_j is also stronger than that of [GLMS20] but nevertheless satisfied for a priori unstable systems. The proof follows the main ideas of [GLMS20].

Lemma 8.17 (Lemma 3.2 of [GLMS20]). *Suppose Λ_ϵ is an NHIM of the Hamiltonian H and T is the associated inner map. Assume that there exists a finite family S_j , $1 \leq j \leq m$, of scattering maps defined on open subsets of Λ_ϵ . Assume that Λ_ϵ is compact.*

Then for every $\delta > 0$, there exists two family of functions $n_i^ : \mathbb{N}^i \rightarrow \mathbb{N}$ and $m_i^* : \mathbb{N}^{2i+1} \times \mathbb{N}^{i+1} \rightarrow \mathbb{N}$ such that for every pseudo-orbit y_i , $0 \leq i \leq N-1$, of the form*

$$y_{i+1} = T^{m_i} \circ S_{j_i} \circ T^{n_i}$$

such that

$$n_i \geq n_i^*(j_0, \dots, j_i), \quad m_i \geq m_i^*(n_0, \dots, n_i, m_0, \dots, m_{i-1}, j_0, \dots, j_i),$$

there exists an orbit $z(t)$ of the Hamiltonian flow and $t_0 < \dots < t_N$ such that

$$d(z(t_i), y_i) < \delta.$$

To prove Proposition 8.4, given any pseudo-orbit of T and S_j , we can use Poincaré recurrence to attach arbitrarily long excursions of iterates of T . This allows us to construct a new pseudo-orbit that satisfies the requirement of Lemma 8.17.

In the rest of the section, any unspecified “measure” stands for Lebesgue measure.

Proof of Proposition 8.4. First, rewrite the pseudo-orbit in the following form

$$x_{i+1} = T^{s_i} \circ S_{j_i}(x_i) =: f_i(x_i), \quad 0 \leq i \leq N-1$$

where $s_i \geq 0$. Note that each f_i maps positive measure sets to positive measure sets, and zero measure sets to zero measure sets. Since each f_i are continuous, then there exists open balls B_i with $x_i \in B_i \subset B_{\delta/2}(x_i)$ such that

$$f_i(B_i) \subset B_{i+1}.$$

Let n_i^*, m_i^* be the functions given by Lemma 8.17 depending on $\delta/2$ and j_i .

By the Poincaré recurrence theorem, there exists $n_0 \geq n_0^*(j_0)$ such that both

$$E'_0 = \{x \in B_0 : T^{k_0}(x) \in B_0\},$$

and $T^{n_0}(E'_0)$ have positive measure. Since

$$f_0 \circ T^{n_0}(E'_0),$$

has positive measure, there exists $l_0 \geq m_0^*(n_0, j_0) - s_0$ such that

$$F'_0 = \{x \in f_0 \circ T^{n_0}(E'_0) : T^{l_0}(x) \in f_0 \circ T^{n_0}(E'_0)\}$$

has positive measure and so does $F_0 = T^{l_0}(F'_0) \subset f_0 \circ T^{n_0}(E'_0) \subset B_1$. Set $m_0 = l_0 + s_0$ and $g_0 = T^{l_0} \circ f_0 \circ T^{n_0} = T^{m_0} \circ S_{j_0} \circ T^{n_0}$, and

$$E_0 = g_0^{-1}(F_0) \cap E'_0.$$

Then $g_0(E_0) = T^{l_0}(F'_0) = F_0$ and both E_0 and F_0 have positive measure.

Inductively, suppose $E_i, F_i, g_i = T^{m_i} \circ S_{j_i} \circ T^{n_i}$ are constructed such that

$$n_i \geq n_i^*(j_0, \dots, j_i), \quad m_i \geq m_i^*(n_0, \dots, n_i, m_0, \dots, m_{i-1}, j_0, \dots, j_i),$$

satisfies

$$E_i \supset \dots \supset E_0,$$

$$F_i = g_i \circ \dots \circ g_0(E_i) \subset B_{i+1}$$

and E_i, F_i have positive measure. See Figure 8.3 for a diagram of the sets involved in the construction.

We set

$$E'_{i+1} = \{x \in F_i : T^{n_{i+1}}(x) \in F_i\},$$

where $n_{i+1} \geq n_{i+1}^*(j_0, \dots, j_{i+1})$ is chosen such that both E'_{i+1} and $T^{n_{i+1}}(E'_{i+1})$ has positive measure. Let $l_{i+1} \geq m_{i+1}^*(n_0, \dots, n_{i+1}, m_0, \dots, m_i, j_0, \dots, j_i) - s_{i+1}$ such that

$$F'_{i+1} = \{x \in f_{i+1} \circ T^{n_{i+1}}(E'_{i+1}) : T^{n_{i+1}}(x) \in f_{i+1} \circ T^{n_{i+1}}(E'_{i+1})\}$$

$m_{i+1} = l_{i+1} + s_{i+1}$, $F_{i+1} = T^{l_{i+1}}(F'_{i+1}) \subset f_{i+1} \circ T^{n_{i+1}}(E'_{i+1}) \subset B_{i+2}$. Our construction ensures

$$g_{i+1} \circ \dots \circ g_0(E_i) = g_{i+1}(F_i) \supset g_{i+1}(E'_{i+1}) \supset F_{i+1},$$

therefore

$$E_{i+1} := (g_{i+1} \circ \dots \circ g_0(E_i))^{-1}(F_{i+1}) \cap E_i$$

is mapped onto F_{i+1} by $g_{i+1} \circ \dots \circ g_0(E_i)$.

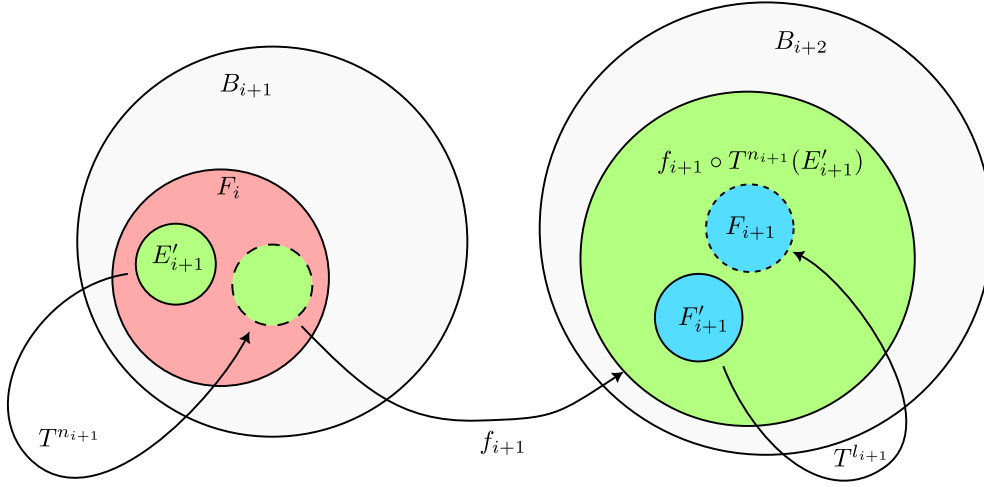


Figure 8.3: Diagram for the choice of the sets E_i , F_i .

Apply the construction for $0 \leq i \leq N-1$, we obtain

$$g_i \circ \dots \circ g_0(E_{N-1}) \subset g_i \circ \dots \circ g_0(E_i) = F_i \subset B_{i+1},$$

for all $0 \leq i \leq N-1$. Pick any $y_0 \in E_N$, then

$$y_{i+1} = g_i(y_i)$$

defines a pseudo-orbit satisfying the condition of Lemma 8.17 and

$$d(y_i, x_i) < \delta/2.$$

Apply Lemma 8.17, we get a real orbit shadowing y_i within $\delta/2$ distance, which shadows x_i within δ distance. $\square$

Chapter 9

Spatial R3BP

In this chapter, we consider the spatial circular restricted three-body problem (RTBP for short), as a model for the motion of spacecraft relative to the Sun-Earth system. We focus on the dynamics near the equilibrium point L_1 located between the Sun and the Earth. We show that we can transfer the spacecraft, at zero energy cost, from a quasi-periodic orbit that is nearly planar relative to the ecliptic to a quasi-periodic orbit of large vertical amplitude. Moreover, we provide several explicit constructions of such trajectories, and also develop an algorithm to design trajectories that achieve the shortest transfer time. Our algorithm is flexible and can be applied to other systems besides Sun-Earth.

For illustration, Figure 9.1 shows the initial and final segments (in blue and green, respectively) of the fastest transfer trajectory between one quasi-periodic orbit with small vertical amplitude, and another with large vertical amplitude.

The model that we consider is a 3-degrees of freedom Hamiltonian system. We construct trajectories that follow closely geometric structures that organize the dynamics. The main geometric object near L_1 is a 4-dimensional center manifold on which the dynamics is nearly integrable. More precisely, in a neighborhood of L_1 the Hamiltonian can be approximated by a high-order Birkhoff normal form, which is an integrable Hamiltonian. In terms of the Birkhoff normal form, the center manifold can be parametrized by a system of symplectic coordinates consisting of two action variables (J_p, J_v) and two angle variables (ϕ_p, ϕ_v). The action J_p describes the horizontal amplitude (relative to the ecliptic) of a quasiperiodic orbit, and J_v describes its vertical amplitude. Restricting to an energy level close to that of L_1 amounts to fixing the action variable J_p . This yields a 3-dimensional sphere which is foliated by 2-dimensional tori, where each torus is uniquely determined by a fixed value of the remaining action variable J_v . A change in J_v corresponds to a change in the vertical amplitude of a quasi-periodic orbit. Since the tori are invariant, by using only the ‘inner flow’ restricted to the 3-dimensional sphere, the vertical amplitude of orbits remains constant. However, the tori do not separate the energy manifold, so there may exist trajectories that move from one torus to another, thus changing the vertical amplitude. In order to obtain such trajectories, we need to use the ‘outer dynamics’, described below.

The 3-dimensional sphere is a normally hyperbolic invariant manifold (NHIM), and has stable and unstable manifolds which go around the Earth and intersect transversally along trajectories homoclinic to the NHIM. By carefully selecting consecutive homoclinic trajectories, we show that it is possible to achieve large changes in the vertical amplitude of orbits. Proving the existence of such trajectories is related to *Arnold diffusion problem* (see the discussion later).

The tool that allows us to systematically select suitable homoclinics at each step is the *scattering map*. This is a map defined on the NHIM, which relates the past asymptotic of a homoclinic point to its future asymptotic. The scattering map was introduced in [DLS00, DLS06a, DLS06b] in the study of Arnold diffusion. When restricted to a suitable 2-dimensional Poincaré section, the scattering map turns out to be symplectic [DLS08, DGR13]. An additional advantage that we exploit in our model is that we obtain two scattering maps, which give us more options in the selection of suitable homoclinics.

We provide a theoretical result (Theorem 9.1) that gives sufficient conditions on a inner dynamics and two scattering maps defined on an annulus inside a NHIM (described in action-angle variables), to ensure the existence of true trajectories that start near the lower boundary of the annulus and end near its upper boundary.

In our model, the action variable corresponds to the vertical amplitude J_v and the annulus to some range of $J_v \in [J_1, J_2]$. Provided that the assumptions of Theorem 9.1 are verified, the orbits of the Iterated Functions System (IFS) formed by the two scattering maps and the inner map that achieve

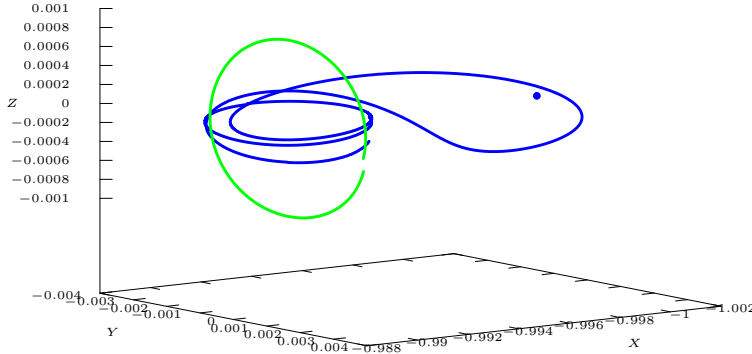


Figure 9.1: Initial segment (blue) and final segment (green) of the fastest transfer trajectory between a quasi-periodic orbit with small vertical amplitude (small Z -oscillation), and another with large vertical amplitude (Z -oscillation of amplitude 0.001, roughly 150000 km). The complete trajectory (not shown here) is very complicated, and goes through many homoclinic jumps. This trajectory is computed in Section 9.11.2. (See also Figures 9.20 and 9.21).

the prescribed gain in the vertical amplitude yield true trajectories that achieve the same gain (up to a small error). To distinguish the orbits of the IFS from true trajectories of the system, we will refer to the former as *pseudo-orbits*.

Before going into more details, we now outline the methodology that we will use. The trajectories designed to change the vertical amplitude J_v are guided by homoclinic orbits that depart and land, asymptotically, at points in the NHIM, depending on the scattering (outer) map used. The vertical amplitude at landing can be higher or lower than the vertical amplitude at departure. The inner dynamics of the NHIM allow us to travel between points with the same vertical amplitude to change, if necessary, the departure points. With a simple simulation of these 3 dynamics—the 2 scattering maps and the inner map—we obtain pseudo-orbits with the desired vertical amplitude gain.

We note that the problem that we consider is not perturbative. Until now, the only available methods for computing the scattering map in such a setting have been numerical [CDMR06, DGR16]. However, purely numerical approaches are computationally intensive and offer little insight into the geometric structures determined by the scattering map.

The highlight of this chapter is that an analytical approximation of the scattering map for the spatial circular RTBP is provided. We describe the scattering map via a generating function depending on old and new variables. Then we approximate the generating function using a Fourier-Polynomial interpolation. As it turns out, the numerical computation of the scattering map at a few points can be used to compute the coefficients of the Fourier-Polynomial interpolation, up to some suitable order, and thus to obtain an analytical formula for the generating function, up to some small error. The outcome of this approximation is referred to as the *Standard Scattering Map* (SSM). It is given explicitly as a perturbation of an integrable twist map. As such, the phase space of the scattering map is organized by KAM tori, elliptic islands, hyperbolic periodic orbits and their stable and unstable manifolds, and resonant zones. See Figure 9.14. The rich geometric structure unveiled by the analytical approximation of the scattering map was not available through previous approaches. Similar computations of the generating function of the scattering map and of its phase space were obtained purely analytically in *uncoupled* pendulum-rotor systems subject to small perturbations of a special type [DS17, DS18]. However, as the unperturbed pendulum-rotor systems considered in those papers are uncoupled, the phase shift phenomenon [DMR08] does not take place, and the unperturbed scattering maps are just the identity. In particular, they are not twist maps, which makes the dynamics different from those considered here.

The main application of the Standard Scattering Map is that it offers an explicit method to find

pseudo-orbits, that is, orbits of the iterated function system consisting of scattering maps and the inner map (induced by the inner flow on the Poincaré section), along which the vertical amplitude J_v grows consistently. The method is versatile, in the sense that one can choose the starting and ending points of such pseudo-orbits. As mentioned earlier, here we compute two scattering maps, and we compare them in terms of the fastest trajectory to achieve the desired change in vertical amplitude.

It is important to note that the orbits of the scattering maps are not equivalent to true trajectories of the system. Rather, we can approximate a segment of a homoclinic trajectory by a concatenation of a finite orbit of the inner dynamics, followed by an application of a scattering map, followed by another finite orbit of the inner dynamics. The map that described this concatenation of orbits is referred to as the *transition map*. The transition map is a map on the NHIM, and each application of the transition map approximates a segment of a homoclinic orbit to the NHIM; see Section 9.1.4. Since we have constructed two scattering maps, we have two corresponding transition maps. To obtain approximate trajectories that change the orbital vertical amplitude, we consider the iterated function system consisting of the two transition maps and the inner map, and we search for optimal trajectories.

Note the order in which our methodology proceeds. First and foremost, we obtain the Standard Scattering Map, which models the asymptotic homoclinic dynamics in a comprehensive and efficient manner, forming the backbone of all subsequent computations. Second, we use the SSM to validate the hypothesis of Theorem 9.1 and conclude the existence of diffusion. However, to design pseudo-orbits it is necessary to work with finite-time segments of trajectories. Third, from the SSM we derive the transition map, which approximates *finite-time* homoclinic segments. The transition map is used to design pseudo-orbits, which can finally be refined into true orbits.

To find optimal pseudo-orbits, we leverage the classic Dijkstra algorithm for finding shortest paths in a graph. A surprising finding is that for an optimal orbit of the iterated function system, rather than always selecting a transition map that grows J_v , sometimes we must select a transition map that decreases J_v , in order to arrive to a place where the next application of a transition map yields a large increase in J_v . Another surprising finding is that an optimal pseudo-orbit involves very few applications of the inner map.

More quantitatively, in Section 9.11 we divide the phase space into a grid of $30 \times 30 = 900$ small cells, and in Section 9.11.2 we obtain a diffusion pseudo-orbit that uses just 17 iterations of the scattering/transition maps plus intermediate iterations of the inner map. We emphasize that only using the image of 7 tori we can have an approximation of the phase space of the scattering map, good enough to be able to design with several algorithms the appropriate diffusion pseudo-orbits. The use of more invariant tori and of a more refined grid does not present additional technical difficulties, and would not modify in a qualitative way the phase space of the scattering maps represented in Figure 9.14, so the optimal paths would not change substantially.

These optimal pseudo-orbits can be refined into true orbits either through theoretical shadowing results or by applying appropriate numerical methods, such as parallel shooting.

Our construction described so far is based on approximating the Hamiltonian near L_1 by a Birkhoff normal form. Since the approximation is quite accurate, the true dynamics associated to the original Hamiltonian follow closely the Birkhoff normal form dynamics. In particular, the trajectories of the true inner dynamics stay close to invariant tori, and the scattering map for the true dynamics is close to the scattering map derived from the normal form approximation. This implies that there exist diffusing trajectories—that change the orbital vertical amplitude by a significant amount—for the original Hamiltonian system.

Our results are related to the Arnold diffusion problem for Hamiltonian systems, claiming that integrable Hamiltonian systems subjected to small perturbations of generic type have ‘diffusing orbits’ along which the action variable changes by an amount independent of the smallness of the perturbation [Arn64]. Arnold proposed a mechanism of diffusion based on transition chains of tori, which are sequences of invariant tori with consecutive heteroclinic connections between consecutive tori. Arnold conjectured: “I believe that this mechanism of instability is applicable to the general case (for example, to the problem of three bodies)”. This conjecture has witnessed significant progress in recent years, including [CG94, BT99, DLS00, Tre02, Tre04, DLS06a, DLS06b, Pif06b, GT08, DH09, CY09, Mat12, KZ15, BKZ16, CX19, Tre12, GL17, GT17, GM22, KZ20]. Some of the progress has been geared towards proving Arnold diffusion in concrete models, under explicit, verifiable conditions on the perturbation. This direction opened up the possibility of implementing Arnold’s mechanism of diffusion in applications, such as to Celestial Mechanics. Notably, some papers, including [DKRS19, GPS25, CFG25], succeeded in providing analytical proofs of Arnold diffusion in some models of the three- and four-body problem. These papers rely on perturbative methods, and therefore they need to assume that certain parameters

(such as ratios of the masses of the bodies, or ratios of the semi-major axes of the orbits) are very small, in fact much smaller than those observed in solar systems. Another line of arguments combine analytical methods with numerical computation (including computer assisted proofs) to show Arnold diffusion in models with realistic parameters, see, e.g. [CGL17b, CG23, FH25].

We follow this latter approach. In the case of the Sun-Earth system we implement Arnold's mechanism of transition chains of tori via analytical tools and numerical methods, obtaining orbits that follow the transition chain and change their vertical amplitude. The system that we consider is *a priori chaotic*, that is, it contains a hyperbolic basic set (see, e.g., [GT17]). Since the system is non-perturbative, we do not obtain a change that is independent of some small parameter. However, we argue that the change is as large as possible for the geometric mechanism at play. Specifically, we obtain a change in the action that spans approximately 70% of the region where primary homoclinic orbits exist. (See Section 9.3.5).

The construction in this chapter can be potentially adapted to astrodynamics applications. Sometimes, a satellite (which typically carries little fuel) ends up on a wrong orbit, and one tries to correct the orbit by exploiting the gravity of Earth, Sun, Moon as much as possible, and firing the satellites' thrusters as little as possible; see, e.g., [Bel04]. While our methodology to change the vertical amplitude of a satellite orbit may be too slow from a practical point of view, by combining zero-cost geometric routes with small thrusts, one may be able to design useful trajectories; see, e.g., [GKL⁺01].

We do not focus on trajectory optimization. Nevertheless, in our setting, we can estimate both the duration (32 years) and the total required thrust (271 m/s) for the pseudo-orbit that exhibits the fastest growth in vertical amplitude. See Section 9.11.2 and Remark 9.19.

Moreover, our methodology can be applied to build transfers involving two or more NHIMs connected by heteroclinic orbits, e.g., the NHIM around L_1 and that around L_2 [DMR08, BHM24].

