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# Geometric properties of the scattering map of a normally hyperbolic invariant manifold

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#### Abstract

Given a normally hyperbolic invariant manifold  $\Lambda$  for a map f, whose stable and unstable invariant manifolds intersect transversally, we consider its associated scattering map. That is, the map that, given an asymptotic orbit in the past, gives the asymptotic orbit in the future.

We show that when f and  $\Lambda$  are symplectic (respectively exact symplectic) then, the scattering map is symplectic (respectively exact symplectic). Furthermore, we show that, in the exact symplectic case, there are extremely easy formulas for the primitive function, which have a variational interpretation as difference of actions.

We use this geometric information to obtain efficient perturbative calculations of the scattering map using deformation theory. This perturbation theory generalizes and extends several results already obtained using the Melnikov method. Analogous results are true for Hamiltonian flows. The proofs are obtained by geometrically natural methods and do not involve the use of particular coordinate systems, hence the results can be used to obtain intersection properties of objects of any type.

We also reexamine the calculation of the scattering map in a geodesic flow perturbed by a quasi-periodic potential. We show that the geometric theory reproduces the results obtained in [Amadeu Delshams, Rafael de la Llave, Tere M. Seara, Orbits of unbounded energy in quasi-periodic perturbations of geodesic flows, Adv. Math. 202 (1) (2006) 64–188] using methods of fast–slow systems. Moreover, the geometric theory allows to compute perturbatively the dependence on the slow variables, which does not seem to be accessible to the previous methods.

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# 1. Introduction

A remarkable tool introduced in [22] 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 [33] introduced the *homoclinic map* to a center manifold.)

The use of the scattering map was crucial for the applications in [25,27,34,35]. 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 paper, 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 [25,27].
- 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 [15, pp. 17, 68] and related ideas in [47]. The scattering map is extremely similar to the scattering matrix in quantum mechanics [55,58]. Indeed, we have followed a notation that matches the definitions in quantum mechanics. For a comparison with the quantum mechanics scattering theory see Appendix A.

The first goal of this paper is to provide a more global definition of the scattering map (in [22, 25,26] 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 8 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 2. First we introduce the wave operators

$$\Omega_{\pm} : W^{s,u}_{\Lambda} \to \Lambda$$
$$x \mapsto x_{\pm}$$

which assign to each point x in the stable (or unstable) manifold, the unique point  $x_+$  (or  $x_-$ ) in  $\Lambda$  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 a "homoclinic channel"  $\Gamma$  where both wave operators are well-defined diffeomorphisms with their images (see Definition 3).

For such homoclinic channel  $\Gamma$  the scattering map is defined as

$$\sigma = \sigma^{\Gamma} = \Omega_{+} \circ \left( \Omega_{-}^{\Gamma} \right)^{-1} \colon \Omega_{-}(\Gamma) \to \Omega_{+}(\Gamma)$$

The goal of this paper 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  $\Gamma$  chosen. The same happens with its domain and image that, in general, are strict subsets of  $\Lambda$ . Nevertheless we will suppress  $\Gamma$  from the notation unless it causes confusion. The end of Section 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 3 we prove that the scattering map is (exact) symplectic provided that the map f and the normally hyperbolic invariant manifold  $\Lambda$  are (exact) symplectic. Some of these results were also established in [33] 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 9) 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 3.4 we show that there is a very compact formula (28) for the *primitive function* of the scattering map. The formula (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 4 and 5 is to develop perturbative formulas for the scattering map. In Section 4 the general setup 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 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 6, we apply the perturbative formula of the scattering map in the case of quasiperiodically perturbed geodesic flows already considered in [26]. In particular, we show that for geodesic flows the scattering map is globally defined in  $\Lambda$ , nevertheless, for the perturbations, there are considerations of domains and monodromy. Even if these considerations were already presented in [22], the global theory of this paper allows to discuss them more fully. We show that the calculations obtained by the formalism in this paper agree with the calculations in [22,26]. The calculations in [22,26] 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 paper, obtain at the same time information of the scattering map both for fast and for slow variables.

## 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 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.

## 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 [29,30,40, 41,56,68]. 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,  $f: M \to M$  a  $C^r$  diffeomorphism,  $r \ge 1$ .

**Definition 1.** Let  $\Lambda \subset M$  be a submanifold invariant under f,  $f(\Lambda) = \Lambda$ . We say that  $\Lambda$  is a normally hyperbolic invariant manifold if there exist a constant C > 0, rates  $0 < \lambda < \mu^{-1} < 1$  and a splitting for every  $x \in \Lambda$ 

$$T_{\mathcal{X}}M = E_{\mathcal{X}}^s \oplus E_{\mathcal{X}}^u \oplus T_{\mathcal{X}}\Lambda$$

in such a way that

$$v \in E_x^s \quad \Leftrightarrow \quad \left| Df^n(x)v \right| \leqslant C\lambda^n |v|, \quad n \ge 0,$$
  

$$v \in E_x^u \quad \Leftrightarrow \quad \left| Df^n(x)v \right| \leqslant C\lambda^{|n|} |v|, \quad n \le 0,$$
  

$$v \in T_x \Lambda \quad \Leftrightarrow \quad \left| Df^n(x)v \right| \leqslant C\mu^{|n|} |v|, \quad n \in \mathbb{Z}.$$
(1)

We will assume that  $\Lambda$  is compact or that f is uniformly  $C^r$  in a neighborhood of  $\Lambda$ . We will also assume without loss of generality that  $\Lambda$  is connected. In the case that  $\Lambda$  is not compact, one has to pay attention to the properties of the map f in a neighborhood of  $\Lambda$  and work out issues such as regularity of extensions, etc.

It follows from (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  $\ell$  being any number such that

$$\ell < \min\left(r, \frac{|\log \lambda|}{\log \mu}\right). \tag{2}$$

We recall that it is possible to introduce a smooth metric (the adapted metric) in M in such a way that C = 1 in (1) at the only price of redefining slightly  $\lambda$ ,  $\mu$ .

Given a normally hyperbolic invariant manifold  $\Lambda$  we define

$$W^{s}_{\Lambda} = \left\{ y \in M \mid d\left(f^{n}(y), \Lambda\right) \leqslant C_{y}\lambda^{n}, \ n \ge 0 \right\},\$$
$$W^{u}_{\Lambda} = \left\{ y \in M \mid d\left(f^{n}(y), \Lambda\right) \leqslant C_{y}\lambda^{|n|}, \ n \leqslant 0 \right\}.$$

Furthermore, for each  $x \in \Lambda$ , we define

$$W_x^s = \left\{ y \in M \mid d\left(f^n(x), f^n(y)\right) \leqslant C_{x,y}\lambda^n, \ n \ge 0 \right\},$$
  
$$W_x^u = \left\{ y \in M \mid d\left(f^n(x), f^n(y)\right) \leqslant C_{x,y}\lambda^{|n|}, \ n \le 0 \right\}$$

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

$$W_{\Lambda}^{s} = \bigcup_{x \in \Lambda} W_{x}^{s},$$
$$W_{\Lambda}^{u} = \bigcup_{x \in \Lambda} W_{x}^{u}.$$
(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 (3) can be expressed as saying that  $\{W_x^s\}_{x \in \Lambda}$ ,  $\{W_x^u\}_{x \in \Lambda}$  give a foliation of  $W^s_{\Lambda}, W^u_{\Lambda}$ , respectively.

We recall that in these circumstances we have that

Λ is a C<sup>ℓ</sup> manifold with ℓ given in (2).
 W<sup>s</sup><sub>A</sub>, W<sup>u</sup><sub>A</sub> are C<sup>ℓ-1</sup> manifolds.
 W<sup>s</sup><sub>X</sub>, W<sup>u</sup><sub>X</sub> are C<sup>r</sup> manifolds.
 The maps x ↦ W<sup>s</sup><sub>X</sub>, W<sup>u</sup><sub>X</sub> are C<sup>ℓ-1-j</sup>, when W<sup>s</sup><sub>X</sub>, W<sup>u</sup><sub>X</sub> are given the C<sup>j</sup> topologies.

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  $W^s_A$ ,  $W^u_A$  do not have any more regularity than that claimed above.

Note that the leaves of the foliation  $\{W_x^s\}_{x \in \Lambda}$  of  $W_A^s$  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  $W^s_A$  is limited by ratios of exponents.

Note that Definition 1 of normal hyperbolicity implies that  $\ell \ge 1$ , but in this paper we assume  $\ell \ge 2$  in order to have  $W_A^s$ ,  $W_A^u C^1$  manifolds. This is important because we will use the implicit function theorem for  $C^{\ell-1}$  regular objects.

For a point  $x \in W_A^s$  (respectively  $x \in W_A^u$ ), we denote by  $x_+$  (respectively  $x_-$ ) the point in  $\Lambda$  which satisfies  $x \in W_{x_+}^s$  (respectively  $x \in W_{x_-}^u$ ).

Note that given a point x, the points  $x_+$ ,  $x_-$  are uniquely defined. Moreover, denoting

$$\Omega_{\pm} : W_{\Lambda}^{s,u} \to \Lambda$$
$$x \mapsto x_{\pm}, \tag{4}$$

these maps, that we call wave operators, are well defined and of class  $C^{\ell}$ . We note that, with the standing assumptions of this paper, these maps are always  $C^1$ .



Fig. 1.