9.1 Setup

9.1.1 The Spatial Circular RTBP

We consider the spatial circular RTBP as a model for the motion of an infinitesimal body (e.g. satellite) under the gravitational influence of two massive bodies, referred to as primaries (e.g. Sun and the Earth). We describe the problem in normalized units, relative to a co-rotating frame XYZ , such that the larger primary of mass $1 - \mu = \mu_1$ is located at $P_1 = (\mu, 0, 0)$, the smaller primary of mass μ is located at $P_2 = (\mu - 1, 0, 0)$, and the vertical component of the motion of the infinitesimal body is given by the Z -coordinate (see Figure 9.2).

In the case of the Sun-Earth system $\mu = 3.040423398444176 \times 10^{-6}$.

The motion of the infinitesimal body relative to these coordinates is given by the autonomous system of equations:

$$\begin{aligned}\ddot{X} - 2\dot{Y} &= \Omega_X, \\ \ddot{Y} + 2\dot{X} &= \Omega_Y, \\ \ddot{Z} &= \Omega_Z,\end{aligned}\tag{9.1}$$

where the effective potential Ω is given by

$$\Omega = \frac{1}{2}(X^2 + Y^2) + \frac{1 - \mu}{r_1} + \frac{\mu}{r_2},$$

with r_1, r_2 representing the distances from the secondary to the larger and the smaller primary, respectively:

$$\begin{aligned}r_1 &= ((X - \mu)^2 + Y^2 + Z^2)^{1/2}, \\ r_2 &= ((X - \mu + 1)^2 + Y^2 + Z^2)^{1/2}.\end{aligned}$$

The phase space is 6-dimensional.

The system has an integral of motion (referred to as the Jacobi integral) given by:

$$C = 2\Omega - (\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2).$$

Equivalently, the equations (9.1) can be described as a 3-degree-of-freedom, autonomous Hamiltonian system given by the Hamiltonian function:

$$H = \frac{1}{2}(P_X^2 + P_Y^2 + P_Z^2) + YP_X - XP_Y - \frac{1 - \mu}{r_1} - \frac{\mu}{r_2},\tag{9.2}$$

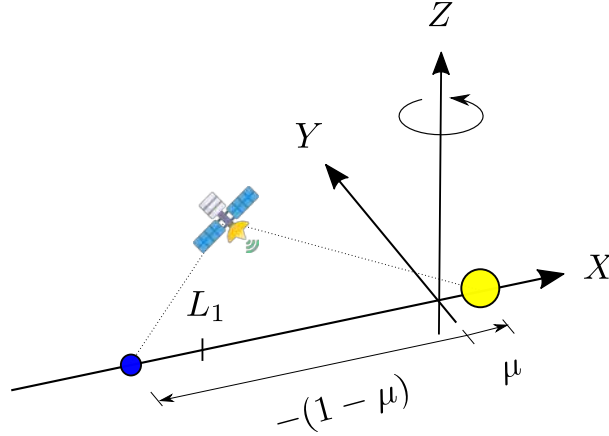


Figure 9.2: Schematic location of the Sun (in yellow), the Earth (in blue), and the equilibrium point L_1 .

where X, Y, Z are the generalized coordinates, $P_X = \dot{X} - Y$, $P_Y = \dot{Y} + X$, $P_Z = \dot{Z}$ are the generalized momenta, and the symplectic form is:

$$dP_X \wedge dX + dP_Y \wedge dY + dP_Z \wedge dZ.$$

We denote by Φ_H the flow of (9.2).

The Hamiltonian function and the Jacobi integral are equivalent integrals of motion, since

$$H = -C/2.$$

As the Hamiltonian (and, equivalently, the Jacobi integral) is preserved along the solutions of the system, each trajectory lies on a 5-dimensional energy manifold M_c corresponding to some energy level $h = -c/2$, that is,

$$M_c = \{H(P_X, P_Y, P_Z, X, Y, Z) = -c/2\}.$$

We are going to focus on the dynamics around the equilibrium point L_1 , which is located between the primaries, and is of Saddle $\times$ Center $\times$ Center – linear stability type (see Figure 9.2). Let us denote by

$$\pm\lambda, \pm i\nu_p, \pm i\nu_v, \text{ with } \lambda, \nu_p, \nu_v \text{ real and positive,}$$

the eigenvalues of the linearized system near L_1 . The quantities $\lambda, -\lambda$ represent the exponential expansion and contraction hyperbolic rates, while ν_p, ν_v represent the frequencies of the planar and vertical components of the motion, respectively. In the case of the Sun-Earth system, $\lambda = 2.5326591740529678$, $\nu_p = 2.0864535642231075$ and $\nu_v = 2.0152106629966386$.

By the Center Manifold Theorem (see e.g., [JM99]), there exists a 4-dimensional invariant center manifold $\Lambda = W^c(L_1)$ that is tangent at L_1 to the generalized eigenspace corresponding to $\pm i\nu_p, \pm i\nu_v$. The manifold Λ is a normally hyperbolic invariant manifold (NHIM) for the flow Φ_H . If we fix the energy level (or, equivalently the Jacobi constant), the restriction of the center manifold $W^c(L_1)$ to the energy level $\{H = -c/2\}$ is a 3-dimensional sphere

$$\Lambda_c = \Lambda \cap M_c,$$

which is a NHIM for the flow Φ_H restricted to the energy manifold M_c .

9.1.2 Local Dynamics around L_1

The Hamiltonian H can be expanded about L_1 , via a symplectic coordinate change

$$(P_X, P_Y, P_Z, X, Y, Z) \mapsto (y_h, J_p, J_v, x_h, \phi_p, \phi_v),$$

as a Birkhoff normal form

$$\mathcal{H}^{(N)} = H_2 + \mathcal{Z}^{(N)} + \mathcal{R}^{(N)},$$

where H_2 denotes the quadratic part of H expressed in terms of the new variables, $\mathcal{Z}^{(N)}$ is a polynomial of degree N that Poisson-commutes with H_2 , and the remainder $\mathcal{R}^{(N)}$ is small in a neighborhood of L_1 (more precisely, of the order of the $(N+1)$ -th power of the distance to L_1). The coordinates x_h, y_h represent the hyperbolic directions of motion. The *action variables* (J_p, ϕ_p) correspond to the *planar* component of the motion, while the *angle variables* (J_v, ϕ_v) corresponds to the *vertical* component. A useful reference for the derivation of such a Birkhoff normal form is [Jor99].

In [DGR16], we performed the computation of this normal form for the spatial circular RTBP up to order $N = 16$. We will use this computation.

The truncated Birkhoff normal form depends only on $x_h y_h, J_p, J_v$,

$$\mathcal{H}_{\text{trunc}}^{(N)} = H_2 + \mathcal{Z}^{(N)} = \lambda x_h y_h + \nu_p J_p + \nu_v J_v + \mathcal{Z}^{(N)}(x_h y_h, J_p, J_v), \quad (9.3)$$

which are integrals of motion for $\mathcal{H}_{\text{trunc}}^{(N)}$. We denote by Φ_N the flow associated to (9.3).

The truncated Birkhoff normal form $\mathcal{H}_{\text{trunc}}^{(N)}$ represents an approximation of the original Hamiltonian H , and therefore the invariant objects for $\mathcal{H}_{\text{trunc}}^{(N)}$ give approximations of the corresponding invariant objects of H . Truncating the normal form at order $N = 16$ ensures that the error between the true dynamics in the NHIM and the dynamics induced by the Birkhoff normal form is within machine precision. See Section 9.3.1. In particular, we consider the center manifold Λ^N for the truncated Birkhoff normal $\mathcal{H}_{\text{trunc}}^{(N)}$, which represents an approximation of Λ . In the action-angle coordinates, we have that

$$\Lambda^N = \{(y_h, J_p, J_v, x_h, \phi_p, \phi_v) \mid y_h = 0, x_h = 0, J_p, J_v \geq 0, \phi_p, \phi_v \in \mathbb{T}\}, \quad (9.4)$$

is parameterized by the symplectic action-angle coordinates $(J_p, J_v, \phi_p, \phi_v)$. This has a symplectic structure given by the form

$$dJ_p \wedge d\phi_p + dJ_v \wedge d\phi_v.$$

The planar Lyapunov periodic orbits correspond to $J_v = 0$ and $J_p > 0$, the vertical Lyapunov periodic orbits to $J_p = 0$ and $J_v > 0$, and the libration point L_1 to $J_p = J_v = 0$, so these coordinates are degenerate when some action $J_{p,v} = 0$, as it is usual with polar coordinates.

For a fixed energy $\mathcal{H}_{\text{trunc}}^{(N)} = h = -c/2$, J_p is given as an implicit function of J_v, ϕ_p, ϕ_v, c . The corresponding NHIM for the truncated system is given by

$$\Lambda_c^N = \Lambda^N \cap \left\{ \mathcal{H}_{\text{trunc}}^{(N)} = -c/2 \right\},$$

and is therefore parameterized by the 3 variables (J_v, ϕ_p, ϕ_v) .

For each fixed value of the vertical action $J_v = \bar{J}_v$, there is a unique invariant torus for the Birkhoff normal form

$$T_{\bar{J}_v}^N = \Lambda_c^N \cap \{J_v = \bar{J}_v\}$$

which is therefore parameterized by the 2 angles (ϕ_p, ϕ_v) . Thus, the NHIM Λ_c^N is foliated by a family of 2-dimensional invariant tori. By comparison, the NHIM Λ_c corresponding to the full Hamiltonian H contains a KAM family of 2-dimensional invariant tori, with gaps between the tori that are exponentially small in the action (see [41] for quantitative estimates). The existence of the NHIM for the full Hamiltonian has been rigorously proven for the planar RTBP in [CR12].

Each of the objects $\Lambda^N, \Lambda_c^N, T_{\bar{J}_v}^N$, have associated stable and unstable (or asymptotic) manifolds of one more dimension than the object itself. The truncated Birkhoff normal form provides an accurate approximation of the local asymptotic manifolds in a neighborhood of L_1 . In particular, the 4-dimensional local stable and unstable manifolds of Λ_c^N are given by

$$W_{\text{loc}}^{s,u}(\Lambda_c^N) = \Lambda_c^N \oplus \Upsilon^{s,u},$$

where $\Upsilon^{s,u}$ is a small interval in the stable (unstable) direction. In practice, we take this interval to be of length $\delta = 10^{-3}$; see Section 9.3.1 for more details.

Once the local stable and unstable manifolds are obtained, the global manifolds are computed by integrating the local ones by the flow Φ_H of (9.2).

9.1.3 Scattering Map

One of the main tools that we use is the scattering map. This is an effective tool to quantify the effect of homoclinic excursions to a NHIM. In general, it can be computed either perturbatively or numerically.

We recall the definition of the scattering map following [DLS08]. We consider a general setting of flow Φ on a manifold M , and assume that there is a normally hyperbolic invariant manifold Λ for the flow. We will assume that the flow as well as the geometric objects referred to below are differentiable enough, without formulating specific assumptions on regularity. (In the case of the spatial circular RTBP the flow is real analytic, and the geometric objects of interest are at least C^1 -differentiable, but not necessarily analytic.)

As a consequence of normal hyperbolicity, the stable manifold $W^s(\Lambda)$ and the unstable manifold $W^u(\Lambda)$ are foliated by stable and unstable manifolds of points $W^s(y)$, $W^u(y)$, respectively, for $y \in \Lambda$. This implies that for each $x \in W^u(\Lambda)$ there exists a unique $x_- \in \Lambda$ such that $x \in W^u(x_-)$, and for each $x \in W^s(\Lambda)$ there exists a unique $x_+ \in \Lambda$ such that $x \in W^s(x_+)$. These correspondences are described via the *wave maps* $\Omega_+ : W^s(\Lambda) \rightarrow \Lambda$ given by $\Omega_+(x) = x_+$, and $\Omega_- : W^u(\Lambda) \rightarrow \Lambda$ given by $\Omega_-(x) = x_-$, respectively.

Assume the following transversality conditions:

- $W^s(\Lambda)$ and $W^u(\Lambda)$ intersect transversally along a homoclinic manifold Γ ;
- The homoclinic manifold Γ is transverse to the stable (unstable) foliation $\{W_x^{s,u}\}_{x \in \Lambda}$ relative to $W^{s,u}(\Lambda)$.

Then, the restrictions Ω_+^Γ , Ω_-^Γ of Ω_+ , Ω_- , respectively, to Γ are local diffeomorphisms. We can always choose Γ so that Ω_+^Γ , Ω_-^Γ are diffeomorphisms onto their images. A homoclinic manifold Γ for which the corresponding restrictions of the wave maps to Γ are diffeomorphisms is referred to as a *homoclinic channel*.

Definition 9.1. Given a homoclinic channel Γ , the scattering map associated to Γ is the diffeomorphism

$$S^\Gamma = \Omega_+^\Gamma \circ (\Omega_-^\Gamma)^{-1}$$

from the $\text{Dom}(S^\Gamma) := \Omega_-^\Gamma(\Gamma) \subseteq \Lambda$ to the $\text{Im}(S^\Gamma) := \Omega_+^\Gamma(\Gamma) \subseteq \Lambda$.

That is, if $x \in \Gamma$ is a homoclinic point and $\Omega_\pm^\Gamma(x) = x_\pm$, then $S^\Gamma(x_-) = x_+$. In general, the domain and range of the scattering map are proper subsets of Λ . There are examples where the local domain of the scattering map cannot be extended to a global one, that is, on the whole Λ , as moving along a loop in Λ leads to lack of monodromy (see [DLS00]).

The scattering map depends on the choice of the homoclinic channel Γ . When we flow the homoclinic channel Γ to $\Phi^t(\Gamma)$, the corresponding scattering maps are conjugate by the flow (see [DLS08, Section 2.3]):

$$S^{\Phi^t(\Gamma)} = \Phi^t \circ S^\Gamma \circ \Phi^{-t}. \quad (9.5)$$

Of course, when Γ and $\Phi^t(\Gamma)$ overlap, for $x \in \Gamma \cap \Phi^t(\Gamma)$, we have $S^{\Phi^t(\Gamma)}(x_-) = S^\Gamma(x_-)$. This means that S^Γ can be continued to $S^{\Phi^t(\Gamma)}$ for some interval of times t , for as long as the corresponding homoclinic channels are well defined and can be continued into one another. We will regard the result of such continuation to the maximal domain as a single scattering map.

When the choice of the homoclinic channel Γ is evident from the context, we drop the superscript from the notation S^Γ .

In the case of a discrete-time dynamical system, the scattering map can be defined in a similar fashion.

A remarkable property of the scattering map is that it is exact symplectic, provided that the manifold and the flow are exact symplectic. We refer to [DLS08] for details.

Remark 9.1. As we shall see in Section 9.3.5, in our model we can construct two scattering maps that are defined on a whole annulus inside the NHIM. In this sense, the scattering maps are globally defined on the annulus. Each of this scattering maps is obtained by a continuation of a locally defined scattering map to a maximal domain. In our model, the scattering map extended to its maximal domain satisfies the monodromy condition, as moving around on a non-trivial loop inside the annulus does not yield a multi-valued map.

9.1.4 Transition map

Assume the general setting from Section 9.1.3.

From the definition of the scattering map associated to Φ^t , it follows that, if $x \in \Gamma$ is a homoclinic point and

$$S(x_-) = x_+, \text{ where } x_\pm \in \Lambda,$$

then

$$\begin{aligned} d(\Phi^{-t_-}(x), \Phi^{-t_-}(x_-)) &\rightarrow 0, \text{ as } t_- \rightarrow \infty, \\ d(\Phi^{t_+}(x), \Phi^{t_+}(x_+)) &\rightarrow 0, \text{ as } t_+ \rightarrow \infty. \end{aligned}$$

This correspondence represents the so-called *transition map* (see [DGR13]).

Definition 9.2. Given $\delta > 0$, let $T_- = T_-(\delta)$, $T_+ = T_+(\delta)$ be the infimum of the positive reals t_- , t_+ , respectively, for which

$$d(\Phi^{-t_-}(x), \Phi^{-t_-}(x_-)) \leq \delta, \quad d(\Phi^{t_+}(x), \Phi^{t_+}(x_+)) \leq \delta. \quad (9.6)$$

Then the *transition map* $\mathcal{T}_\delta : \Phi^{-T_-}(\text{Dom}(S)) \rightarrow \Phi^{T_+}(\text{Im}(S))$ is defined as

$$\mathcal{T}_\delta = \Phi^{T_+} \circ S \circ \Phi^{T_-}.$$

The transition map depends on the choice of the homoclinic channel Γ and on the distance δ to the NHIM.

Thus, for T_-, T_+ large enough, the homoclinic orbit segment $\Phi^{[-T_-, T_+]}(x) = \{\Phi^t(x) \mid t \in [T_-, T_+]\}$ in M is an approximation of the pseudo-orbit $\Phi^{T_+} \circ S \circ \Phi^{T_-}(x_-)$. The former is an orbit segment in the manifold M , while the latter is given by an orbit segment of the inner dynamics $\Phi^{T_-}|_\Lambda$, followed by one application of the scattering map S , followed by another orbit segment of the inner dynamics $\Phi^{T_+}|_\Lambda$.

Remark 9.2. Note that, for the computation of both the scattering map and the transition map, one needs to know the inner dynamics, given by the restriction to the NHIM. Compared to the scattering map, the transition map depends on an extra parameter (the threshold distance δ to the NHIM), and so, different choices of this parameter yield different transition maps.

Remark 9.3. In the setting of Section 9.1.1, we can consider the dynamics of the original flow Φ_H of the RTBP, and the dynamics of the flow Φ_N associated to the Birkhoff normal form, as well as the corresponding NHIMs Λ_c and Λ_c^N , respectively. In each case, we can define a scattering map and a transition map. We denote by S the scattering map corresponding to Φ_H , and by S^N the scattering map corresponding to Φ_N . The map S is defined on some domain in Λ_c , and S^N is defined on some domain in Λ_c^N . Similarly, we denote by $\mathcal{T}_\delta$ the transition map associated to Φ_H , and by $\mathcal{T}_\delta^N$ the transition map associated to Φ_N .

9.1.5 Reduction of the Scattering Map and the Transition Map to a Poincaré Section

We now consider the setting from Section 9.1.1.

In the paper [DGR16] it is shown that, in the case of the spatial circular RTBP, the unstable and stable manifolds of Λ_c^N intersect, giving rise to homoclinic orbits to Λ_c^N . We can select a homoclinic channel Γ_c and consider the scattering map associated to the truncated Birkhoff normal form:

$$S^N : \text{Dom}(S^N) \subseteq \Lambda_c^N \rightarrow \text{Im}(S^N) \subseteq \Lambda_c^N.$$

To reduce the dimensionality of the scattering map, we consider the Poincaré section $\Sigma = \{\phi_p = 0\}$, with associated first return map $\mathcal{F} : \Sigma \rightarrow \Sigma$. Let $\Lambda_c^{N, \Sigma}$ denote the intersection of the NHIM with the Poincaré section:

$$\Lambda_c^{N, \Sigma} = \Lambda_c^N \cap \Sigma.$$

We have shown in [DGR16, Section 3.2] that $\Lambda_c^{N, \Sigma}$ is a normally hyperbolic invariant manifold for $\mathcal{F}$, which we call the *reduced NHIM*. This is a 2-dimensional manifold, that can be parameterized in terms of (J_v, ϕ_v) . It has a symplectic structure given by $dJ_v \wedge d\phi_v$. The scattering map induces a *reduced scattering map*:

$$\sigma^N : \text{Dom}(\sigma^N) \subseteq \Lambda_c^{N, \Sigma} \rightarrow \text{Im}(\sigma^N) \subseteq \Lambda_c^{N, \Sigma}.$$

The reduced scattering map σ^N is exact symplectic. (See [DLS08]).

Inside $\Lambda_c^{N, \Sigma}$ we consider an annulus given by

$$\mathcal{A} = \Lambda_c^{N, \Sigma} \cap \{ J_v \in [J_1, J_2], \phi_v \in [0, 2\pi) \}$$

where $J_1 < J_2$ will be specified in Section 9.3.5.

For each fixed value of $J_v = \bar{J}_v$ in the range, there is a unique invariant curve for $\mathcal{F}$

$$T_{\bar{J}}^{N,\Sigma} = \mathcal{A} \cap \{J_v = \bar{J}_v\}.$$

One can derive the reduced scattering map σ from the full scattering map S^N as follows. Let $x_{\pm}$ be two points related by the scattering map: $x_+ = S^N(x_-)$. Then we flow x_- backwards to the Poincaré section Σ , obtaining a new point $(J_-, \phi_-) \in \Lambda_c^{N,\Sigma}$. Similarly, we flow x_+ forward to Σ , obtaining $(J_+, \phi_+) \in \Lambda_c^{N,\Sigma}$. The reduced scattering map σ^N takes (J_-, ϕ_-) to (J_+, ϕ_+) .

When it is clear from the context, we will abbreviate ‘reduced scattering map’ to just ‘scattering map’. Also, for ease of notation, we will simply write (J, ϕ) for (J_v, ϕ_v) .

The transition map can be reduced to a surface of section in a similar fashion. Let $x \in \Gamma_c^\Sigma = \Gamma_c \cap \Sigma$ be a homoclinic point and

$$\sigma^N(x_-) = x_+, \text{ where } x_{\pm} \in \Lambda_c^\Sigma.$$

In terms of the (J, ϕ) coordinates we can write $x_- = (J_-, \phi_-)$ and $x_+ = (J_+, \phi_+)$. For a given $\delta > 0$ where the Birkhoff normal form applies (see Section 9.3.1), let K_-, K_+ be the smallest positive integers k_-, k_+ , respectively, such that

$$d(\mathcal{F}^{-k_-}(x), \mathcal{F}^{-k_-}(x_-)) < \delta, \quad d(\mathcal{F}^{k_+}(x), \mathcal{F}^{k_+}(x_+)) < \delta. \quad (9.7)$$

Then the transition map is given by

$$\tau_\delta^N = \mathcal{F}^{K_+} \circ \sigma^N \circ \mathcal{F}^{K_-}.$$

Remark 9.4. Since the dynamics along the hyperbolic manifolds $W^{u,s}(\Lambda_c^\Sigma)$ is much faster than the inner dynamics $\mathcal{F}|_{\Lambda_c^\Sigma}$, it may happen that condition (9.7) is satisfied for $K_- = K_+ = 1$. In that case, the transition map is given by

$$\tau_\delta^N = \mathcal{F} \circ \sigma^N \circ \mathcal{F}.$$

Indeed, the transition map used will be of this type.

9.2 Main results

In this section we first provide an abstract result for an iterated function system (IFS) consisting of an inner map (given by the restriction of the dynamics to a NHIM) and finitely many scattering maps, saying that, if the IFS satisfies some verifiable, quantitative conditions, then the system has true ‘diffusing’ orbits. Then, we give the main numerical result of the chapter, which amounts to the numerical verification of the assumptions of the abstract result.

Theorem 9.1. *Assume that $\mathcal{F} : \Sigma \rightarrow \Sigma$ is a diffeomorphism on a manifold Σ , Λ is a 2-dimensional NHIM for $\mathcal{F}$, (I, ϕ) a coordinate system on Λ , $\omega = dI \wedge d\phi$ a symplectic form on Λ , and*

$$\mathcal{A} = [I_1, I_2] \times \mathbb{T}^1 \subset \Lambda.$$

Assume that $W^s(\mathcal{A})$ and $W^u(\mathcal{A})$ intersect along a homoclinic channel Γ_i , $i \in \{1, \dots, L\}$, where $L \geq 1$. Let $f = \mathcal{F}|_{\Lambda}$ be the restriction of $\mathcal{F}$ to Λ and σ_i be the scattering map associated to Γ_i , $i \in \{1, \dots, L\}$.

I. We assume that the inner map f satisfies the following conditions:

(I.i) The map f is an exact symplectic¹ twist map, i.e.

$$\frac{\partial \pi_\phi f}{\partial I}(I, \phi) > 0. \quad (9.8)$$

(I.ii) There exists $\rho_1 > 0$ such that for every $\bar{I} \in [I_1, I_2]$, the level set $\{I = \bar{I}\}$ is invariant under f up to an error of ρ_1 , that is, for all $n \geq 0$ and $\bar{\phi} \in [0, 2\pi)$, we have

$$|\pi_I(f^n(\bar{I}, \bar{\phi})) - \bar{I}| < \rho_1.$$

II. We assume that each scattering map σ_i , $i \in \{1, \dots, L\}$, satisfies the following conditions:

¹A map f on $\mathcal{A}$ is exact symplectic if $f^*(Id\phi) - Id\phi = ds$ for some function s on $\mathcal{A}$.

(II.i) σ_i is globally defined on $\mathcal{A}$, i.e., $\text{dom}(\sigma) \supset \mathcal{A}$;

(II.ii) There exist C^1 -functions $\tilde{\mathcal{L}}_i = \tilde{\mathcal{L}}_i(I, \phi')$ and $\omega_i = \omega_i(I)$ such that

$$\begin{aligned} I' &= I + \frac{\partial \tilde{\mathcal{L}}_i}{\partial \phi'}(I, \phi'), \\ \phi &= \phi' + \omega_i(I) + \frac{\partial \tilde{\mathcal{L}}_i}{\partial \phi'}(I, \phi'), \end{aligned} \quad (9.9)$$

where we denote $\sigma_i(I, \phi) = (I', \phi')$;

(II.iii) There exists $\rho_2 > \rho_1$ such that for every $\bar{I} \in [I_1, I_2]$ there exists $i \in \{1, \dots, L\}$ and $\bar{\phi} \in [0, 2\pi)$ such that

$$\frac{\partial \tilde{\mathcal{L}}_i}{\partial \bar{\phi}'}(\bar{I}, \bar{\phi}') > \rho_2. \quad (9.10)$$

Then, for any neighborhood U_1 of $\{I_1\} \times \mathbb{T}^1$ and U_2 of $\{I_2\} \times \mathbb{T}^1$ in Σ there exists an orbit $\{z_n\}_{n=0, \dots, N}$ of $\mathcal{F}$ in Σ such that

$$z_0 \in U_1 \text{ and } z_N \in U_2.$$

Proof. The proof follows immediately from the following result in [Moe02], and its extensions in [LC07] and [GM22].

Theorem 9.2 ([Moe02]). *Let $\mathcal{A} = [0, 1] \times \mathbb{T}^1$ and $f, g : \mathcal{A} \rightarrow \mathcal{A}$ be two C^1 -diffeomorphisms of the annulus that preserve the boundary circles.*

Assume the following

- (i) f is a twist map;
- (ii) g is an area preserving map;
- (iii) Every essential² f -invariant circle Γ is not invariant under g .

Then, for every pair of open neighborhoods U_0 of $\{0\} \times \mathbb{T}$ and U_1 of $\{1\} \times \mathbb{T}$ in $\mathcal{A}$, there exists an orbit $(x_n)_{n=0, \dots, N}$ of the IFS generated by $\{f, g\}$ such that $x_0 \in U_0$ and $x_N \in U_1$ (the orbit of the IFS is defined at every step by a choice $x_{n+1} = f(x_n)$ or $x_{n+1} = g(x_n)$).

In Theorem 9.2 it is essential that the map g is globally defined on the annulus $\mathcal{A}$. On the other hand, the condition that f preserves the boundary components of the annulus can be replaced by the condition that f is exact symplectic. Also, the conditions that g preserves the boundary components of the annulus and that it does not preserve any essential f -invariant circle can be replaced by the condition that for any essential f -invariant circle, there are points below the circle that are mapped by g to points above the circle.

The theorem extends immediately when instead of a single map g we have finitely many maps $g_1, \dots, g_L$ satisfying (ii) such that every essential f -invariant circle Γ is not invariant under some g_i , $i \in \{1, \dots, L\}$.

Condition (I.i) of Theorem 9.1 in f represents condition (i) of Theorem 9.2. Condition (II.i) on σ_i from Theorem 9.1 ensure that these maps are globally defined on $\mathcal{A}$.

Condition (I.ii) of Theorem 9.1 implies that each essential invariant circle for f is contained within ρ_1 of some I -level set. Conditions (II.ii) and (II.iii) of Theorem 9.1 imply that for each I -level set, there is a scattering map σ_i and a point on the I -level set whose I -coordinate is increased by σ_i by more than $\rho_2 > \rho_1$. Therefore, any essential f -invariant circle fails to remain invariant under at least one of the σ_i . Theorem 9.2 implies that there is a pseudo-orbit $(x_n)_{n=0, \dots, N}$ of the IFS generated by $\{f, \sigma_1, \dots, \sigma_L\}$ such that $x_0 \in U_0$ and $x_N \in U_1$. To obtain a true orbit, we use the following result that follows directly from [GLMS20, Lemma 3.2 and Theorem 3.7].

Theorem 9.3. *Assume that (Σ, ω) is a symplectic manifold of finite symplectic volume, $\mathcal{F} : \Sigma \rightarrow \Sigma$ is a symplectic diffeomorphism, $\Lambda \subseteq M$ is a NHIM for $\mathcal{F}$, $f = \mathcal{F}|_\Lambda$ and σ_i , $i = 1, \dots, L$, is a family of scattering maps on Λ .*

Then every finite pseudo-orbit $\{x_i\}_{i=0, \dots, N}$ of the IFS generated by $\{f, \sigma_1, \dots, \sigma_L\}$ in Λ can be shadowed by a true orbit, that is, for every $\delta > 0$, there exists an orbit $\{z_i\}_{i=0, \dots, N}$ of $\mathcal{F}$ in Σ , with $z_{i+1} = f^{k_i}(z_i)$ for some $k_i > 0$, such that $d(z_i, x_i) < \delta$ for all $i = 0, \dots, N$.

²An essential circle is a simple closed C^0 -curve in $\mathcal{A}$ that is nonhomotopic to zero.

Applying Theorem 9.3 to the $(x_n)_{n=0,\dots,N}$ of the IFS generated by $\{f, \sigma_1, \dots, \sigma_L\}$ yields a true orbit of $\mathcal{F}$ from U_0 to U_1 . $\square$

We now provide an outline of the numerical verification of the conditions of Theorem 9.1. Details are provided in Section 9.9.

Numerical Result 9.1. *Consider the setting from Section 9.1.1.*

- (a) *In Section 9.3 we obtain the approximation of the NHIM Λ_c by Λ_c^N , using the Birkhoff normal form $H_{trunc}^{(N)}$.*
- (b) *In Section 9.3.1 we show that the error in the numerical approximation of the NHIM is less than 10^{-15} (close to machine precision).*
- (c) *In Section 9.3.4 we construct two scattering maps that are globally defined on an annular $\mathcal{A}$ inside Λ_c^N , corresponding to the range $J \in [J_1, J_2]$, where $J_1 = 0.001$ and $J_2 = 0.007$. See Section 9.3.5 for additional details.*
- (d) *In Section 9.4 we rescale $I = 10^3 \cdot J$ and derive series representations of the two scattering maps, which are of the form (9.9).*
- (e) *In Section 9.5 we show that the generating functions $\tilde{\mathcal{L}}_i$ associated to these scattering maps satisfy condition (9.10) for $\rho_2 = 0.1$. By (b), the level sets of I are preserved by the inner map up to an error of $\rho_1 = 10^{-12}$.*
- (f) *In Section 9.6 we verify that the inner map satisfies a twist condition.*

Provided that the conditions (a)–(f) have been verified, then there exists a true, zero-cost orbit of Φ_H along which I changes from $I_1 = 1$ to $I_2 = 7$.

Remark 9.5. A result similar to Theorem 9.1 can be formulated in terms of scattering maps only (without using the inner map). More precisely, assume that we have a family of scattering maps $\{\sigma_1, \dots, \sigma_L\}$ as in Theorem 9.1, and that one of them, say σ_1 , satisfies a twist condition as in (9.8). Also assume that there exist $0 < \rho_1 < \rho_2$ such that

$$\max_{\bar{\phi}'} \left| \frac{\partial \tilde{\mathcal{L}}_1}{\partial \bar{\phi}'}(\bar{I}, \bar{\phi}') \right| < \rho_1,$$

and for each $\bar{I}$ there exists $i \neq 1$ such that

$$\max_{\bar{\phi}'} \frac{\partial \tilde{\mathcal{L}}_i}{\partial \bar{\phi}'}(\bar{I}, \bar{\phi}') > \rho_2.$$

Then there exist an orbit $\{z_n\}_{n=0,\dots,N}$ of $\mathcal{F}$ as in the conclusion of Theorem 9.1.

The main idea is that σ_1 plays the role of the inner dynamics in Theorem 9.1.

In Sections 4–12 below, we compute numerically the flow Φ_N , the corresponding NHIM Λ_c^N , two scattering maps and two transition maps, as well as their reductions to the surface of section Σ . In Section 9.3.1 we give an estimate of the error between the original flow Φ_H and the flow computed via the Birkhoff normal form Φ_N , obtaining that Λ_c^N is an accurate enough numerical approximation of Λ_c . As all subsequent computations are performed via the Birkhoff normal form, to simplify the notation, from now on we drop the superscript/subscript N from the notation for all objects.

9.3 Numerical Scattering Map on a Grid for $C = 3.00088$

Using the methodology presented in the paper [DGR16], we compute the NHIM Λ_c and its stable/unstable manifolds. We show that the asymptotic manifolds intersect transversally along two homoclinic channels, giving rise to two different scattering maps. We compute the scattering maps numerically at a grid of points; they are shown in Figure 9.9.

For our purpose we will use the energy value $C = c := 3.00088$. This value is chosen after the appearance of the equilibrium point L_1 ($c_1 := 3.00090$), but before the appearance of *halo* orbits ($c_{\text{halo}} := 3.00082$). The choice of energy is motivated by two reasons.

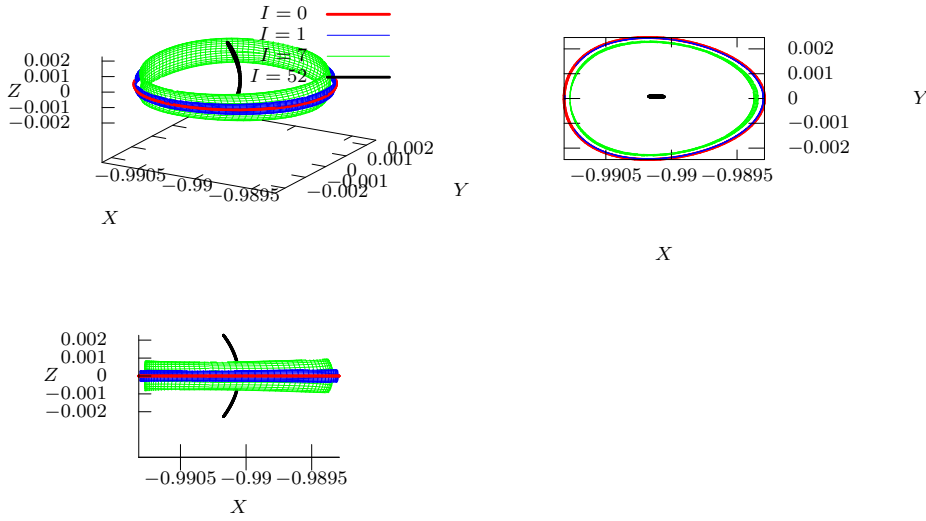


Figure 9.3: The NHIM Λ_c consists of a continuous family of invariant tori around L_1 . The endpoints of the family are the planar and vertical Lyapunov orbits (shown in red and black, respectively). In between, there are 2-d tori of increasing vertical amplitude J . (For clarity, only two of them are shown). The transfer trajectory shown in Figure 9.1 starts at an initial condition very close to the blue torus $I = 1$ and ends very close to the green torus $I = 7$, where $I = 10^3 \cdot J$

Firstly, c is close enough to c_1 so that the dynamics around L_1 is almost integrable. Thus, the (integrable) Birkhoff normal form $H_{\text{trunc}}^{(N)}$ provides a good approximation to the local dynamics. (Section 9.3.1 quantifies the Birkhoff normal form error).

Secondly, c is close enough to c_1 so that we are in the setting of *a priori chaotic Arnold diffusion* (see Section 9).

Fixing the energy value $c = 3.00088$, the NHIM Λ_c consists of a continuous family of 2-dimensional invariant tori around L_1 , which we parametrize by the vertical action J . The vertical action increases along the family from $J = 0$ to $J = J_{\max} := 0.052$. Correspondingly, the planar action J_p decreases from 0.05029 to 0.

Figure 9.3 shows some tori in the NHIM Λ_c .

- $J = 0$ (i.e. $J_p = 0.05029$) corresponds to the unique planar Lyapunov orbit in this energy level.
- $J = 0.052$ (i.e. $J_p = 0$) corresponds to the unique vertical Lyapunov orbit in this energy level.
- Every intermediate action $J \in (0, 0.052)$ corresponds to a 2-dimensional torus located between the planar and the vertical Lyapunov orbits.

As seen in Figure 9.3, the NHIM Λ_c spans a spherical region of radius 0.002 Astronomical Units (AU), or roughly 300000 km around the equilibrium point L_1 .

9.3.1 Accuracy of the Birkhoff normal form

The accuracy of the Birkhoff normal form (BNF) expansion has been tested against numerical integration of the R3BP equations, following the same procedure as in [JM99]. Compute an initial condition on Λ_c by evaluating the BNF up to order $N = 16$. This initial condition is integrated for π units of adimensional time using two different methods:

1. Using the BNF. No numerical integration is needed. As the Hamiltonian is integrable, and we have it integrated, we simply tabulate the solution at time π .
2. Integrate the R3BP equations using a Runge-Kutta-Feldberg numerical integrator of order 7-8, with local error at each step within 10^{-14} .

Then compare the two final conditions.

This test has been performed for several initial conditions on Λ_c . In all cases, the difference in the Euclidean norm for the final condition is less than 10^{-12} adimensional R3BP units. Thus the initial condition was very accurate, in the sense that it is very close to one of the tori computed by the BNF.

In fact, it is known that, due to the hyperbolicity of orbits around the collinear point, errors increase by a factor close to 1500 after π units of time. Therefore the error in the initial condition is less than $10^{-12}/1500$ adimensional units, close to machine precision.

Furthermore, this validity and accuracy of the BNF of order N in a neighborhood of size δ along the unstable/stable coordinates, say for $\delta = 10^{-3}$ and $N = 16$, can also be analytically corroborated using theoretical results, for example from [DG96b]. The bound of the error in a neighborhood of the libration point is there given as a function of the bounds of the Taylor expansion of the Hamiltonian, as well as of the small divisors $k_p\nu_p + k_v\nu_v$ for integers satisfying $|k_p| + |k_v| \leq N$.

It should be noted that the presence of these small divisors is what affects the convergence of these Birkhoff normal forms. Although they depend on the mass ratio μ , they do so very slightly for libration points; see, for instance, [Jor99, JM99]. Therefore, their influence in detecting strong resonances is not noticeable up to normal form orders much higher than $N = 16$.

9.3.2 Homoclinic Orbits

In [DGR16], Section 4.3, we explained in detail how to compute the intersection of the stable and unstable manifolds $W^s(\Lambda_c) \cap W^u(\Lambda_c)$ restricted to the surface of section

$$\mathcal{S} = \{(X, Y, Z, \dot{X}, \dot{Y}, \dot{Z}) : Y = 0, \dot{Y} > 0\}.$$

We find that the asymptotic manifolds do indeed intersect transversally, giving rise to families of homoclinic orbits to the Λ_c . These homoclinics will later be encoded by two scattering maps.

Briefly, the numerical procedure to compute each homoclinic consists of finding two initial conditions y_-, y_+ on the *local* unstable resp. stable manifolds, and a point $x \in \mathcal{S}$ such that: (1) $\Phi_H^t(y_-) = x$; and (2) $\Phi_H^{-s}(y_+) = x$. Then x is a homoclinic point, generating a homoclinic orbit segment from y_- to y_+ .

We would like to emphasize some aspects of this computation:

- We consider **only the first intersection** of the stable and unstable manifolds with the surface of section $\mathcal{S}$. The ‘primary’ homoclinic connections generated in this way travel around the Earth once.
- The initial conditions y_-, y_+ are taken at a distance $\delta = 10^{-3}$ of the NHIM along the unstable/stable coordinates. This guarantees that they are inside the domain where the Birkhoff normal form is accurate.
- At the same time, these initial conditions are sufficiently far from the NHIM so that the homoclinic orbit segment does not wind around L_1 more than once.
- All homoclinics take $5.936738 \leq t + s \leq 6.000688$ time units to go from y_- to y_+ . We will refer to $t + s$ as the ‘flight time’ of the homoclinic. The shortest and longest flight times correspond to the two homoclinics of the Lyapunov orbit. See Figure 9.4.

Following the decomposition of Λ_c into invariant tori, we first study homoclinic orbits from each T_J to itself. Later we will study homoclinic orbits from T_J to nearby tori.

- When $J = 0$, the invariant manifolds $W^u(T_0)$ and $W^s(T_0)$ have 2 transverse intersections in the section $\mathcal{S}$. Hence, the planar Lyapunov orbit T_0 has 2 homoclinic connections with itself. See Figure 9.4.
- For every fixed $J \in (0, 0.01)$, the invariant manifolds $W^u(T_J)$ and $W^s(T_J)$ have 8 transverse intersections. That is, every torus T_J in this domain has 8 homoclinic connections with itself.
- In contrast, for action values J above 0.01, the invariant manifolds $W^u(T_J)$ and $W^s(T_J)$ cease to intersect (at their first intersection with the section $\mathcal{S}$).

Remark 9.6. The planar Lyapunov orbit has two ‘primary’ homoclinics that travel around the Earth (see Figure 9.4). However, one of them makes a longer excursion than the other: the green homoclinic has flight time 5.936738, while the blue one has flight time 6.000688.

Remark 9.7. Each of the 2 intersections in $W^u(T_0) \cap W^s(T_0)$ gives rise to 4 intersections when we increase the dimension of the manifolds $W^u(T_J), W^s(T_J)$ by one. This is expected by Morse theory [Mil63].