#### 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  $W_A^s$ ,  $W_A^u$ .

More precisely, we will assume that there is a normally hyperbolic invariant manifold  $\Lambda$  and a homoclinic manifold  $\Gamma \subset W^s_{\Lambda} \cap W^u_{\Lambda}$  such that  $\forall x \in \Gamma$ :

$$T_x M = T_x W^s_A + T_x W^u_A,$$
  

$$T_x W^s_A \cap T_x W^u_A = T_x \Gamma.$$
(5)

We will refer to (5) by saying that the intersection of  $W^s_{\Lambda}$  and  $W^u_{\Lambda}$  is transversal along  $\Gamma$ .

If *M* is *m*-dimensional,  $\Lambda$  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,  $W_A^s$ ,  $W_A^u$  are  $d_s + c$ ,  $d_u + c$ -dimensional, respectively. Because of Definition 1, we have that  $m = c + d_s + d_u$  and therefore, by (5), the dimension of  $\Gamma$  has to be  $(c + d_s + c + d_u) - m = c$ .

The definition of the scattering map requires that the intersection  $\Gamma$  satisfying (5) satisfies also that for every point  $x \in \Gamma$  we have

$$T_x \Gamma \oplus T_x W^s_{x+} = T_x W^s_{\Lambda},$$
  
$$T_x \Gamma \oplus T_x W^u_{x-} = T_x W^u_{\Lambda}.$$
 (6)

We will refer to (6) by saying that  $\Gamma$  is transversal to the  $W_x^s$ ,  $W_x^u$  foliation, see Fig. 1. Note that to define (6) we assume (5). We also call attention that (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 6.1, we will discuss these phenomenon of monodromy making more geometric the discussion in [22].

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 (5) is satisfied for a map f and manifolds  $\Lambda$ ,  $\Gamma$ , 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 (6) holds in  $C^1$  open sets.



Fig. 2.

**Remark 2.** By the implicit function theorem, if for some  $x^* \in W_A^s \cap W_A^u$  it is verified that  $T_{x^*}W_A^s \cap T_{x^*}W_A^u$  is *c*-dimensional, we can find a locally unique manifold  $\Gamma$  such that

$$T_{x^*}\Gamma = T_{x^*}W^s_{\Lambda} \cap T_{x^*}W^u_{\Lambda}.$$

Moreover, this  $\Gamma$  is  $C^{\ell-1}$ .

Also by the implicit function theorem, if the transversality condition (6) is satisfied for certain  $x^*$  in a manifold  $\Gamma$ , then it is satisfied by all  $x \in \Gamma$  close enough to  $x^*$ .

Given a manifold  $\Gamma$  verifying (5), we can consider the wave operators  $\Omega_{\pm}$  of (4) restricted to  $\Gamma$ . Under assumption (6) we have that  $\Omega_{\pm}$  are local diffeomorphisms from  $\Gamma$  to  $\Lambda$ .

**Definition 3.** We say that  $\Gamma$  is a *homoclinic channel* if:

Γ ⊂ W<sup>s</sup><sub>Λ</sub> ∩ W<sup>u</sup><sub>Λ</sub> verifies (5) and (6).
 The wave operators (Ω<sub>±</sub>)<sub>|Γ</sub>: Γ → Ω<sub>±</sub>(Γ) ⊂ Λ are C<sup>ℓ-1</sup> diffeomorphisms.

Restricting  $\Gamma$  if necessary, from now on we will only consider  $\Gamma \subset W^s_{\Lambda} \cap W^u_{\Lambda}$  such it verifies Definition 3 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

$$\Omega_{\pm}^{\Gamma}:\Gamma\to H_{\pm}^{\Gamma}$$

are  $C^{\ell-1}$  diffeomorphisms. Note that if  $\Gamma$  is a homoclinic channel, so is  $f^n(\Gamma)$  for any  $n \in \mathbb{Z}$ .

**Remark 4.** 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 Fig. 2)

$$\Omega_{+}^{\Gamma} = f^{-1} \circ \Omega_{+}^{f(\Gamma)} \circ f, \tag{7}$$

and analogously

$$\Omega_{-}^{\Gamma} = f \circ \Omega_{-}^{f^{-1}(\Gamma)} \circ f^{-1}.$$
(8)



Fig. 3. Illustration of Definition 5 of the scattering map.

Iterating these formulas, we have for every  $n \in \mathbb{Z}$ ,

$$\Omega_{+}^{\Gamma} = f^{-n} \circ \Omega_{+}^{f^{n}(\Gamma)} \circ f^{n},$$
  
$$\Omega_{-}^{\Gamma} = f^{n} \circ \Omega_{-}^{f^{-n}(\Gamma)} \circ f^{-n}.$$
 (9)

**Definition 5.** Given a homoclinic channel  $\Gamma$  and  $\Omega_{\pm}^{\Gamma} \colon \Gamma \to H_{\pm}^{\Gamma}$  the associated wave operators, we define the scattering map associated to  $\Gamma$ 

$$\sigma^{\Gamma}: H_{-}^{\Gamma} \to H_{+}^{\Gamma}$$

by

$$\sigma^{\Gamma} = \Omega^{\Gamma}_{+} \circ \left(\Omega^{\Gamma}_{-}\right)^{-1}.$$
(10)

See Fig. 3.

#### 2.3. Some elementary properties of the scattering map

### 2.3.1. Regularity properties

We note that, because of the implicit function theorem, the homoclinic channel  $\Gamma$  is as differentiable as the invariant manifolds  $W^s_{\Lambda}$ ,  $W^u_{\Lambda}$ , that is  $C^{\ell-1}$ , where  $\ell$  is given in (2).

Later, we will consider a family of mappings  $f_{\varepsilon}$  which are jointly  $C^r$  in all the variables and in the parameter  $\varepsilon$ . 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.

#### 2.3.2. Invariance properties

It is clear from its definition that the scattering map depends on the homoclinic channel considered.

• We note that if  $\Gamma$  satisfies Definition 3, 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 (7) and (8) and Definition 5 of the scattering map, we easily obtain:

$$f \circ \sigma^{\Gamma} = \sigma^{f(\Gamma)} \circ f. \tag{11}$$

Moreover, iterating f and using (9), we have:

$$\sigma^{f^n(\Gamma)} = f^n \circ \sigma^{\Gamma} \circ f^{-n}.$$
(12)

We call attention to the fact that in (11) and (12) the scattering map on both sides is not the same.

• If we exchange the map f by  $f^{-1}$ , the manifold  $\Lambda$  is still a normally hyperbolic invariant manifold under  $f^{-1}$ . On the other hand, the stable and unstable manifolds are exchanged. Hence, if  $\Gamma$  is a homoclinic channel verifying Definition 3 for the  $W_{\Lambda}^{s,(f)}$ ,  $W_{\Lambda}^{u,(f)}$ , then it is also a homoclinic channel verifying Definition 3 for  $W_{\Lambda}^{s,(f^{-1})}$ ,  $W_{\Lambda}^{u,(f^{-1})}$ , and

$$\Omega_{+}^{\Gamma,(f)} = \Omega_{-}^{\Gamma,(f^{-1})}, \qquad \Omega_{-}^{\Gamma,(f)} = \Omega_{+}^{\Gamma,(f^{-1})}$$
(13)

and

$$\Omega_{\pm}^{\Gamma,(f^n)} = \Omega_{\pm}^{\Gamma,(f)}, \quad n \ge 0.$$

All these properties give

$$\sigma^{\Gamma,(f)} = \left(\sigma^{\Gamma,(f^{-1})}\right)^{-1}, \qquad \sigma^{\Gamma,(f^n)} = \sigma^{\Gamma,(f)}, \quad n \ge 0.$$

#### 2.4. The scattering map in other contexts

#### 2.4.1. 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  $\Lambda$  is a normally hyperbolic invariant manifold for a flow  $\Phi_t$  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

$$v \in E_x^s \quad \Leftrightarrow \quad \left| D\Phi_t(x)v \right| \leqslant C e^{-\beta t} |v|, \quad t \ge 0,$$
  

$$v \in E_x^u \quad \Leftrightarrow \quad \left| D\Phi_t(x)v \right| \leqslant e^{-\beta |t|} |v|, \quad t \le 0,$$
  

$$v \in T_x \Lambda \quad \Leftrightarrow \quad \left| D\Phi_t(x)v \right| \leqslant C e^{\alpha |t|} |v|, \quad t \in \mathbb{R}.$$
(14)

All the properties and definitions given in Section 2.1 are analogous in the case of flows. In particular, the stable and unstable manifolds of  $\Lambda$  are given by

$$W_{\Lambda}^{s} = \left\{ y \in M \mid d(\Phi_{t}(y), \Lambda) \leqslant C_{y} e^{-\beta t}, \ t \ge 0 \right\},\$$
$$W_{\Lambda}^{u} = \left\{ y \in M \mid d(\Phi_{t}(y), \Lambda) \leqslant C_{y} e^{-\beta |t|}, \ t \leqslant 0 \right\}$$

and, for each  $x \in \Lambda$ , we define the stable and unstable manifolds of x as

$$W_x^s = \left\{ y \in M \mid d\left(\Phi_t(x), \Phi_t(y)\right) \leqslant C_{x,y} e^{-\beta t}, \ t \ge 0 \right\},\$$
  
$$W_x^u = \left\{ y \in M \mid d\left(\Phi_t(y), \Phi_t(y)\right) \leqslant C_{x,y} e^{-\beta |t|}, \ t \le 0 \right\}.$$

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  $\Lambda$  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:

$$\Omega_{\pm} \colon W^{s,u}_{\Lambda} \to \Lambda$$
$$x \mapsto x_{\pm}$$

such that  $|\Phi_t(x) - \Phi_t(x_{\pm})| \leq C_{x,x_{\pm}} e^{-\beta|t|}$ , as  $t \to \pm \infty$ .