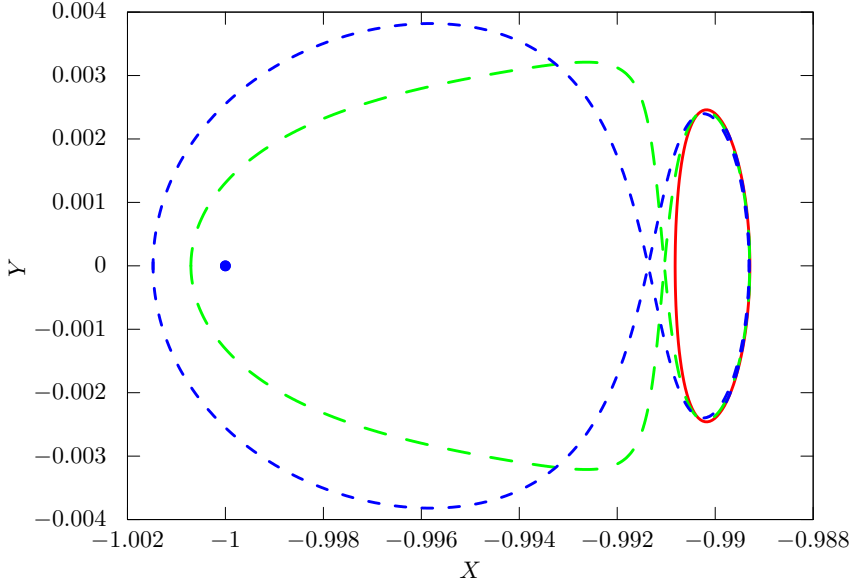


Figure 9.4: Planar Lyapunov orbit (solid line), and its two ‘primary’ homoclinics (dashed). Both homoclinics travel around the Earth once (located at $X = -1 + \mu$).

9.3.3 Computation of Local Transition Map and Scattering Map.

Consider a homoclinic point $x \in \mathcal{S}$ as found in Section 9.3.2, generating a homoclinic orbit segment from $y_- \in W_{loc}^u(\Lambda_c)$ to $y_+ \in W_{loc}^s(\Lambda_c)$, with flight time $t + s$. Let

$$y_- = (y_h^- = \delta, J_p^-, J_v^-, x_h^- = 0, \phi_p^-, \phi_v^-)$$

and

$$y_+ = (y_h^+ = 0, J_p^+, J_v^+, x_h^+ = \delta, \phi_p^+, \phi_v^+)$$

in Birkhoff normal form coordinates. Then, the transition map $\mathcal{T}_\delta: \Lambda_c \rightarrow \Lambda_c$ is given by

$$(J_p^-, J_v^-, \phi_p^-, \phi_v^-) \mapsto (J_p^+, J_v^+, \phi_p^+, \phi_v^+).$$

As explained in Section 9.1.4, the scattering map $S: \Lambda_c \rightarrow \Lambda_c$ is related to the transition map by the flow. Therefore, the scattering map is given by

$$x_- := \Phi^t(J_p^-, J_v^-, \phi_p^-, \phi_v^-) \mapsto x_+ := \Phi_H^{-s}(J_p^+, J_v^+, \phi_p^+, \phi_v^+).$$

Every transverse intersection

$$x \in W^u(T_J) \cap W^s(T_J)$$

implies that there exists a pair of points $x_-, x_+ \in T_J$ such that $W^u(x_-)$ intersects $W^s(x_+)$ at the homoclinic point x . Since this is an open condition, we can define a local scattering map on some open set containing x_- by $x_- \mapsto S(x_-) := x_+$.

In fact, we find that these local scattering maps can be continued to form two *global* scattering maps, which we will denote S_1 and S_2 . They determine the reduced scattering maps, σ_1 and σ_2 (see Section 9.1.5).

9.3.4 Extending the Scattering Map

Let us explain how S_1 is numerically constructed. (S_2 is constructed analogously). The general idea is to compute S_1 on several tori T_J (for example $J = 0.001, 0.002, \dots, 0.007$). This provides a coarse representation of S_1 .

To compute S_1 on a given torus T_J , fix an action $J \in [0.001, 0.007]$. As explained above, $W^u(T_J)$ has 8 transverse intersections with $W^s(T_J)$ in the surface of section $\mathcal{S}$. Four of them, which we will denote x^i for $i = 1, 2, 3, 4$, give rise to 4 pairs of points associated by the local scattering maps:

$$x_+^i = S(x_-^i) \quad \text{for } i = 1, \dots, 4.$$

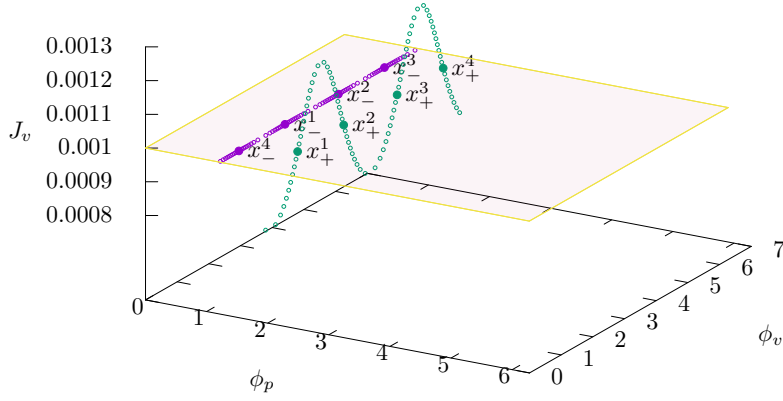


Figure 9.5: Action of the scattering map S_1 on the torus T_J with $J = 0.001$. S_1 maps the purple set to the green set. When the ‘source’ and ‘destination’ tori T_J have the same action ($J = 0.001$ in this picture, corresponding to the translucent plane), S_1 maps the 4 points $x_-^i \in T_J$ to $x_+^i \in T_J$. Fixing the source torus T_J and varying the destination torus $T_{J'}$ to action levels J' near J , the scattering map S_1 is continued to the purple and green sets.

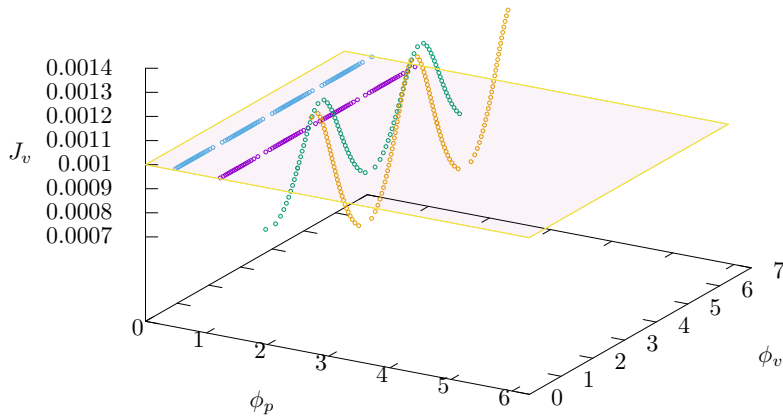


Figure 9.6: Action of scattering maps S_1 and S_2 on the torus T_J with $J = 0.001$. S_1 maps the purple set to the green set, while S_2 maps blue to orange.

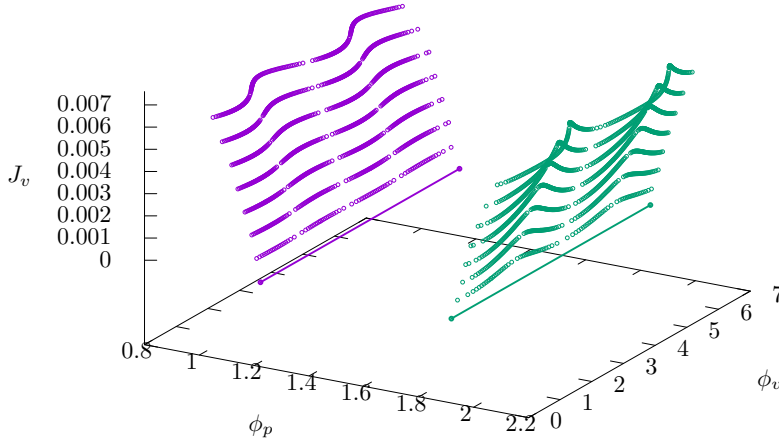


Figure 9.7: S_1 acting on several action levels: $J = 0.001, 0.002, \dots, 0.007$.

Figure 9.5 shows these 4 pairs of points: x_-^i in the domain of S_1 are plotted in purple, while x_+^i in the codomain are plotted in green.

Keeping the action of the source torus fixed to J , vary the action of the destination torus to a new value J' close to J , and recompute the intersection $W^u(T_J) \cap W^s(T_{J'})$, giving rise to 4 new homoclinic points and 4 corresponding pairs of points associated by S_1 . Continue this procedure until the manifolds $W^u(T_J)$ and $W^s(T_{J'})$ cease to intersect, effectively extending the domain of the scattering map S_1 from 4 points to the purple set in Figure 9.5, and the codomain to the green set.

Remark 9.8. Starting with the other 4 homoclinic points, x^i for $i = 5, 6, 7, 8$, and applying the same procedure, gives rise to a different scattering map S_2 . See Figure 9.6. S_1 and S_2 are fundamentally different, as they are not conjugated by the flow in the sense of (9.5).

We repeat this procedure for the tori $J = 0.001, 0.002, \dots, 0.007$. See Figure 9.7.

Remark 9.9. For $J \rightarrow 0$, the torus T_J degenerates into the horizontal Lyapunov periodic orbit T_0 . The 4 homoclinic points x^i converge to a single homoclinic point x for T_0 . Similarly, the 4 pairs x_-^i, x_+^i converge to a single pair x_-, x_+ of points associated by S_1 . Figure 9.7 shows x_-, x_+ as straight lines (all angles $\phi_v \in [0, 2\pi)$ are identified for $J = 0$).

Using the computation of S_1 we compute the reduced scattering map σ_1 . Recall from Section 9.1.5 that the reduced scattering map can be obtained from the full scattering map simply by flowing the points x_-/x_+ backwards/forwards to the Poincaré section $\Sigma = \{\phi_p = 0\}$.

Flowing the purple set backwards to Σ , we obtain a mesh $\{(J, \phi)\}$ discretizing the reduced NHIM Λ_c^Σ . Flowing the green set forwards to Σ , we obtain the image set $\{(J', \phi')\}$ under σ_1 , also on Λ_c^Σ . This way, we have extended the local scattering maps onto a global (reduced) scattering map σ_1 on Λ_c^Σ .

Figure 9.9 (top panel) shows the image set of the global scattering map σ_1 . For example, the green set in Figure 9.5 ($J = 0.001$) corresponds to the lowest curve in Figure 9.9 after flowing it forward.

9.3.5 Domain of the Global Scattering Map

From above, the global scattering maps σ_1, σ_2 are well defined on an annulus $\mathcal{A}$ inside Λ_c^Σ given by

$$\mathcal{A} = \{(J, \phi) : J \in [0.001, 0.007] \text{ and } \phi \in [0, 2\pi)\}. \quad (9.11)$$

For $0.007 < J < 0.01$, we find that the scattering maps can not be defined on the whole torus T_J . For illustration, Figure 9.8 shows the continuation of all 8 local scattering maps when $J = 0.009$. Notice that the purple and blue sets (which belong to the domain of S_1 and S_2 respectively) have become connected, and they form two contractible circles. Moreover, the purple and blue sets do not cover all angles $\phi_v \in [0, 2\pi)$ as before. Thus one can not extend S_i to the whole torus T_J by the flow using

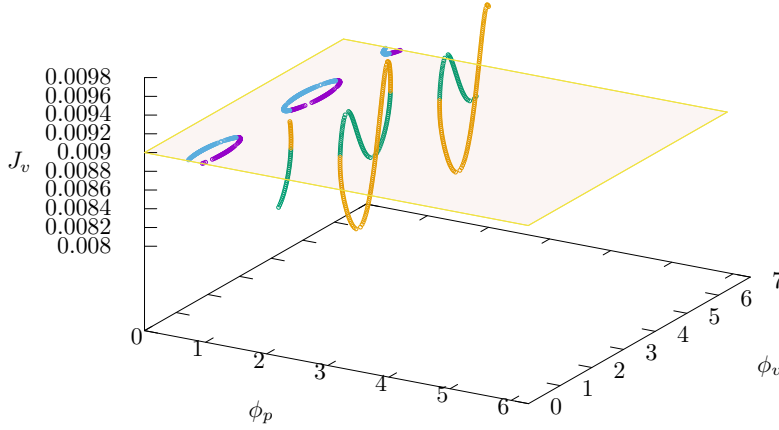


Figure 9.8: Action of scattering maps S_1 and S_2 on the action level $J = 0.009$. S_1 and S_2 have ‘merged’, and they can not be extended to the whole torus.

the conjugacy property (9.5). Consequently, the reduced scattering map σ_i is not defined on the whole invariant curve T_J^Σ .

For the purpose of this chapter, we will restrict the domain of the global scattering maps σ_1, σ_2 to the annulus $\mathcal{A}$.

9.4 Series Representation of the Scattering Map

The goal of this section is to introduce a series representation of the (global, reduced) scattering maps σ_1 and σ_2 . This finite series expansion consists in Equations (9.13)-(9.15) and (9.19) below. It is a more efficient representation than the numerical scattering map computed in the previous section, since it is limited to a small number of terms. Moreover, it allows us to evaluate σ_i , $i = 1, 2$, at any point of its domain.

Note that J and ϕ have different scales: J is of order 10^{-3} , while ϕ is of order 1. To improve numerical conditioning, we scale J as follows:

$$I = 1000J. \quad (9.12)$$

From now on, we will work with the scaled coordinate I instead of J .

The most classical way to represent a symplectic map $(I, \phi) \rightarrow (I', \phi')$ is by a generating function depending on old and new variables. In [DMR08], the scattering map on Lyapunov periodic orbits was shown to be a phase shift $(I, \phi) \rightarrow (I, \phi + \Delta(I))$. Thus, in our setting it is natural to look for a generating function of the form

$$\mathcal{L}(I, \phi') = I\phi' + \Omega(I) + \tilde{\mathcal{L}}(I, \phi'),$$

which will at least be valid for small values of I . The generating function $\mathcal{L}(I, \phi')$ is decomposed into its average part with respect to ϕ' , denoted $\Omega(I)$, and its oscillatory part $\tilde{\mathcal{L}}(I, \phi')$, which satisfies $\int_0^{2\pi} \tilde{\mathcal{L}}(I, \phi') d\phi' = 0$.

Hence, the equations for the scattering map $(I', \phi') = \sigma(I, \phi)$ are given implicitly by

$$\phi = \frac{\partial \mathcal{L}}{\partial I}(I, \phi') = \phi' + \omega(I) + \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi') \quad (9.13a)$$

$$I' = \frac{\partial \mathcal{L}}{\partial \phi'}(I, \phi') = I + \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi'), \quad (9.13b)$$

where $\omega(I) = \Omega'(I)$.

We will approximate both $\tilde{\mathcal{L}}(I, \phi')$ and $\omega(I)$ in Equation (9.13) using finite series expansions. Firstly, since we are going to work with few values of I , we approximate the function $\tilde{\mathcal{L}}(I, \phi')$ using a Fourier-Polynomial interpolation:

$$\tilde{\mathcal{L}}(I, \phi') = - \sum_{n=1}^N \frac{B_n(I)}{n} \cos n\phi' + \sum_{n=1}^N \frac{A_n(I)}{n} \sin n\phi', \quad (9.14)$$

where

$$A_n(I) = \sum_{l=0}^L a_l^{(n)} I^l \quad \text{and} \quad B_n(I) = \sum_{l=0}^L b_l^{(n)} I^l. \quad (9.15)$$

The goal is to find the coefficients $a_l^{(n)}$ and $b_l^{(n)}$. In Section 9.3, we obtained numerically the scattering map σ on a grid of equispaced (I, ϕ) points. See Figure 9.9. It is a simple matter to fit the coefficients to this data, as explained in Section 9.4.1.

Remark 9.10. The SR3BP is invariant with respect to the transformation $(Z, \dot{Z}) \rightarrow (-Z, -\dot{Z})$. Thus, every trajectory passing through the point (X, Y, Z) has a *symmetric trajectory with respect to the XY plane*, which passes through the point $(X, Y, -Z)$. In particular, every heteroclinic trajectory from torus I to torus I' has a symmetric heteroclinic trajectory from torus I to I' . In Birkhoff normal form coordinates, the symmetry $Z \rightarrow -Z$ corresponds to $\phi_v \rightarrow \phi_v + \pi$. This translates to the following fact for the scattering map of the flow. Suppose that $S(J_v, \phi_p, \phi_v) = (J'_v, \phi'_p, \phi'_v)$. Then we have $S(J_v, \phi_p, \phi_v + \pi) = (J'_v, \phi'_p, \phi'_v + \pi)$. Equivalently for the reduced scattering map: Suppose that $\sigma(I, \phi_v) = (I', \phi'_v)$. Then we have $\sigma(I, \phi_v + \pi) = (I', \phi'_v + \pi)$. This implies that the image under the scattering map of any torus is a π -periodic curve (see Figure 9.9). Indeed, we have checked that the curves in Figure 9.9 are π -periodic up to a tolerance of 10^{-6} . From this point on, **we will plot all figures involving ϕ_v in the domain $[0, \pi)$ only.**

9.4.1 Fourier-Polynomial interpolation of the Generating Function

Let I be fixed, and consider equation (9.13b):

$$I' = I + \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'},$$

where

$$\frac{\partial \tilde{\mathcal{L}}}{\partial \phi'} = \sum_{n=1}^N A_n \cos n\phi' + \sum_{n=1}^N B_n \sin n\phi'. \quad (9.16)$$

Given a set of (I', ϕ') values on a grid (data points composing one curve in Figure 9.9), we use the discrete Fourier transform to obtain the Fourier coefficients A_n, B_n .

Remark 9.11. Since we have 128 (I', ϕ') data points for each torus, the maximum possible degree of the Fourier expansion (9.14) is $N = 64$.

Next, let I vary to obtain the Fourier coefficients $A_n(I), B_n(I)$ for each torus $I = 1, 2, \dots, 7$. Figure 9.10 shows the decay of these Fourier coefficients for each torus.

Remark 9.12. We know from Remark 9.10 that the scattering map is π -periodic. Thus, for each torus $I = \text{const}$, its image is a π -periodic curve $I' = \gamma(\phi')$, and the odd Fourier coefficients should all be zero: $A_{2k+1}(I) = B_{2k+1}(I) = 0$ for $k = 0, 1, 2, \dots$. Of course, in Figure 9.10 they are not exactly zero because the numerical data is not exactly π -periodic. From now on, all odd Fourier coefficients are set to zero, to obtain a model that satisfies the theoretical π -periodicity of the scattering map.