To define the scattering map in the case of flows we also assume that there exists a homoclinic channel  $\Gamma$  satisfying Definition 3 and then the maps

$$\Omega_{\pm}^{\Gamma}:\Gamma\to H_{\pm}^{\Gamma}\subset\Lambda$$

are diffeomorphisms. Hence, analogously to (10), we define the scattering map

$$\sigma^{\Gamma} = \Omega_{+}^{\Gamma} \circ \left(\Omega_{-}^{\Gamma}\right)^{-1}$$

It is straightforward to check that these wave operators  $\Omega_{\pm}^{\Gamma}$  for the flow  $\Phi_t$  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:

$$\sigma^{\Gamma} = \sigma^{\Gamma, f_T} = \sigma^{\Gamma, f_{T'}}, \quad \forall T, T' \in \mathbb{R}.$$
(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  $\Phi_t$ . We have that the following properties, completely analogous to the properties of Section 2.3.2, hold:

$$\begin{split} \Omega_{\pm}^{\Gamma,\mathcal{H}} &= \Omega_{\mp}^{\Gamma,-\mathcal{H}}, \\ \Omega_{+}^{\Gamma,\mathcal{H}} &= \Phi_{-t} \circ \Omega_{+}^{\Phi_{t}(\Gamma),\mathcal{H}} \circ \Phi_{t}, \qquad \Omega_{-}^{\Gamma,\mathcal{H}} &= \Phi_{t} \circ \Omega_{-}^{\Phi_{-t}(\Gamma),\mathcal{H}} \circ \Phi_{-t}, \\ \sigma^{\Gamma,\mathcal{H}} &= \left(\sigma^{\Gamma,-\mathcal{H}}\right)^{-1}, \\ \sigma^{\Phi_{t}(\Gamma),\mathcal{H}} &= \Phi_{t} \circ \sigma^{\Gamma,\mathcal{H}} \circ \Phi_{-t}. \end{split}$$

## 2.4.2. 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

$$\|\mathcal{G} - \mathcal{G}_0\|_{\mathcal{C}^r} \ll 1. \tag{16}$$

We first deal with the product case  $\mathcal{H}_0 = (\mathcal{G}_0, \mathcal{L})$ , which is very simple.

**Proposition 6.** Let  $\Lambda$  be a normally hyperbolic invariant manifold under a flow  $\Phi_t$  on a manifold M. Let  $0 < \alpha < \beta$  be the exponential expansion rates corresponding to the normal hyperbolicity of  $\Lambda$ . Let N be another manifold with a flow  $\varphi_t$  with exponential expansion rates less or equal than  $\alpha$ . 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,  $W^s_{\Lambda} \times N = W^s_{\tilde{\lambda}}$  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  $\mathcal{H}_0$ . Since the exponential rates in *N* are smaller or equal than  $\alpha$ , 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

$$\tilde{\sigma}(x,\theta) = \big(\sigma(x),\theta\big).$$

In the skew product case  $\mathcal{H} = (\mathcal{G}, \mathcal{L})$ , provided that  $\mathcal{H}$  is a small perturbation (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

$$\tilde{\sigma}(x,\theta) = \big(\sigma(x,\theta),\theta\big).$$

In particular, in the case of quasi-periodic flows coming from a non-autonomous Hamiltonian vector field of Hamiltonian  $H(x, \theta)$ ,  $\theta = vt$ ,  $v \in \mathbb{R}^d$ , 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  $\theta$  and working with the autonomous flow of the Hamiltonian  $H^*(x, \theta, A) = H(x, \theta) + v \cdot A$  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

$$\sigma^*(x,\theta,A) = \big(\sigma(x,\theta),\theta,\mathcal{A}(x,\theta,A)\big).$$

In the following section we will see that the scattering map for a symplectic map is also symplectic.

## 2.4.3. Center manifolds

Many of the results discussed above generalize to center manifolds of a fixed point [33] or to locally invariant manifolds with boundary.

The standard method to study locally invariant manifolds (see [29]) 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 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.

# 3. Symplectic properties of the scattering map

The main result of this section is that, in case that f is symplectic and  $\Lambda$  is a symplectic manifold (when endowed with the restriction of the symplectic form), the scattering map preserves the restriction of the symplectic form to  $\Lambda$ . A version of this result for a center manifold of a fixed point with a different proof can be found in [33]. These geometric properties will be very important for the perturbative computations of the scattering map in Section 4. In this discussion, we will use Cartan calculus and coordinate free calculations. See [1,8,64].

# 3.1. Notation and some elementary facts on symplectic geometry

When N, M are symplectic manifolds, we say that  $f: N \to M$  is symplectic when

$$f^*\omega_M = \omega_N$$

where  $f^*$  is the pullback 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 pullback 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

$$f^* \alpha_M = \alpha_N + dP^f \tag{17}$$

for some function  $P^f: N \to \mathbb{R}$ . 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 pushforward on forms defined by

$$(f_*\omega_N)(x)(v,w) = \omega_N \left( f^{-1}(x) \right) \left( Df^{-1}(x)v, Df^{-1}(x)w \right) \quad \forall v, w \in T_x M.$$

**Remark 7.** Note that the function  $P^f$  is determined uniquely up to constants when N is connected and  $\alpha_N$ ,  $\alpha_M$  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 [45] and specially [37,38] for a systematic study of the primitive function, including numerical applications.

3.1.1. Formulation of the symplectic properties of the scattering map

**Theorem 8.** Assume that M is endowed with a symplectic (respectively exact symplectic) form  $\omega$  and that  $\omega|_{\Lambda}$  is also symplectic (hence, in particular, the dimension m of M and the dimension c of  $\Lambda$  are even).

Assume that f is symplectic (respectively it is exact symplectic). Assume that there exists a homoclinic channel  $\Gamma$  and so the scattering map  $\sigma^{\Gamma}$  is well defined. Then, the scattering map  $\sigma^{\Gamma}$  is symplectic (respectively exact symplectic).

The main technical tool, from which Theorem 8 follows almost immediately is:

**Lemma 9.** Assume that, with the notations above, we have that  $\omega|_{\Lambda}$  is symplectic, and that  $\Gamma$  is  $C^1$  close to  $\Lambda$  on a neighborhood (hence  $\omega|_{\Gamma}$  is also a symplectic form). *Then,* 

$$\left(\Omega_{+}^{\Gamma}\right)_{*}\omega|_{\Gamma} = \omega|_{\Lambda}.$$
(18)

# 3.2. Proof of Lemma 9

The proof of Lemma 9 is very similar to the proof of absolute continuity of Anosov foliation in [57]. See Fig. 4.

We will prove that given any two-dimensional cell  $\mathcal{B} \subset \Gamma$ , we have

$$\int_{\mathcal{B}} \omega = \int_{\Omega_{+}^{\Gamma}(\mathcal{B})} \omega.$$
<sup>(19)</sup>

To prove (19), we will consider a 3-cell C in  $W^s_{\Lambda}$  whose boundary contains  $\mathcal{B}$ ,  $\Omega^{\Gamma}_+(\mathcal{B})$ . Let  $B:[0,1] \times [0,1] \to \Gamma$  be a parameterization of  $\mathcal{B}$ .



Fig. 4. Illustration of the proof of Lemma 9.

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  $\gamma_z$  geodesic in  $W^s_{\Omega^{\Gamma}_+(y)}$  joining y and  $\Omega^{\Gamma}_+(y)$ . We parameterize these geodesics in such a way that

$$\gamma_z(0) = \Omega_+^{\Gamma}(y),$$
$$\gamma_z(1) = y.$$

We see by the implicit function theorem that the map  $C:[0,1] \times [0,1] \times [0,1] \rightarrow W^s_{\Lambda}$  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 C. We note that

$$\partial \mathcal{C} = \mathcal{B} - \Omega_{+}^{\Gamma}(\mathcal{B}) + \mathcal{R}$$

where  $\mathcal{R}$  is the two-dimensional cell consisting on a union of geodesics in  $W^s_{\mathcal{Q}_+^{\Gamma}(\partial \mathcal{B})}$ .

By Stokes theorem

$$\int_{\partial \mathcal{C}} \omega = \int_{\mathcal{C}} d\omega = 0$$

We therefore have

$$\int_{\mathcal{B}} \omega = \int_{\Omega_{+}^{\Gamma}(\mathcal{B})} \omega - \int_{\mathcal{R}} \omega.$$
(20)

Hence, the desired result (19) will be established when we prove  $\int_{\mathcal{R}} \omega = 0$ .

This is a consequence of the following proposition, which we will also find useful in discussing exactness.

**Proposition 10.** Let  $\mathcal{R}$  be a 2-cell in  $W^s_{\Lambda}$  parameterized by

$$R:[0,1]\times[0,1]\rightarrow W^s_A$$

in such a way that

$$R(z,t) \in W^s_{R(0,t)}, \quad R(0,t) \in \Lambda.$$

That is, we can think of  $\mathcal{R}$  as a union of lines each of which lies in the stable manifold of one point. Then  $\int_{\mathcal{R}} \omega = 0$ .

**Proof.** It consists just in observing that, by the invariance of  $\omega$  under f, we have for every  $n \in \mathbb{N}$ 

$$\int_{\mathcal{R}} \omega = \int_{f^n(\mathcal{R})} \omega$$

and, by the hyperbolicity of  $\Lambda$ , we also have

Area
$$(f^n(\mathcal{R})) \leq C(\lambda \mu)^n$$
,

because the stable coordinates contract at least by  $C\lambda^n$  and the coordinates along  $\Lambda$  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  $\int_{f^n(\mathcal{R})} \omega \leq C \operatorname{Area}(f^n(\mathcal{R}))$ , Proposition 10 is proved.  $\Box$ 

Proposition 10 finishes the proof of the fact that  $\Omega_{+}^{\Gamma}$  is symplectic.

To finish the proof of Lemma 9, 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  $\eta : [0, 1] \to \Gamma$ , we have:

$$\int_{\eta} \alpha = \int_{\Omega_{+}^{\Gamma}(\eta)} \alpha + \mathcal{G}^{\Gamma} \big( \Omega_{+} \big( \eta(1) \big) \big) - \mathcal{G}^{\Gamma} \big( \Omega_{+} \big( \eta(0) \big) \big)$$
(21)

where  $\mathcal{G}^{\Gamma}: \Omega_{+}(\Gamma) \to \mathbb{R}$  is an explicit function which we now compute.

Since the path  $\eta$  is arbitrary, (21) is equivalent to

$$\left(\Omega_{+}^{\Gamma}\right)_{*}\alpha|_{\Gamma} = \alpha|_{\Lambda} + d\mathcal{G}^{\Gamma}.$$
(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

$$\mathcal{G}^{\Gamma}(y) = \int_{\beta} \alpha.$$
<sup>(23)</sup>

The integral defining  $\mathcal{G}^{\Gamma}$  in (23) is independent of the choice of the path  $\beta$  because of Proposition 10.

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

$$\int_{\beta} \alpha - \int_{\widetilde{\beta}} \alpha = \int_{\Sigma} d\alpha = 0.$$

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  $\beta_y$  the shortest geodesic in  $W_y^s$  joining y and  $(\Omega_{\Gamma}^{\Gamma})^{-1}(y)$ .

Denoting  $y_0 = \Omega_+^{\Gamma}(\eta(0)), y_1 = \Omega_+^{\Gamma}(\eta(1))$ , the identity (21) follows because

$$-\eta + \beta_{y_1} + \Omega_+^{\Gamma}(\eta) - \beta_{y_0} = \partial \mathcal{R}$$

where  $\mathcal{R}$  is a two cell satisfying the assumptions of Proposition 10. Then,  $\int_{\partial \mathcal{R}} \alpha = \int_{\mathcal{R}} \omega = 0$ .  $\Box$ 

# 3.3. Proof of Theorem 8

By the  $\lambda$ -lemma (see e.g. [57]) there is an  $n \in \mathbb{N}$  large enough so that  $f^n(\Gamma)$  satisfies the assumptions of Lemma 9.

Similarly  $f^{-n}(\Gamma)$  satisfies the assumptions of Lemma 9 for  $f^{-1}$  in place of f.

We note that, by Eq. (9) with n and -n respectively

$$\sigma^{\Gamma} = \Omega_{+}^{\Gamma} \circ \left(\Omega_{-}^{\Gamma}\right)^{-1} = f^{-n} \circ \Omega_{+}^{f^{n}(\Gamma)} \circ f^{2n} \circ \left[\Omega_{-}^{f^{-n}(\Gamma)}\right]^{-1} \circ f^{-n}.$$
 (24)

Also, by (13), we have that

$$\Omega_{-}^{f^{-n}(\Gamma),(f)} = \Omega_{+}^{f^{-n}(\Gamma),f^{-1}}.$$

Hence, the map  $\sigma^{\Gamma}$  is symplectic (respectively exact symplectic) as desired.

# 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  $\Lambda$  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 (28), which gives the primitive function of the scattering map in terms of the primitive function of f and formula (29) which gives the analogous formula for flows. Formula (28) is given by the difference of two sums computed along the homoclinic intersection. In Theorem 14, we show that formula (28) converges exponentially fast together with some of its derivatives.

## 3.4.1. Some elementary properties

We recall that in Section 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 11.** If  $f: N \to M$  and  $g: M \to V$  are exact symplectic diffeomorphisms with primitives  $P^f: N \to \mathbb{R}$  and  $P^g: M \to \mathbb{R}$ , respectively, then we have:

(1) The primitive  $P^{g \circ f}$  of  $g \circ f$  is given by

$$P^{g \circ f} = P^f + P^g \circ f. \tag{25}$$

(2) If  $g \circ f = \text{Id then}$ 

$$P^g + P^f \circ g = 0. (26)$$

(3) 
$$P^{f^n} = \sum_{j=0}^{N-1} P^f \circ f^j.$$
(27)

**Proof.** The proof of (11) is only the following computation:

$$(g \circ f)^* \alpha_V = f^* g^* \alpha_V = f^* (\alpha_M + dP^g)$$
$$= \alpha_N + dP^f + df^* P^g$$
$$= \alpha_N + d(P^f + P^g \circ f).$$

The other parts of the proposition are easy consequences of (25).  $\Box$ 

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.

## 3.4.2. Formulas for the primitive function of the scattering map

In this section we study a  $C^r$  symplectic diffeomorphism  $f: M \to M$  which has a normally hyperbolic invariant manifold  $\Lambda$  such that  $\omega_{|\Lambda}$  is non-degenerate, and also a homoclinic channel  $\Gamma$  verifying Definition 3, so that there exists a scattering map  $\sigma = \sigma^{\Gamma}: H^{-} \to H^{+}$  as in (10). Again, we are assuming that the map f is uniformly  $C^r$  in a neighborhood of the manifold  $\Lambda$  and of the homoclinic channel  $\Gamma$ .

In the case that the map f is exact symplectic we know that the same is true for the scattering map. The next Theorem 12 gives us a very effective formula for the primitive of the scattering map  $\sigma$  in terms of the primitive of f.

The main results of this section are Theorem 12 which establishes (28), a formula for the primitive function of  $\sigma$ , Theorem 13, which provides an analogous formula (29) for flows, and Theorem 14 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, we will obtain formulas very similar to (28) and (29) for other objects. The results of Theorem 14 will therefore, have further applicability.

**Theorem 12.** Let  $f: M \to M$  be a  $C^r$  exact symplectic diffeomorphism which has a normally hyperbolic invariant manifold  $\Lambda$  such that  $\omega_{|\Lambda|}$  is non-degenerate, and a homoclinic channel  $\Gamma$ verifying Definition 3, so that there exists a scattering map  $\sigma = \sigma^{\Gamma} : H^{-} \to H^{+}$  as in (10). Then, the primitive for  $\sigma$  is given by

$$P^{\sigma} = \lim_{N_{\pm} \to \infty} \sum_{j=1}^{N_{-}} P^{f} \circ f^{-j} \circ \left(\Omega_{-}^{\Gamma}\right)^{-1} - P^{f} \circ f^{-j}$$
$$+ \sum_{j=0}^{N_{+}-1} P^{f} \circ f^{j} \circ \left(\Omega_{+}^{\Gamma}\right)^{-1} \circ \sigma - P^{f} \circ f^{j} \circ \sigma.$$
(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 (15) that is independent of T.

**Theorem 13.** 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  $\Lambda$  such that  $\omega_{|\Lambda}$  is non-degenerate, and a homoclinic channel  $\Gamma$ verifying Definition 3, so that there exists a scattering map  $\sigma = \sigma^{\Gamma} : H^{-} \to H^{+}$  as in (10).

Then, the primitive  $P^{\sigma}$  is given by

$$P^{\sigma} = \lim_{T_{\pm} \to \infty} \int_{-T_{-}}^{0} (\alpha \mathcal{H} + H) \circ \Phi_{t} \circ (\Omega_{-}^{\Gamma})^{-1} - (\alpha \mathcal{H} + H) \circ \Phi_{t}$$
$$+ \int_{0}^{T_{+}} (\alpha \mathcal{H} + H) \circ \Phi_{t} \circ (\Omega_{+}^{\Gamma})^{-1} \circ \sigma - (\alpha \mathcal{H} + H) \circ \Phi_{t} \circ \sigma$$
(29)

where we denote  $\alpha \mathcal{H} = i_{\mathcal{H}} \alpha$ .

The convergence of the series in (28) and the integrals in (29) is guaranteed by the following result.