Let now the index n of the Fourier coefficient be fixed, and consider the polynomial approximation of $A_n(I)$ and $B_n(I)$ given in equation (9.15). Alternatively, given a set of $L + 1$ data points $(I_0, A_n(I_0)), \dots, (I_L, A_n(I_L))$, we will express the polynomials (9.15) in Newton's form

$$A_n(I) = \sum_{l=0}^L \tilde{a}_l^{(n)} N_l(I) \quad \text{and} \quad B_n(I) = \sum_{l=0}^L \tilde{b}_l^{(n)} N_l(I), \quad (9.17)$$

where $\tilde{a}_l^{(n)}, \tilde{b}_l^{(n)}$ are the *divided differences*, and $N_l(I)$ are Newton's basis polynomials

$$N_0(I) = 1, \quad N_l(I) := \prod_{i=0}^{l-1} (I - I_i) \quad \text{for } l = 1, \dots, L.$$

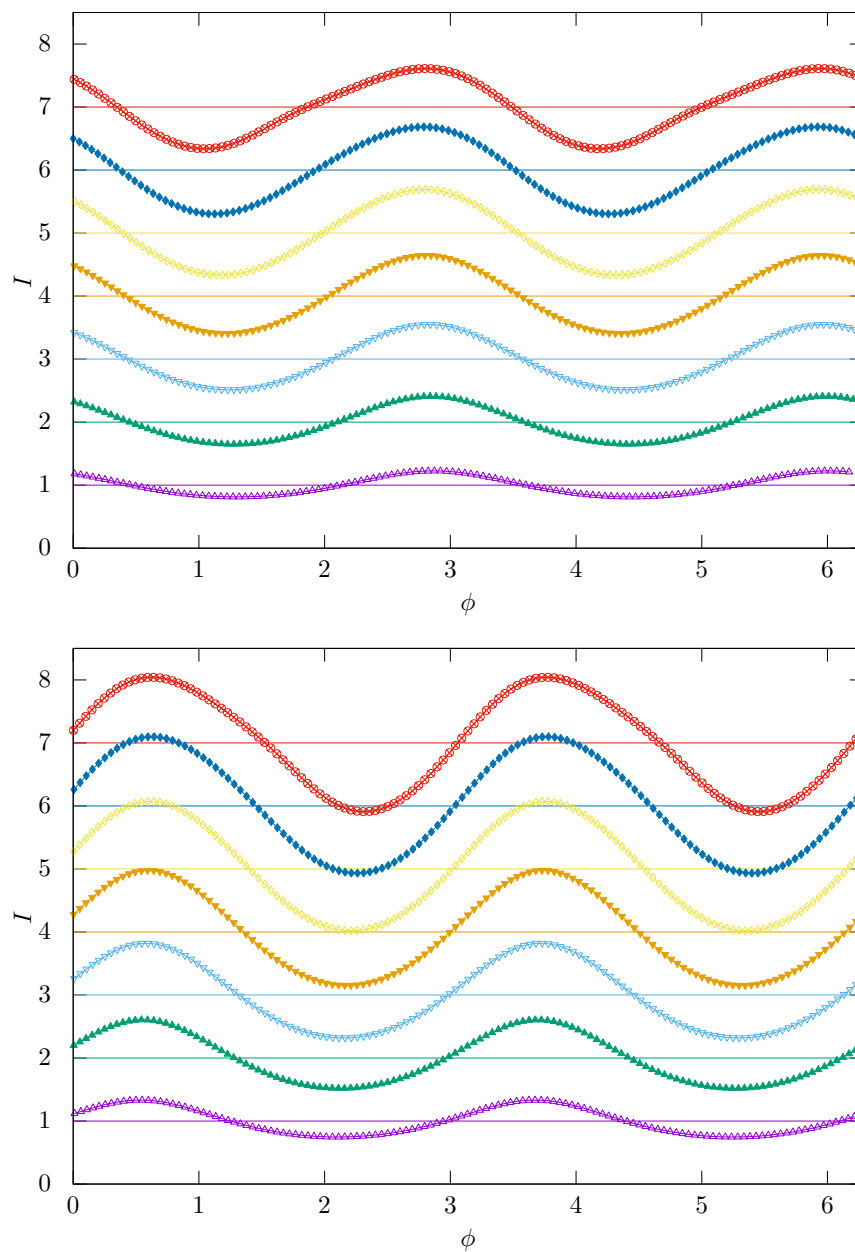


Figure 9.9: Image under the scattering map of several tori ($I = 1, 2, \dots, 7$). Above: action of σ_1 , below: action of σ_2 . A torus $\{(I, \phi) : I = \text{const}, \phi \in [0, 2\pi)\}$ and its image are plotted using the same color. Notice that the curves are π -periodic.

n	$\tilde{a}_1^{(n)}$	$\tilde{a}_2^{(n)}$	$\tilde{a}_3^{(n)}$	$\tilde{a}_4^{(n)}$	$\tilde{a}_5^{(n)}$	$\tilde{a}_6^{(n)}$	$\tilde{a}_7^{(n)}$
2	0.178180	-0.020025	0.000401	-0.000251	0.000046	0.000019	-0.000022
4	0.011726	-0.004878	0.001114	-0.000129	0.000039	-0.000006	0.000001
6	0.000712	-0.000519	0.000295	-0.000065	0.000004	-0.000000	-0.000001
8	0.000147	-0.000064	0.000027	-0.000012	0.000002	0.000000	0.000000
n	$\tilde{z}_1^{(n)}$	$\tilde{z}_2^{(n)}$	$\tilde{z}_3^{(n)}$	$\tilde{z}_4^{(n)}$	$\tilde{z}_5^{(n)}$	$\tilde{z}_6^{(n)}$	$\tilde{z}_7^{(n)}$
2	-0.097275	-0.005156	0.002856	-0.000574	0.000143	0.000003	-0.000016
4	-0.017677	0.003403	0.000242	-0.000067	0.000004	-0.000000	-0.000003
6	-0.002965	0.001408	-0.000332	0.000035	-0.000008	0.000002	-0.000000
8	-0.001045	0.000566	-0.000206	0.000053	-0.000009	0.000002	-0.000000

(a) Scattering map σ_1 .

n	$\tilde{a}_1^{(n)}$	$\tilde{a}_2^{(n)}$	$\tilde{a}_3^{(n)}$	$\tilde{a}_4^{(n)}$	$\tilde{a}_5^{(n)}$	$\tilde{a}_6^{(n)}$	$\tilde{a}_7^{(n)}$
2	0.136664	-0.019375	0.001251	-0.001067	0.000499	-0.000153	0.000031
4	-0.020745	0.001757	0.000921	-0.000221	0.000089	-0.000028	0.000006
6	-0.004644	0.001886	-0.000222	-0.000027	-0.000001	0.000001	-0.000000
8	-0.000049	0.000048	-0.000051	0.000015	0.000000	0.000000	-0.000000
n	$\tilde{z}_1^{(n)}$	$\tilde{z}_2^{(n)}$	$\tilde{z}_3^{(n)}$	$\tilde{z}_4^{(n)}$	$\tilde{z}_5^{(n)}$	$\tilde{z}_6^{(n)}$	$\tilde{z}_7^{(n)}$
2	0.253827	-0.011566	-0.001286	0.000406	-0.000226	0.000067	-0.000018
4	0.034009	-0.008888	0.000925	-0.000160	0.000086	-0.000022	0.000006
6	0.000823	-0.000764	0.000505	-0.000121	0.000025	-0.000008	0.000001
8	0.000400	-0.000113	0.000069	-0.000035	0.000007	0.000000	0.000000

(b) Scattering map σ_2 .

Table 9.1: Divided differences $\tilde{a}_l^{(n)}, \tilde{b}_l^{(n)}$ of the first Fourier coefficients $A_n(I), B_n(I)$. All odd Fourier coefficients are zero and thus not listed (see Remark 9.12). All constant terms of the Newton expansion $\tilde{a}_0^{(n)}, \tilde{b}_0^{(n)}$ are zero, and thus not listed (see Remark 9.14). Notice that the two coefficients $\tilde{a}_1^2$ and $\tilde{b}_1^2$ (in red) are much larger than the rest of coefficients for both scattering maps σ_1, σ_2 . For the scattering map σ_1 , the coefficient $\tilde{a}_2^2$ (in blue) is much larger than the rest of coefficients in the last six columns, i.e. $\tilde{a}_j^n$ for $j \geq 2$. For the scattering map σ_2 , the two coefficients $\tilde{a}_2^2$ and $\tilde{b}_2^2$ are much larger than the rest with $j \geq 2$.

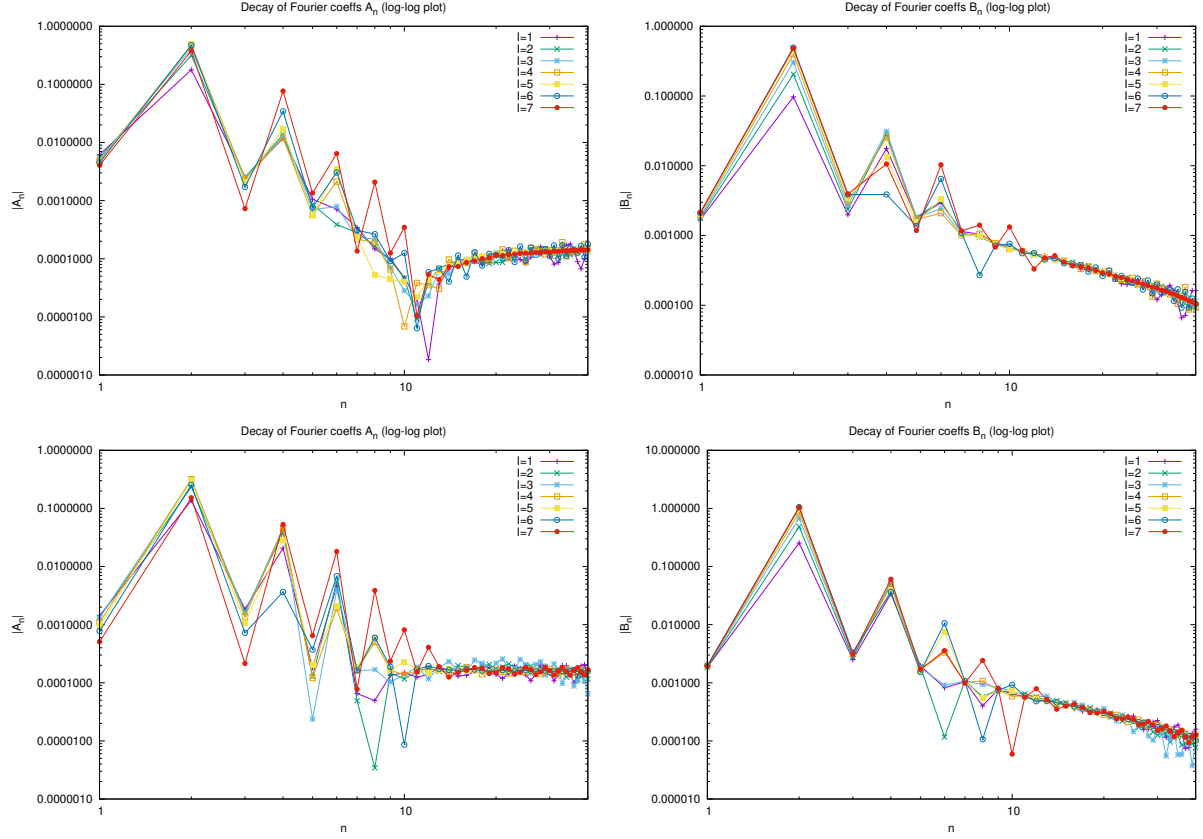


Figure 9.10: Decay of Fourier coefficients (log-log plot) for the scattering map σ_1 (above) and σ_2 (below).

Given the values $A_n(I)$ at $I = 0, 1, 2, \dots, 7$ obtained in the previous step (resp. $B_n(I)$), we use polynomial interpolation (Newton's 'divided differences' algorithm) to obtain the coefficients $\tilde{a}_l^{(n)}$ (resp. $\tilde{b}_l^{(n)}$). The divided differences of the first 8 Fourier coefficients are listed in Table 9.1.

Remark 9.13. Since we only have 8 data points for each Fourier coefficient, the maximum possible degree of the Newton expansion (9.17) is $L = 7$.

Remark 9.14. The constant terms $\tilde{a}_0^{(n)}, \tilde{b}_0^{(n)}$ of the Newton expansion are all zero, since $\tilde{a}_0^{(n)} = A_n(0) = 0$ and $\tilde{b}_0^{(n)} = B_n(0) = 0$ for all n .

9.4.2 Polynomial interpolation of the Frequency $\omega(I)$

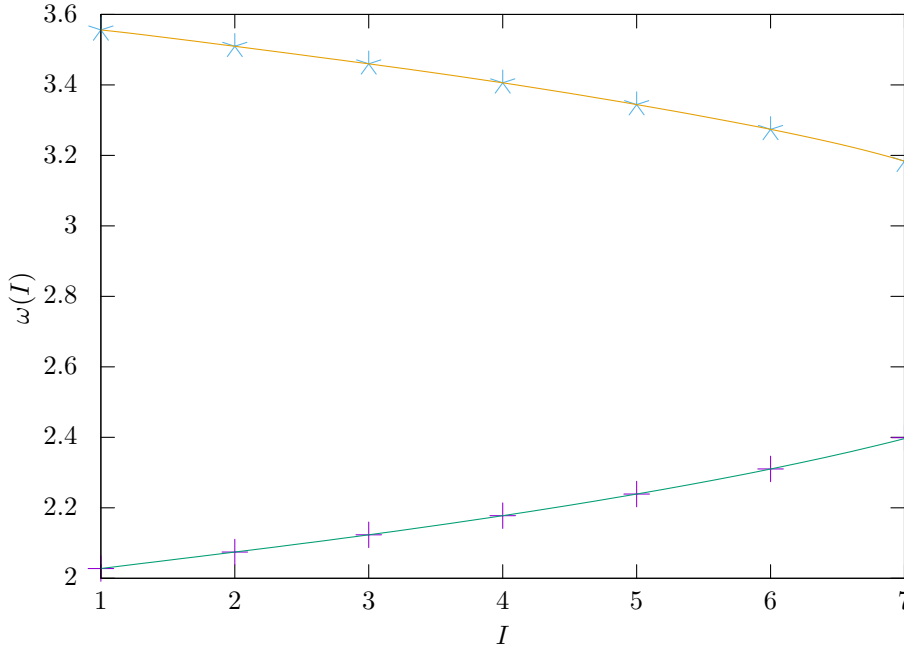
Finally, we approximate the frequency $\omega(I)$ in Equation (9.13).

Frequency $\omega(I)$ at $I = 1, 2, \dots, 7$.

For action levels $I = 1, 2, \dots, 7$ we have available the scattering map data $(I, \phi) \rightarrow (I', \phi')$, so the frequency $\omega(I)$ can be obtained from Equation (9.13a) as

$$\omega(I) = \phi - \phi' - \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi'). \quad (9.18)$$

In an exact calculation, $\omega(I)$ should be independent of ϕ . Numerically, using Equation (9.18) to approximate the value of $\omega(I)$ would yield slightly different values for $\omega(I)$ depending on the data point (I, ϕ) , and indeed depending on ϕ . Thus, we will compute $\omega(I)$ as the *average* of Equation (9.18) over all $\phi \in [0, 2\pi)$.

Figure 9.11: Frequency function $\omega(I)$ for σ_1 (in green) and σ_2 (yellow).

$\tilde{c}_0$	$\tilde{c}_1$	$\tilde{c}_2$	$\tilde{c}_3$	$\tilde{c}_4$	$\tilde{c}_5$	$\tilde{c}_6$
2.027748	0.046673	0.001164	0.000489	-0.000046	0.000016	0.000003

(a) Scattering map σ_1 .

$\tilde{c}_0$	$\tilde{c}_1$	$\tilde{c}_2$	$\tilde{c}_3$	$\tilde{c}_4$	$\tilde{c}_5$	$\tilde{c}_6$
3.555994	-0.046434	-0.001651	-0.000143	-0.000115	0.000046	-0.000026

(b) Scattering map σ_2 .

Table 9.2: Divided differences $\tilde{c}_l$ of function $\omega(I)$. Notice that the coefficient $\tilde{c}_0$ (in red) is much larger than the rest of coefficients of this table, and larger than those of Table 9.1, for both scattering maps σ_1 and σ_2 . Notice also that $\tilde{c}_1$ (in blue) is much larger than the rest of coefficients of the last five columns, i.e $\tilde{c}_j$ for $j \geq 2$, of this table, and larger than the double of those coefficients of the last 6 columns of Table 9.1 for both scattering maps σ_1 and σ_2 .

Frequency $\omega(I)$ at an arbitrary I -value.

Similarly to what we did in Section 9.4.1 with the Fourier coefficients $A_n(I)$, $B_n(I)$, we use the Newton series representation of $\omega(I)$:

$$\omega(I) = \sum_{l=0}^L \tilde{c}_l N_l(I). \quad (9.19)$$

Given the values $\bar{\omega}(I)$ at $I = 1, 2, \dots, 7$, obtained in the previous step, we use polynomial interpolation to obtain the coefficients $\tilde{c}_l$. The frequency function $\omega(I)$ is plotted in Figure 9.11.

Remark 9.15. Since we only have 7 data points for ω , the maximum possible degree of the Newton expansion (9.19) is $L = 6$.

This completes the series representation of the scattering map, consisting of Equations (9.14)-(9.15) and (9.19).

9.4.3 Applying the Scattering Map

We will use equations (9.13) to apply the scattering map $(I', \phi') = \sigma(I, \phi)$. Note that (9.13) give I', ϕ' *implicitly* as functions of I, ϕ . However, ϕ' can be obtained from Equation (9.13a) as a fixed point of

$$\phi' = f(\phi'; I, \phi) = \phi - \omega(I) - \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi').$$

We simply use fixed point iteration, starting with the initial approximation $\phi'_0 = \phi - \omega(I)$. We require an absolute error smaller than 10^{-5} in the fixed point to stop the iteration. There is no point in requiring higher precision, because the error of our series representation in the angle variable is larger than 10^{-2} ; see Table 9.4 (bottom panel).

Once ϕ' is known, I' is obtained directly from Equation (9.13b).

9.5 Approximation Error

Now we have two different representations of the scattering map:

- The **numerical scattering map** $\sigma(I, \phi)$ was obtained in Section 9.3 using Birkhoff normal forms and numerical continuation of the invariant manifolds. It was calculated on a relatively coarse grid of points (Figure 9.9).
- The **standard scattering map (SSM)** $\tilde{\sigma}(I, \phi)$ consists in the Fourier-Polynomial interpolation (9.14)-(9.15) and (9.19). The series approximation has been derived in Section 9.4 from the numerical map, so it is not as precise. However, it has the advantage that it can be evaluated at any desired point (I, ϕ) .

To measure the quality of the series approximation, we do the following:

1. Read the numerical scattering map from file as a table:

$$(I', \phi') = \sigma(I, \phi).$$

We have its values on a grid of points (I, ϕ) .

2. Evaluate the standard scattering map (SSM) *on the same grid*:

$$(\tilde{I}', \tilde{\phi}') = \tilde{\sigma}(I, \phi).$$

3. Find the approximation error, defined as the *maximum over all grid points* of

$$(\epsilon_I, \epsilon_\phi) = \left(\left| \tilde{I}' - I' \right|, \left| \tilde{\phi}' - \phi' \right| \right).$$

Remark 9.16. To better test the quality of the series approximation, we also compute the approximation error on a new set of data, independent of the original one. That is, we extend the original data set $I = 1, 2, \dots, 7$, used to derive $\tilde{\sigma}$ with the new data set $I = 0.5, 1.5, 2.5, \dots, 6.5$. See Figure 9.12. Thus, only for testing purposes, we use 14 tori. As shown in Tables 9.4, 9.5, the errors in the independent data set are comparable to those of the original data set.

Of course, the approximation error depends on the chosen degree (N, L) of the Fourier-Polynomial interpolation. For illustration, Figure 9.12 compares the quality of a low order versus a high order approximation.

We will distinguish two different settings. In the *local* setting, one is interested in an accurate representation of the scattering map in a neighborhood of $I = 0$, whereas in the *global* setting, one is interested in an accurate representation in the whole domain of the global scattering map.

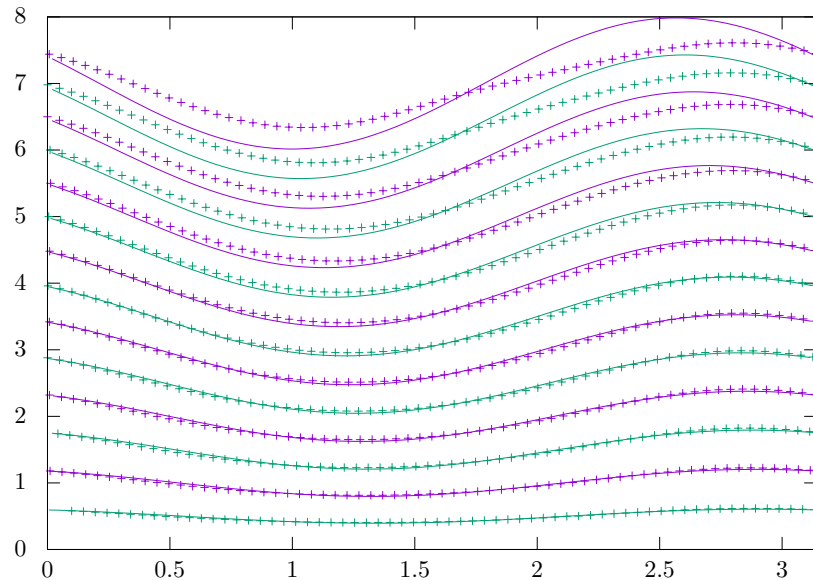
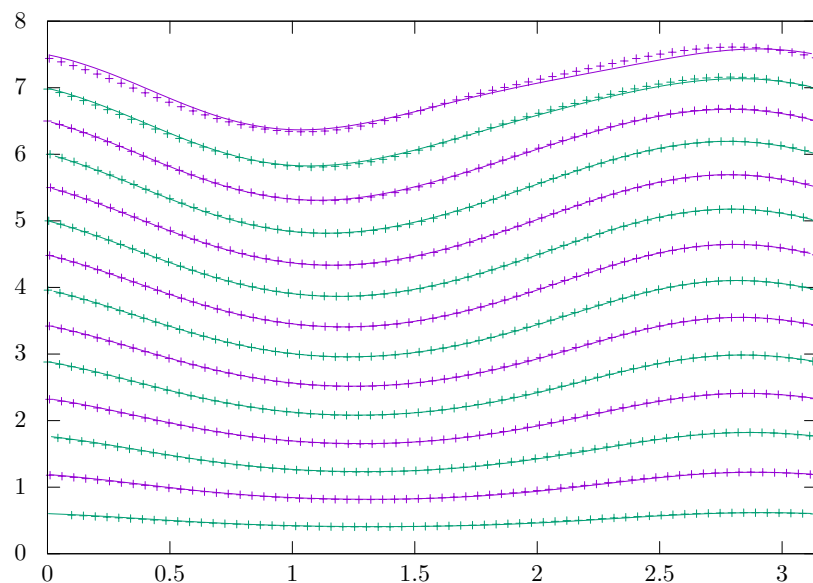
(a) $N = 2, L = 2$ (b) $N = 4, L = 5$

Figure 9.12: Image of the numerical scattering map (points) versus the standard scattering map (SSM) of degree N, L (lines). For testing purposes, we check the approximation error both on the original data set $I = 1, 2, \dots, 7$ (in purple) and on the independent data set $I = 0.5, 1.5, 2.5, \dots, 6.5$ (in green).