**Theorem 14.** Under our standing assumptions let  $\Psi$  be a  $C^m$  function in a neighborhood of  $\Lambda$ .

We have the following bounds for all  $j \in \mathbb{N}$ ,  $0 \leq k \leq \min(m, \ell, r)$ . For any  $\lambda > \lambda$ ,  $\mu > \mu$ , we have:

$$\|D^{k}(\Psi \circ f^{j} \circ (\Omega_{+}^{\Gamma})^{-1} \circ \sigma - \Psi \circ f^{j} \circ \sigma)\|_{C^{0}(H_{-})} \leqslant C \|\Psi\|_{C^{k}} j^{k} (\tilde{\lambda} \tilde{\mu}^{k})^{j},$$
$$\|D^{k}(\Psi \circ f^{-j} \circ (\Omega_{-}^{\Gamma})^{-1} - \Psi \circ f^{-j})\|_{C^{0}(H_{-})} \leqslant C \|\Psi\|_{C^{k}} j^{k} (\tilde{\lambda} \tilde{\mu}^{k})^{j}.$$
(30)

Analogous inequalities are valid for the case of flows.

Of course, to apply Theorem 14 to (28) and (29), we just have to take  $\Psi = P^f \in C^{r-1}$  (or  $\Psi = \alpha \mathcal{H} + H$ ), hence m = r - 1.

#### 3.4.3. A variational interpretation

We recall that the well-known Hamilton variational principle states that, under some nondegeneracy 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

$$\mathcal{L}(\gamma) = \int_{-\infty}^{+\infty} \left( -\alpha \dot{\gamma}(t) + H \circ \gamma(t) \right) dt$$

or, if  $\alpha = p dq$ , and  $\gamma(t) = (\gamma^q(t), \gamma^p(t))$ ,

$$\mathcal{L}(\gamma) = \int_{-\infty}^{+\infty} \left(-\gamma^p(t)\dot{\gamma}^q(t) + H \circ \gamma(t)\right) dt.$$

Hence, Theorems 12 and 13 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 [13] can be interpreted as a 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 [5–7] 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  $P^{\sigma}$  over all homoclinic intersections [13,14,18,44, 48,49].

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,  $\gamma$ , the mapping  $\dot{\gamma} \mapsto \frac{\partial}{\partial \gamma} L$  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 [4].

## 3.4.4. Proof of Theorem 12

The formula (28) is closely related to the following formula, which is true for any  $N_-, N_+ \in \mathbb{N}$ :

$$\sigma = f^{-N_{+}} \circ \Omega_{+}^{\Gamma^{N_{+}}} \circ f^{N_{+}+N_{-}} \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}}$$
(31)

where we have denoted  $\Gamma^n = f^n(\Gamma)$ , for  $n \in \mathbb{Z}$ .

The formula (31) is a consequence of the formula (9) for the wave operators.

To compute the primitive function  $P^{\sigma}$  of the scattering map  $\sigma$ , we start from (31) and apply Eqs. (25)–(27). We obtain, for any  $N_-, N_+ \in \mathbb{N}$ , the following formula in the reference manifold N:

$$\begin{split} P^{\sigma} &= P^{f^{-N_{-}}} + P^{(\Omega_{-}^{\Gamma^{-N_{-}}})^{-1}} \circ f^{-N_{-}} + P^{f^{N_{+}+N_{-}}} \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}} \\ &+ P^{\Omega_{+}^{\Gamma^{N_{+}}}} \circ f^{N_{+}+N_{-}} \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}} \\ &+ P^{f^{-N_{+}}} \circ \Omega_{+}^{\Gamma^{N_{+}}} \circ f^{N_{+}+N_{-}} \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}} \\ &= -(P^{f} \circ f^{-N_{-}} + \dots + P^{f} \circ f^{-1}) + P^{(\Omega_{-}^{\Gamma^{-N_{-}}})^{-1}} \circ f^{-N_{-}} \\ &+ (P^{f} + \dots + P^{f} \circ f^{N_{+}+N_{-}-1}) \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}} \\ &+ P^{\Omega_{+}^{\Gamma^{N_{+}}}} \circ f^{N_{+}+N_{-}} \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}} \\ &- (P^{f} \circ f^{-N_{+}} + \dots + P^{f} \circ f^{-1}) \circ \Omega_{+}^{\Gamma^{N_{+}}} \circ f^{N_{+}+N_{-}} \circ \left(\Omega_{-}^{\Gamma^{-N_{-}}}\right)^{-1} \circ f^{-N_{-}}. \end{split}$$

Now, we use formula (9) for the wave operators, obtaining

$$(\Omega_{-}^{\Gamma^{-N_{-}}})^{-1} \circ f^{-N_{-}} = f^{-N_{-}} \circ (\Omega_{-}^{\Gamma})^{-1},$$

$$f^{N_{+}+N_{-}} \circ (\Omega_{-}^{\Gamma^{-N_{-}}})^{-1} \circ f^{-N_{-}} = f^{N_{+}} \circ (\Omega_{-}^{\Gamma})^{-1},$$

$$\Omega_{+}^{\Gamma^{N_{+}}} \circ f^{N_{+}+N_{-}} \circ (\Omega_{-}^{\Gamma^{-N_{-}}})^{-1} \circ f^{-N_{-}} = \Omega_{+}^{\Gamma^{N_{+}}} \circ f^{N_{+}} \circ (\Omega_{-}^{\Gamma})^{-1} = f^{N_{+}} \circ \sigma$$

which give, using them in the formula for the primitive  $P^{\sigma}$ :

$$\begin{split} P^{\sigma} &= - \left( P^{f} \circ f^{-N_{-}} + \dots + P^{f} \circ f^{-1} \right) + P^{(\Omega_{-}^{\Gamma^{-N_{-}}})^{-1}} \circ f^{-N_{-}} \\ &+ \left( P^{f} \circ f^{-N_{-}} + \dots + P^{f} \circ f^{-1} \right) \circ \left( \Omega_{-}^{\Gamma} \right)^{-1} + \left( P^{f} + \dots + P^{f} \circ f^{N_{+}-1} \right) \circ \left( \Omega_{-}^{\Gamma} \right)^{-1} \\ &+ P^{\Omega_{+}^{\Gamma^{N_{+}}}} \circ f^{N_{+}} \circ \left( \Omega_{-}^{\Gamma} \right)^{-1} - \left( P^{f} + \dots + P^{f} \circ f^{N_{+}-1} \right) \circ \sigma. \end{split}$$

Now we observe that, by Lemma 9 and the  $\lambda$ -lemma applied to the normally hyperbolic invariant manifold  $\Lambda$ , the wave operators  $\Omega_{\pm}^{\Gamma^{\pm N_{\pm}}}$  are exact symplectic and converge to the identity map when  $N_{\pm} \to \infty$ . 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  $N_{\pm} \to \infty$ , we obtain

$$P^{\sigma} = \lim_{N_{\pm} \to \infty} \sum_{j=-1}^{-N_{-}} P^{f} \circ f^{j} \circ \left(\Omega_{-}^{\Gamma}\right)^{-1} - P^{f} \circ f^{j}$$
$$+ \sum_{j=0}^{N_{+}-1} P^{f} \circ f^{j} \circ \left(\Omega_{+}^{\Gamma}\right)^{-1} \circ \sigma - P^{f} \circ f^{j} \circ \sigma$$
(32)

which is formula (28).

#### 3.4.5. Proof of Theorem 13

The proof of Theorem 13 is an easy consequence of the fact that the primitive of the Hamiltonian flow  $\Phi_t$  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:

$$d\frac{d}{dt}P^{\Phi_t} = \frac{d}{dt}(\Phi_t)^*\alpha$$
$$= (\Phi_t)^*(di_{\mathcal{H}}\alpha + i_{\mathcal{H}}d\alpha) = d((\Phi_t)^*(\alpha\mathcal{H} + H))$$

Once we know the primitive of the Hamiltonian flow  $\Phi_T$ , we can consider the corresponding scattering map  $\sigma = \sigma^{\Gamma, \mathcal{H}}$  which, by (15), is independent of *T*. We compute the primitive of  $\sigma$  simply applying formula (28) for this case and using the following facts:

$$P^{\Phi_T} \circ \Phi_{jT} = \int_0^T (\alpha \mathcal{H} + H) \circ \Phi_t \circ \Phi_{jT} dt = \int_{jT}^{(j+1)T} (\alpha \mathcal{H} + H) \circ \Phi_t dt,$$
  

$$P^{\Phi_T} \circ \Phi_{-jT} = \int_0^T (\alpha \mathcal{H} + H) \circ \Phi_t \circ \Phi_{-jT} dt = \int_{-jT}^{-(j-1)T} (\alpha \mathcal{H} + H) \circ \Phi_t dt,$$
  

$$\sum_{j=0}^{N_+ - 1} P^{\Phi_T} \circ \Phi_{jT} = \int_0^{TN_+} (\alpha \mathcal{H} + H) \circ \Phi_t dt,$$
  

$$\sum_{j=1}^{N_-} P^{\Phi_T} \circ \Phi_{-jT} = \int_{-TN_-}^0 (\alpha \mathcal{H} + H) \circ \Phi_t dt.$$

With these expressions one easily obtains formula (29) by calling  $T_{\pm} = T N_{\pm} \rightarrow \pm \infty$ .

## 3.4.6. Proof of Theorem 14

We present the proof for the first estimates in (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 (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 1 we have:

$$d(f^{j} \circ (\Omega_{+}^{\Gamma})^{-1} \circ \sigma(x), f^{j} \circ \sigma(x)) \leq C\lambda^{j},$$
$$d(f^{-j} \circ (\Omega_{-}^{\Gamma})^{-1}(x), f^{-j}(x)) \leq C\lambda^{j}.$$

For higher derivatives the argument is more complicated.