N	L			
	0	1	2	3
2	0.540000	0.134772	0.041698	0.037342
4	0.540000	0.145286	0.019337	0.011640
6	0.540000	0.151078	0.019536	0.013382

N	L		
	0	1	2
2	0.156427	0.052403	0.015123
4	0.156427	0.049706	0.016311
6	0.156427	0.049634	0.016270

Table 9.3: Local approximation error ϵ_I (top panel) and ϵ_ϕ (bottom panel) as a function of N, L for the first scattering map σ_1 .

9.5.1 Local Approximation Error

For definiteness, let us fix the local domain to be

$$\mathcal{A}_{\text{loc}} = \{(I, \phi) : I \in [1, 3] \text{ and } \phi \in [0, 2\pi)\}.$$

We have computed the approximation error over the local domain $\mathcal{A}_{\text{loc}}$ as a function of the degree (N, L) of the Fourier-Polynomial interpolation; see Table 9.3.

Remark 9.17. Only the grid points (I, ϕ) belonging to the local domain (i.e. tori $I = 1, 2, 3$) are used in the computation of the local approximation error.

The error of the Fourier-Polynomial interpolation model decreases as N and L increase, but not monotonically. If we want an approximation error $\epsilon = \max\{\epsilon_I, \epsilon_\phi\}$ less than 0.05, then it is enough to take $N = 2$ and $L = 2$. Notice that the improvement is mild beyond that point. Indeed, Figure 9.12a shows that $N = L = 2$ gives a good approximation in the local domain $\mathcal{A}_{\text{loc}}$.

Thus, it is natural to choose $N = L = 2$ to obtain an accurate model for the local scattering map. In fact, as discussed before (Remark 9.12), we neglect the odd Fourier coefficients $A_1(I)$ and $B_1(I)$ due to the symmetry of the problem, and just keep the even ones $A_2(I)$ and $B_2(I)$.

Therefore, in the local setting, an **accurate model** for the scattering map is given by the Fourier-Polynomial interpolation

$$\tilde{\mathcal{L}}(I, \phi') = -\frac{B_2(I)}{2} \cos 2\phi' + \frac{A_2(I)}{2} \sin 2\phi',$$

where

$$A_2(I) = \tilde{a}_0^{(2)} + \tilde{a}_1^{(2)}I + \tilde{a}_2^{(2)}I(I-1)$$

$$B_2(I) = \tilde{b}_0^{(2)} + \tilde{b}_1^{(2)}I + \tilde{b}_2^{(2)}I(I-1),$$

$$\omega(I) = \tilde{c}_0 + \tilde{c}_1(I-1) + \tilde{c}_2(I-1)(I-2),$$

are polynomials of degree 2 in I , determined by only 9 coefficients. These coefficients were given in Tables 9.1 and 9.2.

This part of the generating function can also be written as $\tilde{\mathcal{L}}(I, \phi') = C_2(I) \cos(2\phi' - 2\phi'_0)$, a cosine function of period π at angle ϕ' . The corresponding Standard Scattering Map (SSM) can thus be used as a universal local model around saddle-center libration points of the R3BP problem, and its cosine expression explains the shape of the KAM curves in Figure 9.14.

9.5.2 Global Approximation Error

Suppose now that we are now interested in an accurate representation in the whole domain of the scattering map

$$\mathcal{A} = \{(I, \phi) : I \in [1, 7] \text{ and } \phi \in [0, 2\pi)\}. \quad (9.20)$$

The approximation error over the global domain is given in Table 9.4. If we want an approximation error $\epsilon = \max\{\epsilon_I, \epsilon_\phi\}$ less than 0.1, we need to increase the degree of Fourier-Polynomial interpolation

N	L							
	0	1	2	3	4	5	6	7
2	0.680000	0.963414	0.495653	0.261042	0.385496	0.131751	0.219163	0.094550
4	0.680000	0.975219	0.618115	0.276085	0.387552	0.087317	0.156552	0.021123
6	0.680000	0.996139	0.656461	0.266668	0.381078	0.107612	0.144998	0.013382
8	0.680000	1.003501	0.657922	0.287596	0.367730	0.110813	0.148937	0.013159
10	0.680000	1.007927	0.647908	0.287781	0.356098	0.105846	0.149545	0.012512

N	L						
	0	1	2	3	4	5	6
2	0.449508	0.268271	0.157380	0.065119	0.148788	0.068206	0.121809
4	0.449508	0.270152	0.169874	0.074112	0.150692	0.085074	0.132709
6	0.449508	0.269731	0.169564	0.076822	0.153570	0.083003	0.132714
8	0.449508	0.269683	0.169068	0.079125	0.155540	0.083914	0.131502
10	0.449508	0.269748	0.169407	0.080213	0.157050	0.085329	0.131450

Table 9.4: Global approximation error ϵ_I (top panel) and ϵ_ϕ (bottom panel) as a function of N, L for the standard scattering map σ_1 . The error is evaluated in the original data set $I = 1, 2, \dots, 7$.

N	L							
	0	1	2	3	4	5	6	7
2	0.680000	0.782085	0.367800	0.198887	0.233913	0.071975	0.104571	0.077636
4	0.680000	0.822172	0.465488	0.201108	0.227997	0.035848	0.062120	0.032394
6	0.680000	0.841491	0.497539	0.205914	0.224239	0.048805	0.052237	0.022763
8	0.680000	0.848342	0.499856	0.219921	0.216637	0.050972	0.053874	0.023362
10	0.680000	0.852520	0.491977	0.219181	0.209180	0.049182	0.054193	0.023105

N	L						
	0	1	2	3	4	5	6
2	0.370667	0.210922	0.112123	0.063086	0.107801	0.040273	0.067627
4	0.370667	0.213108	0.123612	0.057792	0.107593	0.040863	0.062113
6	0.370667	0.212718	0.122866	0.059556	0.109339	0.039459	0.062510
8	0.370667	0.212655	0.122537	0.059490	0.110579	0.039398	0.061885
10	0.370667	0.212716	0.122826	0.059643	0.111556	0.039633	0.061842

Table 9.5: Global approximation error ϵ_I (top panel) and ϵ_ϕ (bottom panel) as a function of N, L for the standard scattering map σ_1 . The error is evaluated in the independent data set $I = 0.5, 1.5, 2.5, \dots, 6.5$. Compare to the original data set in Table 9.4.

to $N = 4$ and $L = 5$. In fact, Figure 9.12b shows that $N = 4$, $L = 5$ gives a good approximation in the global domain $\mathcal{A}$.

From now on, we will use $N = 4$, $L = 5$ as our model for the global scattering map σ_1 .

A similar analysis suggests that $N = 4$, $L = 6$ be used for the global scattering map σ_2 .

9.6 Inner Map

Recall that the *inner flow* refers to the restriction of the R3BP flow to the normally hyperbolic invariant manifold Λ_c , while the *inner map* refers to the restriction of the first return map $\mathcal{F}$ to Λ_c^Σ . Abusing notation, the inner map will still be called $\mathcal{F}$.

As explained in Section 9.1.1, the R3BP flow on the center manifold $W^c(L_1)$ consists simply on a translation on the 2-torus,

$$\begin{aligned} \dot{J}_p &= 0, & \dot{\phi}_p &= \frac{\partial H}{\partial J_p} =: \nu_p(J_p, J_v), \\ \dot{J}_v &= 0, & \dot{\phi}_v &= \frac{\partial H}{\partial J_v} =: \nu_v(J_p, J_v). \end{aligned}$$

The value of the planar and vertical frequencies ν_p , ν_v of the torus are obtained differentiating the Hamiltonian in Birkhoff normal form.

Upon restriction to the NHIM Λ_c , we get rid of the planar action J_p , which can be recovered if necessary using the energy condition, so the inner flow is

$$\dot{J}_v = 0, \quad \dot{\phi}_p = \nu_p(J_v), \quad \dot{\phi}_v = \nu_v(J_v). \quad (9.21)$$

Finally, the first return map of the inner flow to the section Σ is

$$J'_v = J_v, \quad \phi'_v = \phi_v + \frac{2\pi\nu_v(J_v)}{\nu_p(J_v)}.$$

In terms of the scaled coordinates I, ϕ , the inner map $\mathcal{F}: \Lambda_c^{N,\Sigma} \rightarrow \Lambda_c^{N,\Sigma}$ is given by

$$I' = I, \quad \phi' = \phi + \nu(I), \quad (9.22)$$

where we have introduced the new function

$$\nu(I) := \frac{2\pi\nu_v(I/1000)}{\nu_p(I/1000)}.$$

As seen in Figure 9.13, the inner shift $\nu(I)$ decreases almost linearly with I . In particular, this shows that the inner map $\mathcal{F}$ is a twist map.

9.7 Phase Space of the Scattering Map

In Sections 9.4 and 9.5, we have obtained a series representation of the scattering maps $\sigma(I, \phi)$ with small approximation error. This representation is valid on an annulus $\mathcal{A}$ inside the NHIM (see Equation (9.20)). Thus we can now iterate the scattering map in $\mathcal{A}$.

To explore the global phase space of the scattering map, we perform the following experiment: Take 300×300 initial conditions evenly distributed in $\mathcal{A}$, and iterate each initial condition 100 times by the scattering map. The resulting phase space portrait is shown in Figure 9.14.

Notice that the scattering map (9.13), rewritten as

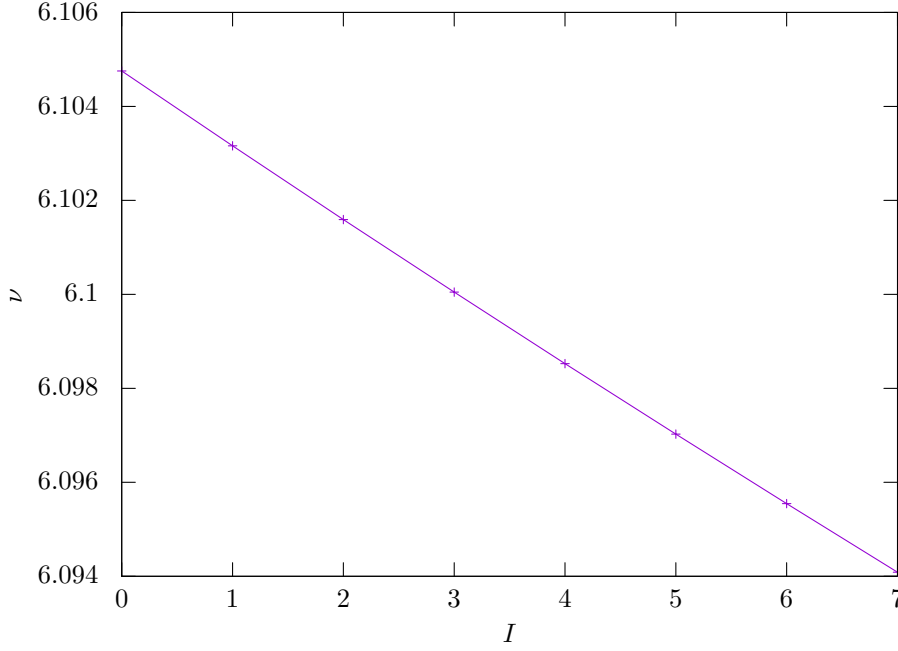
$$\phi' = \phi - \omega(I) - \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi') \quad (9.23a)$$

$$I' = I + \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi') \quad (9.23b)$$

can be seen as a perturbation of the integrable map $(I, \phi) \mapsto (I' = I, \phi' = \phi - \omega(I))$, as long as the derivatives of $\tilde{\mathcal{L}}$ are small enough. The frequency $-\omega(I)$ represents the *phase shift* of the map $(I, \phi) \mapsto (I' = I, \phi' = \phi - \omega(I))$.

Since $\omega'(I) \neq 0$ (see Figure 9.11), the integrable map $(I, \phi) \mapsto (I, \phi - \omega(I))$ is a twist map. Below we check that the scattering map is also a twist map. (See ‘Twist Condition’).

By KAM theory (for an area preserving map given by its generating function; see, for instance, [AA68, Har02]), when the derivatives of $\tilde{\mathcal{L}}$ are small, we expect that many of the invariant tori of the integrable twist map persist.

Figure 9.13: The inner shift $\nu(I)$.

Phase Shift

The phase shift of the scattering map (9.23) is $\phi' - \phi = -\omega(I) - \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi')$. The divided differences of $\omega(I)$ are listed in Table 9.2. From these data we see that $|\tilde{c}_0| \gg |\tilde{c}_1| \gg |\tilde{c}_j|$ for $j = 2, \dots, 6$. Comparing with Table 9.1, we notice that $|\tilde{c}_0| \gg |\tilde{a}_j^n|, |\tilde{b}_j^n|$, $j = 1, \dots, 7$, $n = 2, 4, 6, 8$. This implies that $\frac{\partial \tilde{\mathcal{L}}}{\partial I}$ is much smaller than $\omega(I)$, which is non-zero, at least for I small enough. This argument could be used to assert that the phase shift is non-zero in the local domain $\mathcal{A}_{\text{loc}}$.

To deal with the global domain $\mathcal{A}$, we determine the range of I values where the phase shift is non-zero. The phase shift is bounded by

$$-\omega(I) - \max_{\phi'} \left| \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi') \right| \leq -\omega(I) - \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi') \leq -\omega(I) + \max_{\phi'} \left| \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi') \right|.$$

We have computed these bounds explicitly, using the series expansions of $\omega(I)$ and $\frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi')$. The result is shown in Figure 9.15. Note that the phase shift for σ_1 is non-zero for all $I \in [1, 7]$, while the phase shift for σ_2 (modulo π) is non-zero except possibly for a small range of I values close to $I = 7$.

Twist Condition

Let us compute the twist of the scattering map (9.23):

$$\frac{\partial \phi'}{\partial I}(I, \phi') = -\omega'(I) - \frac{\partial^2 \tilde{\mathcal{L}}}{\partial I^2}(I, \phi') - \frac{\partial^2 \tilde{\mathcal{L}}}{\partial \phi' \partial I}(I, \phi') \frac{\partial \phi'}{\partial I}.$$

Thus

$$\frac{\partial \phi'}{\partial I}(I, \phi') = -\frac{\omega'(I) + \frac{\partial^2 \tilde{\mathcal{L}}}{\partial I^2}}{1 + \frac{\partial^2 \tilde{\mathcal{L}}}{\partial \phi' \partial I}}, \quad (9.24)$$

provided that the denominator is non-zero.

We have computed the twist (9.24) explicitly on the global domain $\mathcal{A}$, using the series expansions of $\omega(I)$ and $\tilde{\mathcal{L}}(I, \phi')$. The result is shown in Figure 9.16. Note that the twist for both σ_1 and σ_2 is non-zero in $\mathcal{A}$.

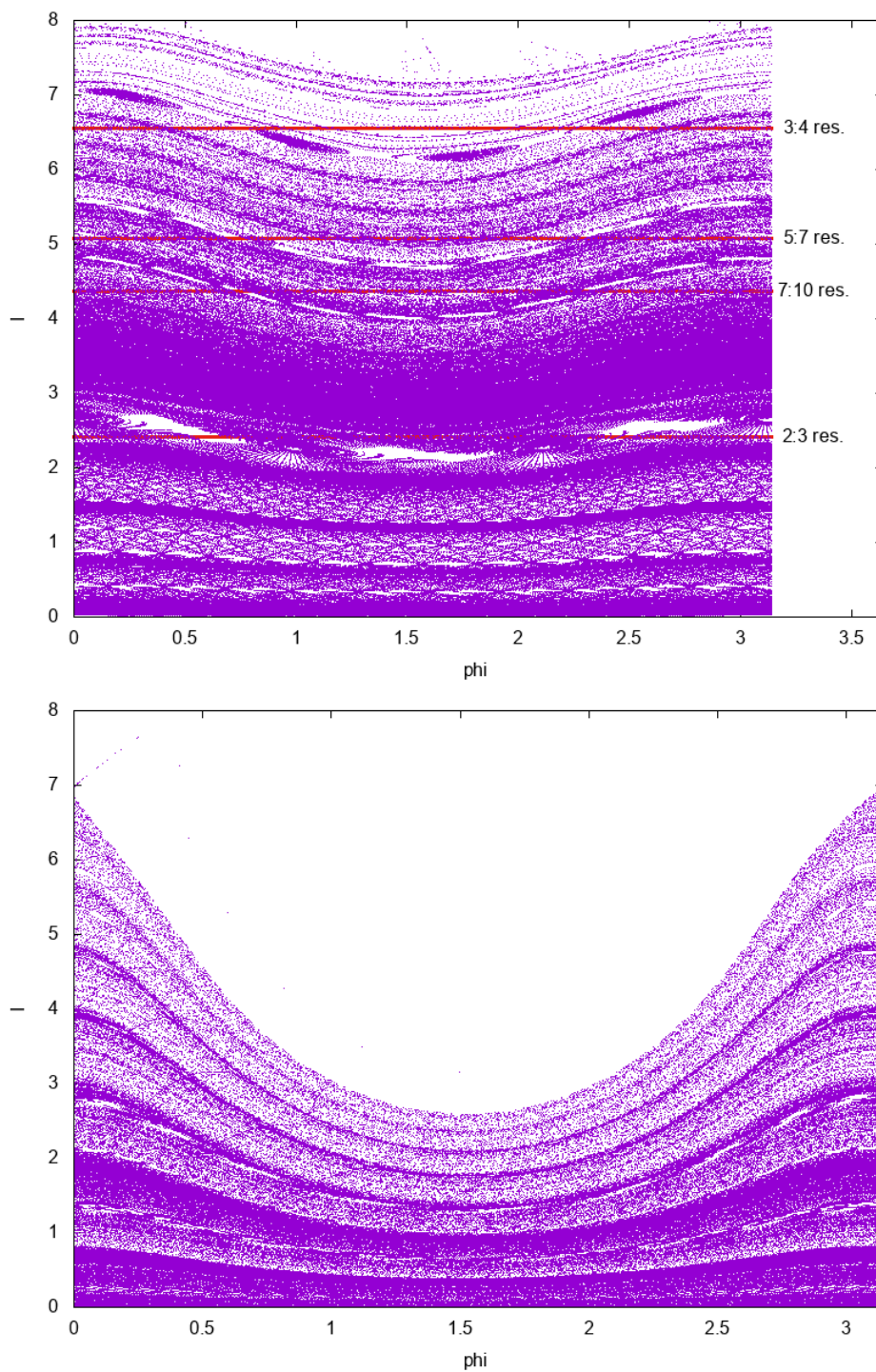


Figure 9.14: Phase portrait of the scattering maps σ_1 (above) and σ_2 (below). The theoretical location of the main resonances, found in Section 9.8, is superimposed in red.