We start by choosing a system of coordinates on a neighborhood  $\mathcal{U}$  of  $\Lambda$  in  $W^s_{\Lambda}$ . Similar choices are quite standard in [29].

We observe that we can identify  $\mathcal{U}$  with a neighborhood of the zero section of the stable bundle. More concretely, we associate to  $(x, \xi)$ , with  $x \in \Lambda, \xi \in E_x^s$ ,  $|\xi| \leq \delta$ , the point

$$\exp_x^{W_x^s}(\xi) \tag{33}$$

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  $\Lambda$  and that the map f is also uniformly differentiable in a neighborhood of  $\Lambda$ . These assumptions are automatic if  $\Lambda$  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 the zero section of  $E_{\Lambda}^s$  to its image in  $W_{\Lambda}^s$ , which is independent of x.

In this system of coordinates, the map f restricted to  $\mathcal{U}$  takes the form

$$(x,\xi) \mapsto \left(f_0(x), f_x(\xi)\right). \tag{34}$$

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  $\Lambda$  have  $\xi$  coordinate equal to zero and that the invariance of  $\Lambda$  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  $f_{f_0^{j-1}(x)} \circ \cdots \circ f_x(\xi) \equiv f_{x,j}(\xi)$ .

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

$$\left(\Omega_{+}^{\Gamma}\right)^{-1}(H_{+})\subset\mathcal{U}.$$

Indeed, by the  $\lambda$ -lemma, we have that for some finite J,  $\Gamma^{\pm j} = f^{\pm j}(\Gamma) \subset \mathcal{U}$ , for  $j \ge J$ . Then, we will obtain the estimate (30) for  $j \ge J$ . The desired result follows just changing the constant C.

In the system of coordinates  $(x, \xi)$ , we can write  $(\Omega_{+}^{\Gamma})^{-1}$  by

$$(x,0)\mapsto (x,\Phi(x)).$$

Hence, in this system of coordinates, the desired result, formula (30), is implied by estimates

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$$\left| D_x^k \Psi \left( f_0^j(x), f_{x,j} \left( \Phi(x) \right) \right) - D_x^k \Psi \left( f_0^j(x), 0 \right) \right| \leqslant C \|\Psi\|_{C^k} j^k \left( \tilde{\lambda} \tilde{\mu}^k \right)^j.$$
(35)

The main idea in the proof of (35) is that, if we apply the Faa Di Bruno formula for the derivatives in (35) we will obtain derivatives of highly iterated functions (except for one term). The derivatives of highly iterated functions will be estimated in Proposition 15 below. The remaining term will be estimated because it is the difference of two terms that have close arguments.

**Proposition 15.** With the notations above we have:

For  $n \ge 1$ :

$$\|D^{n}f_{0}^{j}(x)\|_{C^{0}(\Lambda)} \leq (n-1)!j^{n}(\tilde{\mu}^{n})^{j}.$$
(36)

For  $m \ge 1$ ,  $n \ge 0$ :

$$\left\| D_x^n D_{\xi}^m f_{x,j}(\xi) \right\|_{C^0(\mathcal{U})} \leqslant C_{n,m} j^{n+m} \left( \tilde{\lambda} \tilde{\mu}^{n+m} \right)^j \tag{37}$$

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 [21]. The dependence on parameters of the derivatives of highly iterated functions were considered in [2,9].

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  $1 \le i \le n, 0 \le k \le j$ . 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,

$$T_n \leqslant T_{n-1}F_{n-1},$$
  
$$F_n \leqslant F_{n-1} + j.$$

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 (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  $D_x^{\tilde{n}} D_{\xi}^{\tilde{m}} f_{f_{\tilde{j}}(x)}(\xi)$  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:

$$T_{n,m} \leqslant T_{n-1,m} F_{n-1,m}; \qquad T_{n,m} \leqslant T_{n,m-1} F_{n,m-1}; F_{n,m} \leqslant F_{n-1,m} + j; \qquad F_{n,m} \leqslant F_{n,m-1} + j.$$

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  $\xi$ ) 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  $\xi$  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 (37) by multiplying the upper bound for each of the terms by the upper bound on the number of terms.  $\Box$ 

The bound (35) is an easy consequence of Proposition 15.

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  $\Phi$  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

$$\left\| D_x^m f_{x,j} \left( \Phi(x) \right) \right\|_{C^0(\mathcal{U})} \leqslant C j^m \left( \tilde{\lambda} \tilde{\mu}^m \right)^j$$
(38)

where C depends on the  $C^m$  norm of  $\Phi$  and the combinatorial coefficients, but is independent of j.

Coming back to the proof of inequality (35), we compute the derivatives of the expression  $\Psi(f_0^j(x), f_{x,j}(\Phi(x)))$  and see that most of the terms that we obtain are already considered in Proposition 15 or in (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:

$$D_{x}\Psi(f_{0}^{j}(x), f_{x,j}(\Phi(x))) = (D_{1}\Psi)(f_{0}^{j}(x), f_{x,j}(\Phi(x)))D_{x}f_{0}^{j}(x) + (D_{2}\Psi)(f_{0}^{j}(x), f_{x,j}(\Phi(x)))D_{x}f_{x,j}(\Phi(x)).$$
(39)

The second term of (39) above is controlled in (38):

$$\left| (D_2 \Psi) \left( f_0^J(x), f_{x,j} \left( \Phi(x) \right) \right) D_x f_{x,j} \left( \Phi(x) \right) \right| \leq C \|\Psi\|_{C^1(\mathcal{U})} j(\tilde{\lambda} \tilde{\mu})^j.$$

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 15

$$\begin{split} \big| (D_{1}\Psi) \big( f_{0}^{j}(x), f_{x,j} \big( \Phi(x) \big) \big) D_{x} f_{0}^{j}(x) - (D_{1}\Psi) \big( f_{0}^{j}(x), 0 \big) D_{x} f_{0}^{j}(x) \big| \\ & \leq \|\Psi\|_{C^{2}(\mathcal{U})} \|f_{x,j} \circ \Phi\|_{C^{0}(\Lambda)} \|D_{x} f_{0}^{j}\|_{C^{0}(\mathcal{U})} \\ & \leq \|\Psi\|_{C^{2}(\mathcal{U})} (\tilde{\lambda}\tilde{\mu})^{j}. \end{split}$$

These last two bounds imply immediately inequality (35) for k = 1.

For higher derivatives, we note that all the derivatives of the second term in (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  $\Psi$  is not differentiated. The collection of these terms is of the form:

$$\sum_{k=i_1+\dots+i_k} C_{k,i_1,\dots,i_k} (D_1^{i_1} \Psi) (f_0^j(x), f_{x,j}(\Phi(x))) D_x^{i_2} f_0^j(x) \cdots D_x^{i_k} f_0^j(x).$$
(40)

The combinatorial coefficients  $C_{k,i_1,...,i_k}$  are the same coefficients that appear in the Faa Di Bruno expansion of  $D_x^k \Psi(f_0^j(x), 0)$ ). Namely,

$$D_{x}^{k}\Psi(f_{0}^{j}(x),0) = \sum_{k=i_{1}+\dots+i_{k}} C_{k,i_{1},\dots,i_{k}}(D_{1}^{i_{1}}\Psi)(f_{0}^{j}(x),0)D_{x}^{i_{2}}f_{0}^{j}(x)\cdots D_{x}^{i_{k}}f_{0}^{j}(x).$$

Therefore, we see that

$$D_{x}^{k}\Psi(f_{0}^{j}(x), f_{x,j}(\Phi(x))) - D_{x}^{k}\Psi(f_{0}^{j}(x), 0)$$

$$= \sum_{k=i_{1}+\dots+i_{k}} C_{k,i_{1},\dots,i_{k}}[(D_{1}^{i_{1}}\Psi)(f_{0}^{j}(x), f_{x,j}(\Phi(x))) - (D_{1}^{i_{1}}\Psi)(f_{0}^{j}(x), 0)]$$

$$\cdot D_{x}^{i_{2}}f_{0}^{j}(x)\cdots D_{x}^{i_{k}}f_{0}^{j}(x) + O(||\Psi||_{C^{k}(\mathcal{U})}j^{k}(\tilde{\lambda}\tilde{\mu}^{k})^{j}).$$

We can use the mean value theorem and (38) for m = 0, to obtain

$$\left| \left( D_1^{i_1} \Psi \right) \left( f_0^j(x), 0 \right) - \left( D_1^{i_1} \Psi \right) \left( f_0^j(x), f_{x,j} \left( \Phi(x) \right) \right) \right| \leq C \|\Psi\|_{C^{k+1}(\mathcal{U})} \tilde{\lambda}^j.$$

The other factors are bounded in Proposition 15.

# 4. A geometric framework for a perturbative calculation of the scattering map

In the applications in [22,25–27] the scattering map was computed perturbatively in several models.

The goal of this section is to present a geometrically natural setup for a perturbative calculation of the scattering map which will be carried out in the next section. As we will see, the final results

in Theorems 31 and 32 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  $\sigma_{\varepsilon}$  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.

#### 4.1. Deformation theory

Deformation theory was introduced in singularity theory [65] but soon was used in volume and symplectic geometry [3,51,67]. In [2,21] 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  $\omega_N$ ,  $\omega_M$  (respectively  $\omega_N = d\alpha_N$ ,  $\omega_M = d\alpha_M$ ).