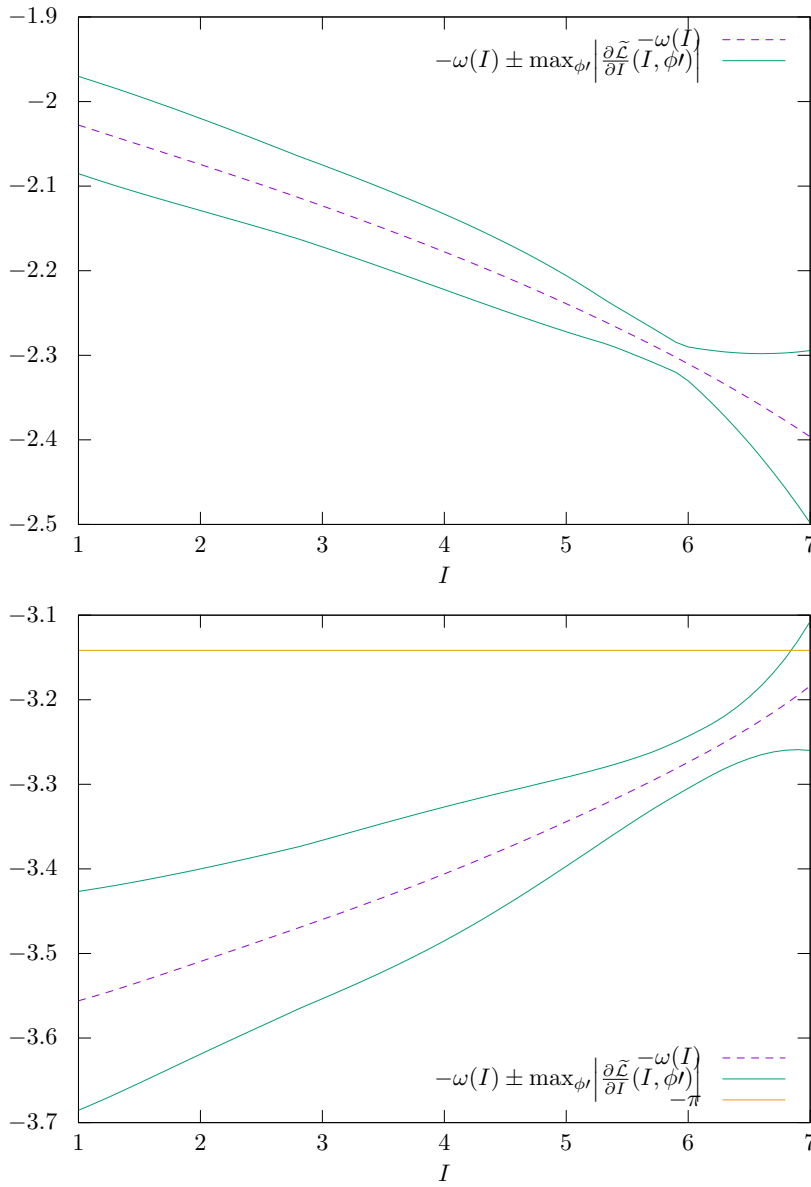
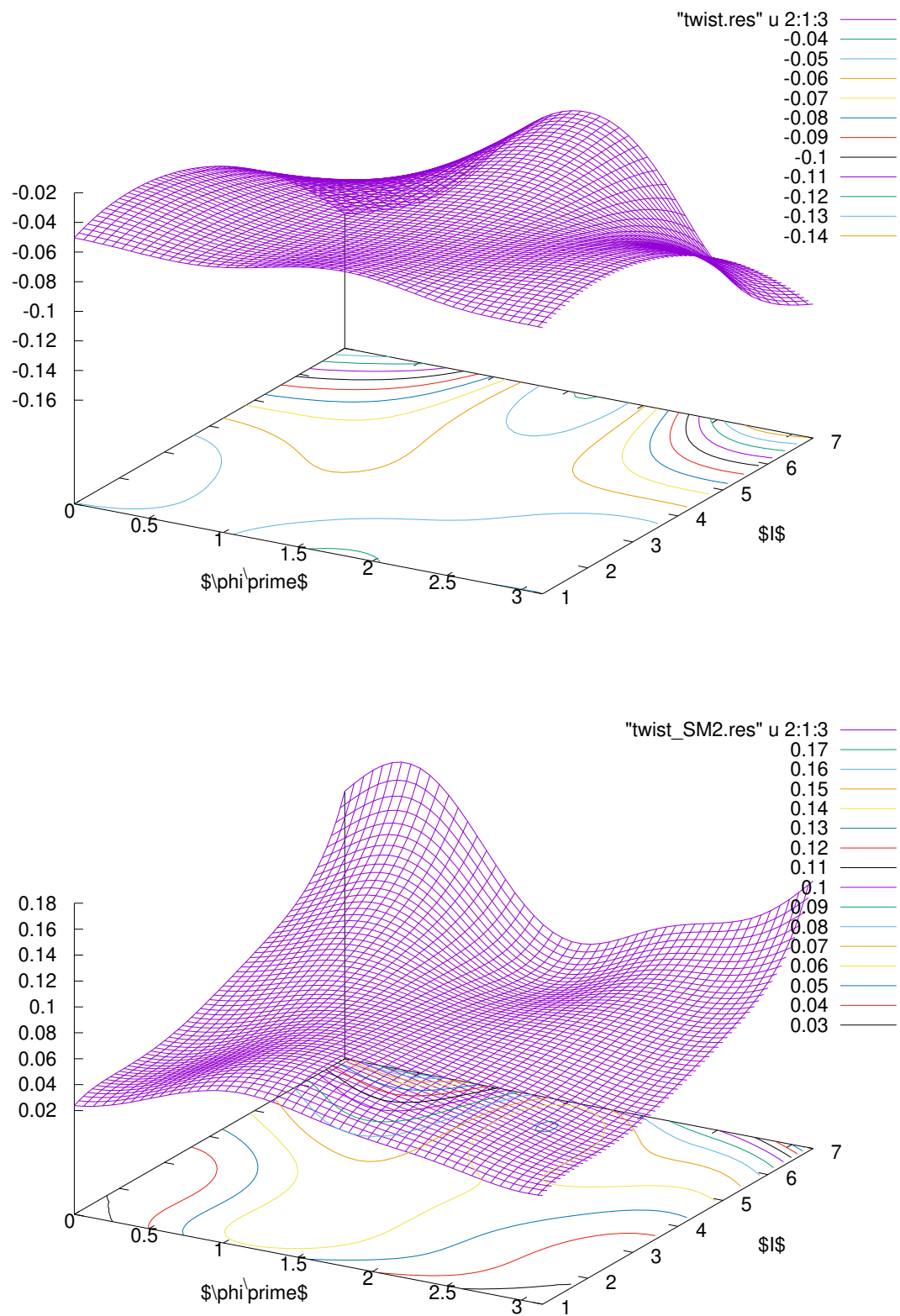


Figure 9.15: Enclosure of the phase shift for the scattering map σ_1 (above) and σ_2 (below). The phase shift $-\omega(I) - \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi')$ is enclosed inside the green lines.

Figure 9.16: Twist for the scattering map σ_1 (above) and σ_2 (below).

9.8 KAM tori and resonant zones for the Scattering Maps

As seen in Figure 9.14, the phase portrait of the scattering maps σ_1, σ_2 is filled up with invariant curves and some resonant zones between them. Recall from Section 9.7 that both σ_1 and σ_2 are twist maps. To compute these invariant curves, we now introduce the exponential form in the sine-cosine Fourier expansion (9.16) of $\frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}$

$$\frac{\partial \tilde{\mathcal{L}}}{\partial \phi'} = \sum_{n=1}^N A_n \cos n\phi' + \sum_{n=1}^N B_n \sin n\phi' = \sum_{n=-N, n \neq 0}^N C_n e^{in\phi'},$$

where $C = (C_{-N}, \dots, C_{-1}, C_1, \dots, C_N) \in \mathbb{C}^{2N}$ satisfies

$$C_n = \frac{1}{2}(A_n - iB_n), \quad C_{-n} = \frac{1}{2}(A_n + iB_n) = \overline{C_n}, \quad \text{for } n > 0.$$

Notice that for $\tilde{\mathcal{L}} = 0$, or equivalently $C = 0$, any torus $I = I_0$ is invariant since then $I' = I_0$ in the expression (9.23b) of a scattering map, with an inner dynamics $\phi' = \phi - \omega_0$ given by (9.23a), where $\omega_0 := \omega(I_0)$.

For $|\tilde{\mathcal{L}}|$ small enough, or equivalently $|C|$ small enough, a lot of these invariant curves survive. An invariant curve $I = I_0 + h(\phi)$ of a scattering map (9.23) satisfies $I' = I_0 + h(\phi')$, that is

$$h(\phi') = h\left(\phi' + \omega(I) + \frac{\partial \tilde{\mathcal{L}}}{\partial I}(I, \phi')\right) + \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi'), \quad \text{where } I = I_0 + h(\phi).$$

Expanding in C and h we get

$$h(\phi') = h(\phi' + \omega_0) + \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi') + O(hC).$$

Writing $h(\phi') = \sum_{n=-N, n \neq 0}^N h_n e^{in\phi'}$ we get

$$\sum h_n e^{in\phi'} = \sum e^{in\omega_0} h_n e^{in\phi'} + \sum C_n e^{in\phi'} + O(hC),$$

which, equating Fourier coefficients, gives

$$h_n = -\frac{C_n}{e^{in\omega_0} - 1} + O(C^2) \quad \text{for } 0 < |n| \leq N.$$

For this approximate formula one needs that $\frac{n\omega_0}{2\pi} \notin \mathbb{Z}$ for $|n| \leq N$ (non-resonant condition), and one sees that, up to order $O(C^2)$, the coefficients $h_n = O(C)$ are uniquely determined by C . KAM theorem consists in proving the convergence of these expansions for *diophantine frequencies* ω_0 , using that σ_1 and σ_2 are twist maps.

Resonant Zones for σ_1

Resonant zones for the symplectic map (9.13), or, equivalently, (9.23), where the KAM theorem does not provide invariant curves for small $\mathcal{L}$, appear around the values I such that $\frac{\omega(I)}{\pi}$ is a rational number. In the global setting,

$$\omega(I) = \Omega'(I) \approx \sum_{l=0}^L c_l N_l(I),$$

where the coefficients c_l are given in table 9.2 for both scattering maps σ_1 and σ_2 .

In particular for σ_1 (a totally analogous study for σ_2 can be carried out) $\frac{\omega(0)}{\pi} = 0.630128\dots$, which is not too far for $2/3$ whose continued fraction is $[1, 2]$, which means that

$$\frac{2}{3} = [1, 2] = \frac{1}{1 + \frac{1}{2}}.$$

Therefore for I such that $\frac{\omega(I)}{\pi} = \frac{2}{3}$, which happens to be $I \approx 2.4175$, there should appear a resonance, indeed the largest one, since the width of the ‘eyes’ of a resonance is related to the denominator, in this case 3.

Other close rationals to $2/3$ are given by close modified continued fractions. For instance

$$[1, 2, 1] = \frac{1}{1 + \frac{1}{2 + \frac{1}{1}}} = \frac{3}{4}.$$

We can compute some of the largest ones, ordered by their denominators:

I	$\frac{\omega(I)}{\pi}$	continued fraction
2.4175	$\frac{2}{3}$	$[1, 2]$
6.5550	$\frac{3}{4}$	$[1, 2, 1]$
5.0752	$\frac{5}{7}$	$[1, 2, 2]$
4.3631	$\frac{7}{10}$	$[1, 2, 3]$
3.9523	$\frac{9}{13}$	$[1, 2, 4]$

The continued fraction of $\frac{2}{3}$ can be also written as $[1, 1, 1]$, and smaller resonant values can be obtained for smaller continued fractions like $[1, 1, 1, 3] = \frac{7}{11} = 0.636363\dots$, etc

For the scattering map σ_1 , the two main resonances are clearly visible near $I \approx 2.4175$ and $I \approx 6.5550$. See Figure 9.14 (top panel).

9.9 Arnold diffusion

In this section we give details on the verification of the Numerical Result 9.1. Specifically, we verify numerically that the conditions of Theorem 9.1 are satisfied.

Let

$$\mathcal{A} = \{(I, \phi) \mid I \in [1, 7], \phi \in [0, 2\pi)\}$$

be the annulus where we want to show diffusion. The inner map f is $\mathcal{F}$ restricted to $\mathcal{A}$, and the system of scattering maps is either one of $\{\sigma_1\}$, $\{\sigma_2\}$, or $\{\sigma_1, \sigma_2\}$. Recall that f is a twist map. In Section 9.7 we verified numerically that σ_1 and σ_2 are twist maps as well.

As seen in Table 9.1, the harmonics of $\tilde{\mathcal{L}}_i$ for both scattering maps σ_1 and σ_2 , particularly those of degree two, are not zero, so that the inner map and any of these scattering maps can not have common invariant curves, and by Theorem 9.1 both the double dynamical systems $\{\mathcal{F}, \sigma_1\}$ and $\{\mathcal{F}, \sigma_2\}$ formed by the inner map and one of the scattering maps have diffusing pseudo-orbits along $\mathcal{A}$.

Even more, for the two scattering maps described in Table 9.1, one sees that the difference between the respective coefficients C_n is greater than 0.04 for the coefficients $C_{\pm 1}$ due to $\tilde{a}_1$. This, together with the fact that the magnitude of the denominator $e^{\pm i\omega_0} - 1$ in the formula of $h_{\pm 1}$ is much smaller than 1, prevents the two scattering maps from having common invariant curves, which, on the other hand, is clearly observed in the juxtaposition of the curves found numerically for the two scattering maps. This implies that the double dynamical system $\{\sigma_1, \sigma_2\}$ also has diffusing orbits along the NHIM.

We can take advantage of these dynamics to construct fast diffusing pseudo-orbits obtained from the triple dynamical system $\{\mathcal{F}, \sigma_1, \sigma_2\}$ formed by the inner map and the two scattering maps. We will give explicit constructions of diffusing pseudo-orbits, including fast ones, in Section 9.11.

Once such pseudo-orbits are obtained, the Shadowing Lemma [GLMS20, Theorem 3.7] gives true orbits that shadow the pseudo-orbits, thus achieving Arnold diffusion.

Note that the above construction of diffusing pseudo-orbits assumes that the inner dynamics is derived from the Birkhoff normal form approximation, which is given by an integrable Hamiltonian. However, the original Hamiltonian is not integrable, and the NHIM Λ_c^Σ for the original Hamiltonian is not foliated by circles invariant under the true inner map. We will now argue the existence of diffusing orbits for the original system.

Recall that the inner map for the Birkhoff normal form is an integrable twist map, and the global error in the numerical integration of orbits with initial condition (J, ϕ_p, ϕ_v) is less than $10^{-12}/5000$; see Section

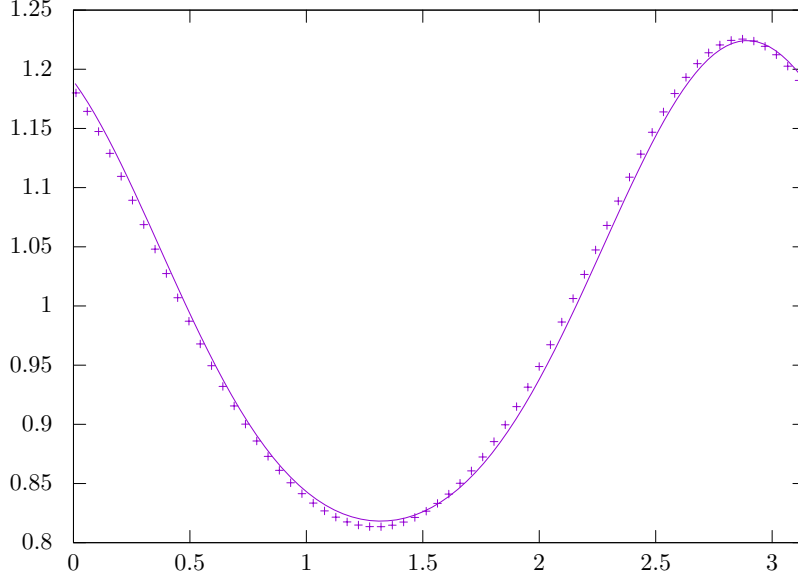


Figure 9.17: Image of the action level $I = 1$ by the numerical scattering map (points) versus the scattering map series $N = 4, M = 5$ (lines).

9.3. (We recall $J = J_v$ is the vertical amplitude of the motion.) Since each level set of J is preserved by the inner dynamics $\mathcal{F}$ for the Birkhoff normal form, and since $I = 1000J$, it follows that each essential invariant circle Γ for the inner map $\mathcal{F}$ for the original Hamiltonian is less than $\rho_1 = 10^{-12} < 10^{-9}/1500$ away from a level set of I .

We also know from Section 9.3.4 that the scattering maps σ_1, σ_2 are globally defined on $\mathcal{A}$. Moreover, for each I in the interval $[1, 7]$, the oscillation,

$$\sup_{\phi} \frac{\partial \tilde{\mathcal{L}}_1}{\partial \phi'}(I, \phi') - \inf_{\phi} \frac{\partial \tilde{\mathcal{L}}_1}{\partial \phi'}(I, \phi')$$

corresponding to σ_1 , is bigger than $\rho_2 = 0.2$.

To see this, note that the smallest oscillations in Figure 9.12b happen for the action level $I = 1$. Zooming in that action level (Figure 9.17), it is clear that the oscillation is bigger than $\rho_2 = 0.2$. Alternatively, approximate the image of $I = 1$ by the truncated Fourier-Polynomial interpolation consisting of the dominant coefficients

$$I' = I + \tilde{a}_1^{(2)} \cos 2\phi' + \tilde{b}_1^{(2)} \sin 2\phi',$$

where $\tilde{a}_1^{(2)} = 0.178180$ and $\tilde{b}_1^{(2)} = -0.097275$ (See Table 9.1). This function has oscillations of size twice its amplitude $\sqrt{(\tilde{a}_1^{(2)})^2 + (\tilde{b}_1^{(2)})^2} = 0.203003$.

Similarly, the oscillation of $\frac{\partial \tilde{\mathcal{L}}_2}{\partial \phi'}$ corresponding to σ_2 is bigger than 0.3.

These facts imply that no essential invariant circle Γ for $\mathcal{F}$ is invariant under σ_1 or σ_2 . Therefore, Theorem 9.1 applies and there are orbits of the IFS $\{\mathcal{F}, \sigma_1\}$, as well as orbits of the IFS $\{\mathcal{F}, \sigma_2\}$, that go from the lower boundary of the annulus $\mathcal{A}$ to its upper boundary.

Again, the Shadowing Lemma [GLMS20, Theorem 3.7] gives true orbits that shadow the obtained pseudo-orbits, thus achieving Arnold diffusion.

9.10 Time Estimates for Inner and Transition Map

One of our main goals is to estimate the drift time spent by drift orbits, constructed in Section 9.11. As an intermediate step, we measure the time spent on one iterate of the inner map ('inner time', or t_{in}), and the time spent on one iterate of the transition map ('outer time', or t_{out}).

In terms of the R3BP inner flow (9.21), one application of the inner map corresponds to integrating an initial condition $(J_v, \phi_p = 0, \phi_v) \in \Lambda_c^\Sigma$ during the amount of time that it takes to return to the section

Σ . Thus, each iterate of the inner map takes time

$$t_{\text{in}} = \frac{2\pi}{\nu_p}.$$

Numerically, we find that $2.0764 < \nu_p(I) < 2.0781$, and therefore the inner time is bounded by

$$3.0235 < t_{\text{in}} < 3.0261.$$

In terms of the R3BP flow, one application of the transition map corresponds to a (segment of) a homoclinic trajectory from $y_- \in W_{\text{loc}}^u(\Lambda_c)$ to $y_+ \in W_{\text{loc}}^s(\Lambda_c)$. As noted in Subsection 9.3.2, the flight time of homoclinic segments is bounded by

$$5.936738 \leq t_{\text{out}} \leq 6.000688.$$

Therefore in our setting we find that outer times t_{out} are approximately twice as long as inner times t_{in} .

9.11 Drift Orbits

In Section 9.9 we provided numerical evidence that the conditions of Theorem 9.1 are fulfilled, hence there exist trajectories that exhibit Arnold diffusion, characterized by a drift in the scaled vertical amplitude I (see (9.12)). Our arguments do not provide a way to find such orbits, much less those orbits that drift ‘fast’.

In this section, we propose different algorithms to produce drift orbits, i.e., orbits of the iterated function system (IFS) consisting of the inner and outer map, whose action variable I increases from $I = 1$ to $I > 7$. We produce two different type of orbits:

- Orbits of the iterated function system $\{\mathcal{F}, \sigma_1\}$, $\{\mathcal{F}, \sigma_2\}$, or $\{\mathcal{F}, \sigma_1, \sigma_2\}$. These orbits are a realization of the existence Theorem 9.1. We look for short orbits, i.e. we try to minimize the number of iterates. However, it is important to realize that **these orbits do not directly translate to pseudo-orbits for the R3BP flow** (since one iterate of the scattering map does not correspond to a segment of homoclinic trajectory).
- Orbits of the iterated function system $\{\mathcal{F}, \tau_1\}$, $\{\mathcal{F}, \tau_2\}$, or $\{\mathcal{F}, \tau_1, \tau_2\}$. These are also a realization of the existence Theorem 9.1, and they **directly translate to pseudo-orbits of the R3BP flow**. Each iterate of the transition map corresponds to a segment of homoclinic trajectory. Using the time estimates of Section 9.10, we can estimate the total drift time of the pseudo-orbit as:

$$t = n_0 t_{\text{in}} + n_1 t_{\text{out}} + n_2 t_{\text{out}},$$

where n_0 , n_1 and n_2 denote the number of iterates of $\mathcal{F}$, τ_1 and τ_2 respectively. Keeping an eye on Astrodynamics applications, we want to minimize the total drift time.

9.11.1 Double Dynamical System $\{\mathcal{F}, \sigma_i\}$. Greedy Algorithm.

In Section 9.8 we already established that σ_i ($i = 1, 2$) has many invariant curves. All iterates of σ_i either belong to an invariant curve, or are confined between two invariant curves. Thus it is not possible to cross from $I = 1$ to $I > 7$ using just one scattering map σ_i .

However, according to Theorem 9.1, one can combine the inner and outer map to produce drift orbits. Now we will explicitly construct such drift orbits for the double dynamical system $\{\mathcal{F}, \sigma_i\}$.

Let us partition the domain $\mathcal{A}$ of the scattering map into three sets:

$$\mathcal{A} = \mathcal{A}_- \cup \mathcal{A}_0 \cup \mathcal{A}_+.$$

$\mathcal{A}_+$ denotes the subdomain where σ gains action, $\mathcal{A}_-$ where it loses action, and $\mathcal{A}_0$ where it neither gains nor loses action:

$$\begin{aligned} \mathcal{A}_+ &= \{(I, \phi') \mid I' - I > 0\} = \left\{ (I, \phi') \mid \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi') > 0 \right\} \\ \mathcal{A}_- &= \{(I, \phi') \mid I' - I < 0\} = \left\{ (I, \phi') \mid \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi') < 0 \right\} \\ \mathcal{A}_0 &= \{(I, \phi') \mid I' - I = 0\} = \left\{ (I, \phi') \mid \frac{\partial \tilde{\mathcal{L}}}{\partial \phi'}(I, \phi') = 0 \right\}. \end{aligned}$$

These sets are readily identified in Figure 9.18. For the first scattering map, $\mathcal{A}_0$ roughly consists of two vertical lines at $\phi' \approx 0.5$ and $\phi' \approx 2$, and $\mathcal{A}_+$ roughly consists of the vertical strip $(I, \phi') \in [1, 7] \times (2, 0.5)$. For the second scattering map, $\mathcal{A}_0$ roughly consists of two vertical lines at $\phi' \approx 1.25$ and $\phi' \approx 3$, and $\mathcal{A}_+$ roughly consists of the vertical strip $(I, \phi') \in [1, 7] \times (3, 1.25)$.