Given a  $C^r$  family of one-to-one mappings

$$f_{\varepsilon}: N \to M$$

that is, the map  $(x, \varepsilon) \mapsto f_{\varepsilon}(x)$  is a  $\mathcal{C}^r$  map in all its arguments for  $r \ge 1$ , we can define vector fields  $\mathcal{F}_{\varepsilon}$  by

$$\frac{d}{d\varepsilon}f_{\varepsilon} = \mathcal{F}_{\varepsilon} \circ f_{\varepsilon}.$$
(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  $f_{\varepsilon}$  is  $C^r$ ,  $r \ge 1$ , 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 (41).

In what follows, we will assume that the regularity is high enough so that we can identify  $f_{\varepsilon}$  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  $f_{\varepsilon}$ . We will use the convention that, given a family denoted by italic letters  $f_{\varepsilon}$ , its generator will be denoted by the same letter in calligraphic capitals.

A perturbative calculation of the family  $f_{\varepsilon}$  will be for us a prescription to compute  $\mathcal{F}_{\varepsilon}$ .

**Remark 16.** 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 a strict submanifold of M of positive codimension it could well happen that  $f_{\varepsilon}(N) \cap f_{\varepsilon}(N) = \emptyset$  when  $\varepsilon \neq \varepsilon$ . 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 17.** If  $f_{\varepsilon}: N \to M$  and  $g_{\varepsilon}: M \to V$  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

$$\mathcal{H}_{\varepsilon} = \mathcal{G}_{\varepsilon} + (g_{\varepsilon})_* \mathcal{F}_{\varepsilon} \tag{42}$$

where  $(g_{\varepsilon})_*$  is the pushforward:

$$(g_{\varepsilon})_{*}\mathcal{F}_{\varepsilon} = Dg_{\varepsilon} \circ g_{\varepsilon}^{-1} \mathcal{F}_{\varepsilon} \circ g_{\varepsilon}^{-1} = (Dg_{\varepsilon}\mathcal{F}_{\varepsilon}) \circ g_{\varepsilon}^{-1}.$$
(43)

(2) If  $g_{\varepsilon} \circ f_{\varepsilon} = \text{Id then}$ 

$$\mathcal{G}_{\varepsilon} + (g_{\varepsilon})_* \mathcal{F}_{\varepsilon} = 0. \tag{44}$$

The proof of the first item of Proposition 17 is a simple computation. The second item is a consequence of (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 pushforward of vector fields (43) does not require that  $g_{\varepsilon}$  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  $f_{\varepsilon}$  is a smooth family of exact symplectic maps so is  $dP^{f_{\varepsilon}}$ . The primitive function  $P^{f_{\varepsilon}}$  is defined uniquely up to additive constants. We will assume that these constants are chosen in such a way that  $P^{f_{\varepsilon}}$  is also smooth.

To study the relations with geometry, we are interested in studying conditions on  $\mathcal{F}_{\varepsilon}$  that guarantee that  $f_{\varepsilon}$  remains symplectic (respectively exact symplectic) when  $f_0$  is.

**Proposition 18.** Let  $f_{\varepsilon}: N \to M$  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  $f_{\varepsilon}$  to be symplectic is:

$$di_{\mathcal{F}_{\varepsilon}}\omega_M \in \operatorname{Ker} f_{\varepsilon}^* \tag{45}$$

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  $f_{\varepsilon}$  to be exact symplectic is that there exists a family of functions  $\psi_{\varepsilon} : N \to M$  such that:

$$f_{\varepsilon}^{*}(i_{\mathcal{F}_{\varepsilon}}\omega_{M}) = d\psi_{\varepsilon}.$$
(46)

(3) In the case that f<sub>ε</sub> are diffeomorphisms, we have:
(a) If f<sub>0</sub> is symplectic, f<sub>ε</sub> is symplectic if and only if

$$di_{\mathcal{F}_s}\omega_M = 0. \tag{47}$$

(b) If f<sub>0</sub> is exact symplectic, f<sub>ε</sub> is exact symplectic if and only if there exists a family of functions F<sub>ε</sub>: M → ℝ such that:

$$i_{\mathcal{F}_{\varepsilon}}\omega_M = dF_{\varepsilon}.\tag{48}$$

**Proof.** If  $f_0$  is symplectic,  $f_{\varepsilon}$  is symplectic if and only if  $\frac{d}{d\varepsilon}f_{\varepsilon}^*\omega_M = 0$ . Using Cartan's magic formula, we rewrite

$$\frac{d}{d\varepsilon} f_{\varepsilon}^{*} \omega_{M} = f_{\varepsilon}^{*} [di_{\mathcal{F}_{\varepsilon}} \omega_{M} + i_{\mathcal{F}_{\varepsilon}} d\omega_{M}]$$
$$= f_{\varepsilon}^{*} [di_{\mathcal{F}_{\varepsilon}} \omega_{M}].$$

Hence,  $f_{\varepsilon}$  remains symplectic if and only if  $f_{\varepsilon}^*[di_{\mathcal{F}_{\varepsilon}}\omega_M] = 0$ , which is condition (45). In the case that  $f_{\varepsilon}$  is a diffeomorphism, the necessary and sufficient condition for  $f_{\varepsilon}$  to verify (45) is (47).

In the case that  $f_0$  is exact symplectic, proceeding as before and recalling the definition of the primitive of  $f_{\varepsilon}$  (17), we see that a necessary and sufficient condition for  $f_{\varepsilon}$  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 (46) with  $\psi_{\varepsilon} = \frac{d}{d\varepsilon} P^{f_{\varepsilon}} - f_{\varepsilon}^* i_{\mathcal{F}_{\varepsilon}} \alpha_M$ .

In the case that  $f_{\varepsilon}$  is a diffeomorphism, this is equivalent to (48), if we take

$$F_{\varepsilon} = (f_{\varepsilon})_* \left(\frac{d}{d\varepsilon} P^{f_{\varepsilon}}\right) - i_{\mathcal{F}_{\varepsilon}} \alpha_M. \qquad \Box$$
(49)

For exact symplectic deformations, we will refer to  $F_{\varepsilon}$  in (48) as the *Hamiltonian for*  $f_{\varepsilon}$  (note, however that it 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 (42) simplifies enormously in the case that the two families are exact and admit Hamiltonians.

**Proposition 19.** If  $f_{\varepsilon}: N \to M$  and  $g_{\varepsilon}: M \to V$  are exact symplectic diffeomorphisms generated by their Hamiltonians  $F_{\varepsilon}: M \to \mathbb{R}$  and  $G_{\varepsilon}: V \to \mathbb{R}$  respectively, then we have:

(1) If we define  $h_{\varepsilon} = g_{\varepsilon} \circ f_{\varepsilon}$ , its Hamiltonian  $H_{\varepsilon}$  is given by

$$H_{\varepsilon} = G_{\varepsilon} + F_{\varepsilon} \circ g_{\varepsilon}^{-1}.$$
<sup>(50)</sup>

(2) If  $g_{\varepsilon} \circ f_{\varepsilon} = \text{Id then}$ 

$$G_{\varepsilon} + F_{\varepsilon} \circ g_{\varepsilon}^{-1} = 0.$$
<sup>(51)</sup>

In the case of families of exact symplectic diffeomorphisms  $f_{\varepsilon}$ , sometimes will be useful to work with the primitive function of the family  $P^{f_{\varepsilon}}$ . The next Proposition 20 gives us the effect of the deformation on the primitive, and it is a direct consequence of (49).

**Proposition 20.** If  $f_{\varepsilon} : N \to M$  is a smooth family of exact symplectic diffeomorphisms generated by its Hamiltonian  $F_{\varepsilon} : M \to \mathbb{R}$  and  $P^{f_{\varepsilon}}$  is its primitive, then we have the following formula:

$$\frac{d}{d\varepsilon}P^{f_{\varepsilon}} = f_{\varepsilon}^{*}(\alpha_{M}\mathcal{F}_{\varepsilon} + F_{\varepsilon}) = f_{\varepsilon}^{*}(i_{\mathcal{F}_{\varepsilon}}\alpha_{M} + F_{\varepsilon}).$$
(52)

## 4.2. Perturbation theory of normally hyperbolic invariant manifolds

The perturbation theory for normally hyperbolic invariant manifolds is a very classical subject [29,41,56,60,68]. 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  $k_0 : N \to \Lambda$  is a diffeomorphism, then there is a  $C^1$  open set of maps that also possess a normally hyperbolic invariant manifold  $\Lambda^f$ . 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 the  $C^1$  neighborhood of  $f_0$ , one can find a diffeomorphism  $k: N \to \Lambda^f$  in such a way that

$$f \circ k = k \circ r \tag{53}$$

where  $k = N \rightarrow M, r : N \rightarrow N$ .

**Remark 21.** Note, however, that the solutions of (53) are far from unique. If k, r are solutions of (53) and  $h: N \to N$  is any diffeomorphism, we have

$$f \circ (k \circ h) = (k \circ h) \circ (h^{-1} \circ r \circ h)$$

so that

$$k = k \circ h,$$
  

$$\tilde{r} = h^{-1} \circ r \circ h$$
(54)

is also a solution of (53).

The idea is that k is a parameterization of the manifold  $\Lambda$ , 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 (53) can be obtained from a solution (k, r) by applying (54) with a conveniently chosen h.