A simple strategy to produce drift orbits is to *always apply the scattering map if it increases the action* (even if the action gain $I' - I$ is small). Otherwise, apply the inner map.

This ‘greedy’ algorithm is guaranteed to produce a drift orbit independently of the initial condition, due to the following simple observations: In our model’s domain $\mathcal{A}$ of validity,

- The inner map $(I', \phi') = \mathcal{F}(I, \phi)$, given in Equation (9.22), is a twist map with frequency $\nu(I) \approx 6.1$ on the universal cover (see Figure 9.13), or $\nu(I) \approx -0.2$ on the base space (where angles are identified modulo π). Thus the angle ϕ decreases approximately by 0.2 radians at every iterate of the inner map.
- Hence, for any given point $(I, \phi) \in \mathcal{A}$, its forward orbit by the inner map eventually enters $\mathcal{A}_+$.
- If (I, ϕ) already belongs to $\mathcal{A}_+$, we apply the scattering map, increasing the action. Else, we apply the inner map until the orbit enters $\mathcal{A}_+$, and then apply the scattering map.

For example, Figure 9.19 shows the drift orbit produced starting from the initial condition $(I = 1, \phi = 0)$. Notice that the drift orbit produced by $\{\mathcal{F}, \sigma_1\}$ is much longer than the one produced by $\{\mathcal{F}, \sigma_2\}$. However, as explained before, these orbits do not directly translate to pseudo-orbits of the R3BP flow, and we don’t have control over their drift time.

9.11.2 Triple Dynamical System $\{\mathcal{F}, \tau_1, \tau_2\}$. Shortest-Time Algorithm.

The algorithms described in previous sections are relatively simple to implement, but they yield sub-optimal pseudo-orbits in terms of their drift time. Now we focus on finding the optimal drift time. This is specially challenging when combining three dynamical systems (inner map, transition map 1, and transition map 2) to construct the pseudo-orbit. Obviously we can’t consider all the possible combinations of $\{\mathcal{F}, \tau_1, \tau_2\}$, since this number grows exponentially with respect to the length of the orbit. The main idea is to leverage the classic Dijkstra algorithm [Dij59] for finding shortest paths in a graph.

First we partition the domain $\mathcal{A}$ into a uniform grid of $m \times n$ two-cells (rectangles) of equal size by dividing $I \in [1, 7]$ into m intervals and $\phi \in [0, \pi)$ into n intervals. (In practice, we will use $m = n = 30$, so the grid consists of 900 small cells).

We introduce a *directed* graph $G = \langle V, E \rangle$ whose vertices V represent the different cells. An edge $e \in E$ from $u \in V$ to $v \in V$ means that the center point (I, ϕ) of cell u is mapped into cell v either by $\mathcal{F}$, τ_1 , or τ_2 . In each case, the edge records the ‘distance’ between cells, defined as the integration time corresponding to applying $\mathcal{F}$, τ_1 , resp. τ_2 .

More precisely, an edge from u to v is a pair $e = (\text{map}, \text{distance})$, where

- $e = (\mathcal{F}, t_{\text{in}})$ if (I, ϕ) is mapped into v by the inner map;
- $e = (\tau_1, t_{\text{out}})$ if (I, ϕ) is mapped into v by the first transition map;
- $e = (\tau_2, t_{\text{out}})$ if (I, ϕ) is mapped into v by the second transition map;
- $e = (\emptyset, \infty)$ if (I, ϕ) is not mapped into v by neither map.

On rare occasions, τ_1 and/or τ_2 can map the center point (I, ϕ) to the same cell as the inner map. If this happens, the inner map is preferred since it takes shorter time, so we set the edge to $(\mathcal{F}, t_{\text{in}})$.

Remark 9.18. The image (I', ϕ') of (I, ϕ) by the transition map may be outside $\mathcal{A}$. However, this can only happen when $I' > 7$ (by construction, $I' < 0$ can never happen). In this case, we associate u with the closest cell v to the point (I', ϕ') , namely the cell containing $(7, \phi')$.

Given a source cell s and a destination cell t , Dijkstra’s algorithm applied to G provides the **shortest (directed) path in the graph** from s to t in terms of the distance defined above.

Notice that this path does not exactly correspond to an orbit of the IFS, since we have only considered iterates of center points to construct G (and the orbit does not necessarily pass through center points, but rather through arbitrary cell points). However, this path clearly *informs* the choice of map $\{\mathcal{F}, \tau_1, \tau_2\}$ that we should apply when the orbit passes through a given cell.

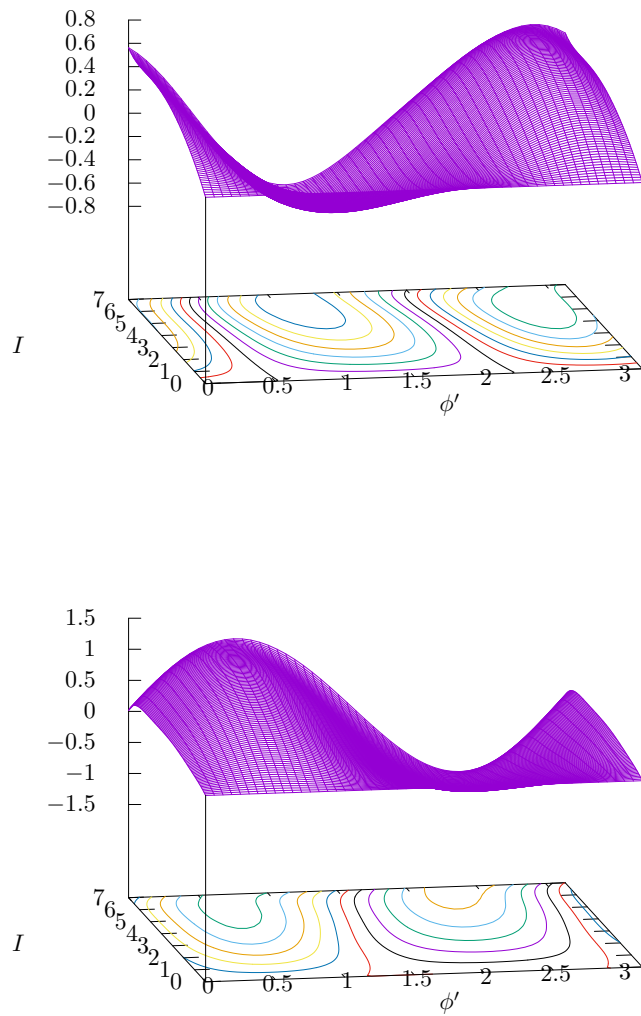


Figure 9.18: The function $\frac{\partial \tilde{L}}{\partial \phi'}(I, \phi')$ for σ_1 (above) and σ_2 (below). Note that the function $\phi' \rightarrow \frac{\partial \tilde{L}}{\partial \phi'}(I_0, \phi')$ attains its maximum at $\phi' \approx 2.8$ (above) and $\phi' \approx 0.6$ (below).

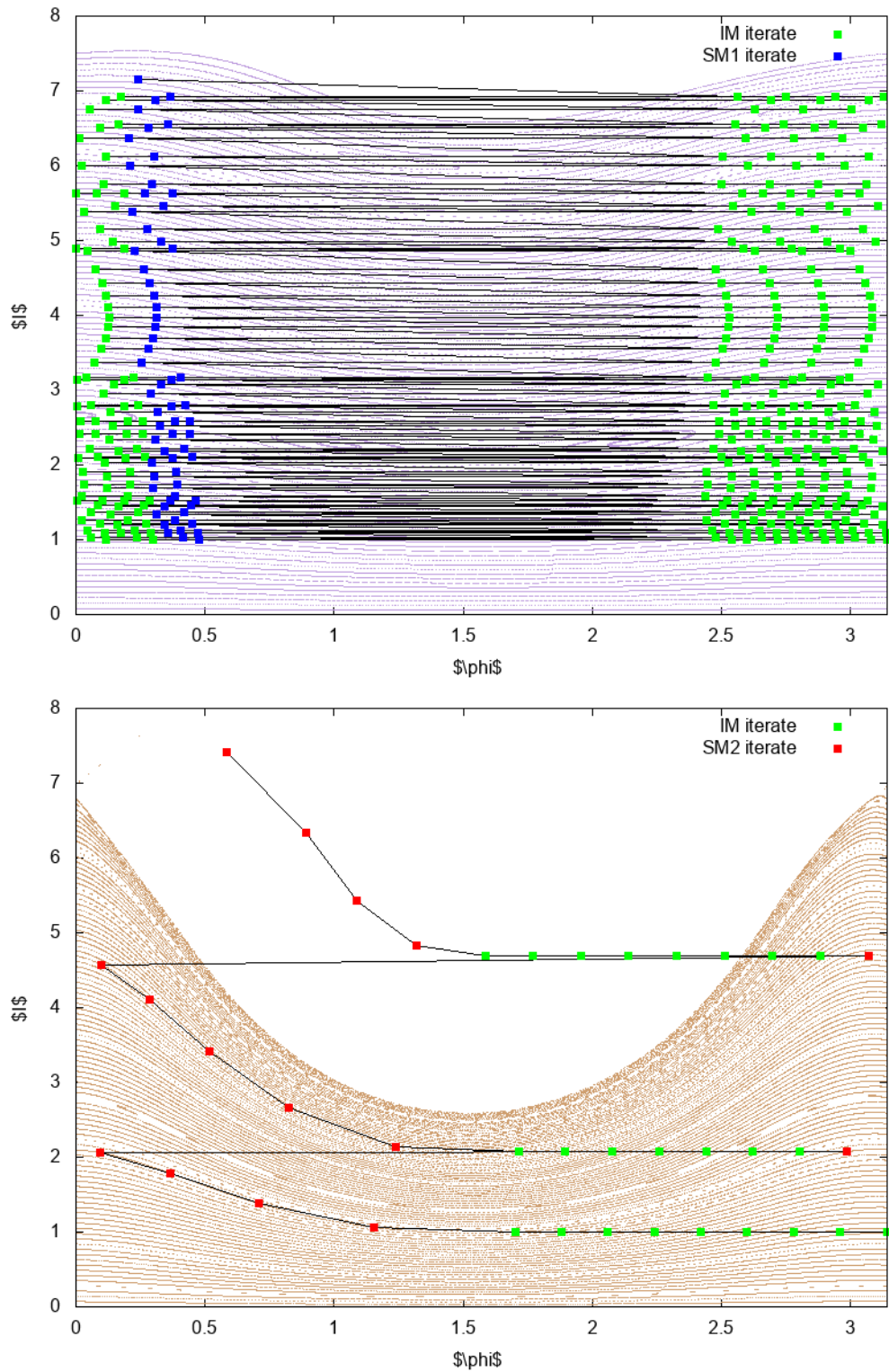


Figure 9.19: Drift orbit of $\{\mathcal{F}, \sigma_1\}$ (top panel) and $\{\mathcal{F}, \sigma_2\}$ (bottom panel) using the greedy algorithm. Green points correspond to iterates of the inner map; blue (resp. red) points correspond to iterates of the first (resp. second) scattering map. Iterates have been joined by line segments to make the orbit more visible. For reference, the orbit is shown against a background consisting of the phase space of the scattering map.

For example, suppose that the current iterate is inside cell u , and the shortest path from u to t starts with, say,

$$u \xrightarrow{(\tau_1, t_{\text{out}})} v \longrightarrow \dots \longrightarrow t.$$

Then, the best choice given the available information is to apply the first transition map to the current iterate.

Our algorithm to construct optimal orbits (shortest drift time) is given next.

Algorithm 1 Shortest-Time Algorithm

```

1: procedure ORBITSHORTESTTIME( $x, y$ )  $\triangleright$  Shortest-time orbit from point  $x \in \mathcal{A}$  to (a neighborhood
   of) point  $y \in \mathcal{A}$ 
2:    $t \leftarrow \text{cell}(y)$   $\triangleright$  Destination cell
3:    $\text{orbit} \leftarrow x$   $\triangleright$  Initialize orbit with  $x$ 
4:   while  $x \notin \text{neighborhood}(y)$  do  $\triangleright$  End when close enough to  $y$ 
5:      $u \leftarrow \text{cell}(x)$   $\triangleright$  Update current cell
6:      $\text{path} \leftarrow \text{Dijkstra}(u, t)$   $\triangleright$  Shortest path from  $u$  to  $t$ 
7:     if  $\text{path}$  starts with  $\mathcal{F}$  then
8:        $x \leftarrow \mathcal{F}(x)$ 
9:     else if  $\text{path}$  starts with  $\tau_1$  then
10:       $x \leftarrow \tau_1(x)$ 
11:     else  $\triangleright$   $\text{path}$  starts with  $\tau_2$ 
12:        $x \leftarrow \tau_2(x)$ 
13:     end if
14:      $\text{orbit} \leftarrow \text{concat}(\text{orbit}, x)$   $\triangleright$  Add iterate  $x$  to orbit
15:   end while
16:   return  $\text{orbit}$ 
17: end procedure

```

Figure 9.20 shows the shortest-time orbit from $x = (I, \phi) = (1, 1.5)$ to a neighborhood of $y = (I, \phi) = (7, 1.5)$. The corresponding pseudo-orbit for the SR3BP flow takes time $34t_{\text{in}} + 17t_{\text{out}} \approx 204$ SR3BP time units, i.e. about 32 years (optimal drift time). Compare this to the orbits obtained in previous sections.

Notice that the optimal orbit uses all three dynamics ($\mathcal{F}$, τ_1 and τ_2) for maximum flexibility.

Notice that some iterates actually *decrease* the action. The key point is that, sometimes, one needs to take an iterate that decreases action in order to quickly move to a region where it later increases sharply. This way the pseudo-orbit's time is globally optimized.

Finally, from the orbit of the IFS $\{\mathcal{F}, \tau_1, \tau_2\}$ we can construct a pseudo-orbit by concatenating segments of trajectories of the SR3BP flow. Each iterate of the inner map $\mathcal{F}$ corresponds to its flow suspension, which is integrated using the Birkhoff normal form. Each iterate of the transition map τ_1 or τ_2 corresponds to a finite piece of homoclinic trajectory, which is computed by continuation of those previously found in Section 9.3.

Figure 9.21 illustrates the construction of the pseudo-orbit corresponding to the orbit in Figure 9.20: First, τ_1 is applied once; this corresponds to the blue homoclinic segment. Then $\mathcal{F}$ is applied three times; this corresponds to the green segment. Next, τ_2 is applied once; this corresponds to the homoclinic red segment. Notice that all segments start and end on the Poincaré section Σ (endpoints are marked with squares). This construction would continue until the whole pseudo-orbit is obtained (not displayed).

Remark 9.19. We have obtained a pseudo-orbit, not a true trajectory of the SR3BP. The endpoints of consecutive segments do not exactly match in positions or velocities, but the discontinuities are small (as is apparent in Figure 9.21). In fact, the velocity discontinuities $\Delta v = \|(\Delta \dot{X}, \Delta \dot{Y}, \Delta \dot{Z})\|$, are smaller than 3.5×10^{-4} . Since the complete pseudo-orbit consists of 27 consecutive segments, the total required thrust is less than $26 \times 3.5 \times 10^{-4} \approx 0.0091$ non-dimensional SR3BP units. When converted into metric units, this amounts to 271 m/s.

Of course, to this pseudo-orbit one can apply shadowing results [GLMS20, Theorem 3.7] to establish the existence of a true SR3BP trajectory that shadows it. For applications, however, obtaining the pseudo-orbit is often the crucial step, since it is ultimately refined in a much more realistic model than the SR3BP, e.g. using JPL's Ephemeris.

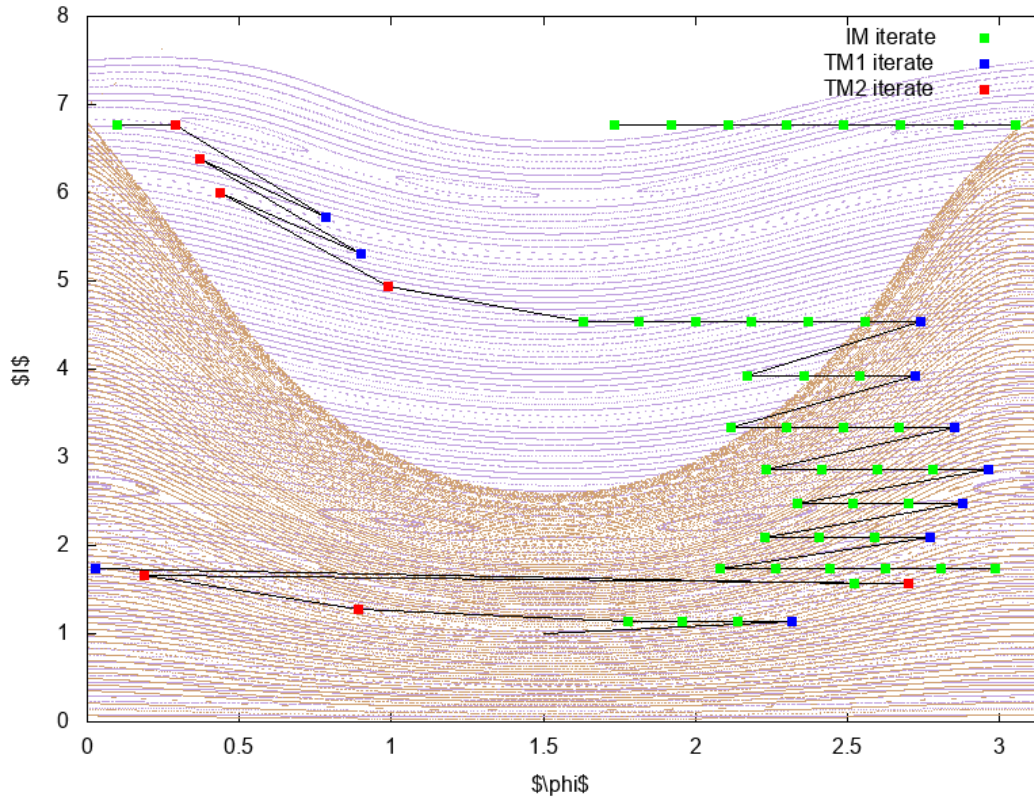


Figure 9.20: Drift orbit of the triple system $\{\mathcal{F}, \tau_1, \tau_2\}$ using the shortest path algorithm. Notice that some iterates of the transition map actually *reduce* the action, in order to increase it more efficiently overall.

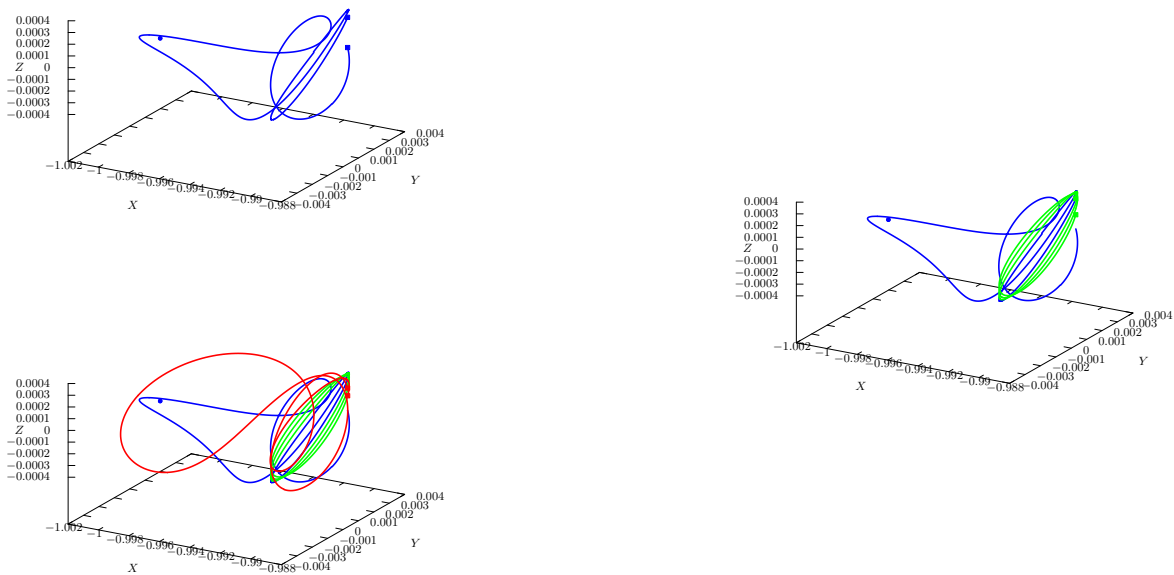


Figure 9.21: Top left: Trajectory segment corresponding to the first application of τ_1 in Figure 9.20 (endpoints are marked with squares). The Earth is represented by a blue circle (not to scale). Middle right: Segments corresponding to $\tau_1 \circ \mathcal{F}^3$. Bottom left: Segments corresponding to $\tau_1 \circ \mathcal{F}^3 \circ \tau_2$.

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