**Remark 22.** The study of Eq. (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 (53). This method has several desirable properties. For example, it can be used to validate numerical calculations and it leads to efficient algorithms. See [39].

For the purposes of this paper, it is enough to point out that the classical persistence theory of normally hyperbolic invariant manifolds implies the existence of solutions of (53). Moreover, the use of (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

$$f \circ k^{s,u} = k^{s,u} \circ r^{s,u} \tag{55}$$

where  $k^{s,u}: E^{s,u} \to M$  and  $E^{s,u}$  is a bundle over  $N, r^{s,u}: E^{s,u} \to E^{s,u}$  is a bundle map and

$$k^{s,u}(\xi, 0) = k(\xi),$$
  

$$r^{s,u}(\xi, 0) = r(\xi),$$
  

$$D_2 k^{s,u}(\xi, 0) E^{s,u}_{\xi} = E^{s,u}_x$$

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 1.

The following is a reformulation of the classical results in the above language (see [29,41]).

**Theorem 23.** Let  $f_{\varepsilon}: M \to M$  be a  $C^r$  family of diffeomorphisms,  $r \ge 2$ . Assume that  $\Lambda \subset M$  is a normally hyperbolic invariant manifold for  $f_0$  with rates  $\lambda$ ,  $\mu$  as in Definition 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 (53), and  $C^{\ell-1}$  families  $k_{\varepsilon}^{s,u}, r_{\varepsilon}^{s,u}$  defined on the unit ball bundle, satisfying (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 23 are non-unique. We now proceed to fix a suitable ones.

If  $f_{\varepsilon}$ ,  $k_{\varepsilon}$ ,  $r_{\varepsilon}$  satisfy (53), taking derivatives with respect to  $\varepsilon$  we obtain that their generators (see Proposition 17) verify on  $k_{\varepsilon}(N) = \Lambda_{\varepsilon}$ ,

$$\mathcal{F}_{\varepsilon} + (f_{\varepsilon})_* \mathcal{K}_{\varepsilon} = \mathcal{K}_{\varepsilon} + (k_{\varepsilon})_* \mathcal{R}_{\varepsilon}$$
(56)

where

$$\mathcal{R}_{\varepsilon} : N \to TN,$$
  
$$\mathcal{F}_{\varepsilon} : M \to TM,$$
  
$$\mathcal{K}_{\varepsilon} : k_{\varepsilon}(N) = \Lambda_{\varepsilon} \to TM$$

If  $x \in \Lambda_{\varepsilon}$ , by Definition 1, we have that

$$T_x M = E_x^{s,\varepsilon} \oplus E_x^{u,\varepsilon} \oplus T_x \Lambda_{\varepsilon}.$$
(57)

If we define the projections  $\Pi_x^{s,\varepsilon}$ ,  $\Pi_x^{u,\varepsilon}$ ,  $\Pi_x^{c,\varepsilon}$  associated to (57), we will call

$$\mathcal{F}_{\varepsilon}^{\alpha}(x) = \Pi_{x}^{\alpha,\varepsilon} \mathcal{F}_{\varepsilon}(x), \qquad \mathcal{K}_{\varepsilon}^{\alpha}(x) = \Pi_{x}^{\alpha,\varepsilon} \mathcal{K}_{\varepsilon}(x)$$

for  $\alpha = s, u, c$ .

Due to the fact that (57) is invariant under  $f_{\varepsilon}$  we have that

$$\Pi^{\alpha,\varepsilon} \circ (f_{\varepsilon})_* = (f_{\varepsilon})_* \circ \Pi^{\alpha,\varepsilon}.$$

Writing (56) as

$$\mathcal{F}_{\varepsilon} = \mathcal{K}_{\varepsilon} - (f_{\varepsilon})_* \mathcal{K}_{\varepsilon} + (k_{\varepsilon})_* \mathcal{R}_{\varepsilon},$$

and taking projections over the splitting (57) we obtain that

$$\Pi^{\alpha,\varepsilon}\mathcal{F}_{\varepsilon} = \Pi^{\alpha,\varepsilon}\mathcal{K}_{\varepsilon} - \Pi^{\alpha,\varepsilon}(f_{\varepsilon})_{*}\mathcal{K}_{\varepsilon} + \Pi^{\alpha,\varepsilon}(k_{\varepsilon})_{*}\mathcal{R}_{\varepsilon}$$

for  $\alpha = s, u, c$ . Since  $(k_{\varepsilon})_* \mathcal{R}_{\varepsilon}$  is tangent to the invariant manifold  $\Lambda_{\varepsilon}$ , (56) is equivalent to

$$\mathcal{F}_{\varepsilon}^{s} = \mathcal{K}_{\varepsilon}^{s} - (f_{\varepsilon})_{*} \mathcal{K}_{\varepsilon}^{s},$$
  

$$\mathcal{F}_{\varepsilon}^{u} = \mathcal{K}_{\varepsilon}^{u} - (f_{\varepsilon})_{*} \mathcal{K}_{\varepsilon}^{u},$$
  

$$\mathcal{F}_{\varepsilon}^{c} = \mathcal{K}_{\varepsilon}^{c} - (f_{\varepsilon})_{*} \mathcal{K}_{\varepsilon}^{c} + (k_{\varepsilon})_{*} \mathcal{R}_{\varepsilon}.$$
(58)

We know that  $k_{\varepsilon}, r_{\varepsilon}$  are not unique. A particularly useful choice of them is the following.

**Theorem 24.** There exist unique  $k_{\varepsilon}$ ,  $r_{\varepsilon}$  such that

$$\mathcal{K}_{\varepsilon}^{c} = 0. \tag{59}$$

**Proof.** If we fix (59), then the solution of the third equation in (58) is clearly  $\mathcal{F}_{\varepsilon}^{c} = (k_{\varepsilon})_{*}\mathcal{R}_{\varepsilon}$ . The  $\mathcal{K}_{\varepsilon}^{s}$ ,  $\mathcal{K}_{\varepsilon}^{u}$  are determined uniquely by (58) because, by the definition of the invariant bundles, a sufficiently large power of  $f_{\varepsilon*}$  is a contraction on  $E_{\varepsilon}^{s}$  and a sufficiently large power of  $f_{\varepsilon*}^{-1}$  is a contraction on  $E_{\varepsilon}^{s}$ .  $\Box$ 

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 4.3 when we discuss symplectic properties, the normalization (59) is also natural from the symplectic point of view and leads to interesting symplectic consequences.

**Remark 25.** Equation (56) can be used as the basis of a formal perturbation expansion that can be carried out to high orders in  $\varepsilon$ .

If we assume that  $f_{\varepsilon}$ ,  $\mathcal{F}_{\varepsilon}$  can be expanded in powers of  $\varepsilon$ , we obtain after equating terms of order *n* in  $\varepsilon$ 

$$(f_0)_*\mathcal{K}^n - \mathcal{K}^n = \mathcal{F}^n + (k_0)_*\mathcal{R}^n + \mathcal{A}_n(\) \tag{60}$$

where  $\mathcal{A}_n$  is a polynomial expression involving  $\mathcal{K}_1, \ldots, \mathcal{K}_{n-1}, \mathcal{R}_1, \ldots, \mathcal{R}_{n-1}$  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 (1), and then Eq. (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 (60) can be carried out up to the order  $\ell - 1$  which appears as a limit of the regularity of the manifold in Theorem 23.

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 [22,25– 27,34,35]. In such a case, the dynamics by  $f_0$  on  $\Lambda$  has a simple expression and one can carry out the perturbation theory to all orders less or equal than r in  $\varepsilon$ . 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  $f_{\varepsilon}$  is analytic, the manifold  $\Lambda_{\varepsilon}$  is not  $C^{\infty}$  in  $\varepsilon$  and much less analytic.

### 4.3. Symplectic properties of normally hyperbolic invariant manifolds

In this section we study the effect of symplectic properties of  $f_{\varepsilon}$  on the manifold  $A_{\varepsilon}$ . Since the deformation method deals very well with geometric properties [2,3,45], we will obtain very simple formulas.

The main result of this section is:

**Theorem 26.** In the same conditions of Theorem 23, assume furthermore that

- (A) *M* is endowed with a symplectic form  $\omega$  (respectively  $\omega = d\alpha$  is an exact symplectic form) and  $\omega|_A$  is a symplectic form.
- (B)  $(f_{\varepsilon})_*\omega = \omega$  (respectively  $(f_{\varepsilon})_*\alpha = \alpha + dP^f$ ).

Let  $k_{\varepsilon}$ ,  $r_{\varepsilon}$  be as in Theorem 24, that is,  $\mathcal{K}_{\varepsilon}$  satisfies (59). Then:

- (1)  $k_{\varepsilon}^* \omega \equiv \omega_N$  is a symplectic form (respectively exact symplectic form) in N. It is independent of  $\varepsilon$ .
- (2) The vector field  $\mathcal{R}_{\varepsilon}$  is Hamiltonian (respectively exact Hamiltonian) with respect to  $\omega_N$ . Moreover, its local Hamiltonian (respectively global Hamiltonian) is

$$R_{\varepsilon} = F_{\varepsilon} \circ k_{\varepsilon} \tag{61}$$

where  $F_{\varepsilon}$  is a local Hamiltonian for  $f_{\varepsilon}$  (respectively a global Hamiltonian).

Formula (61) can be considered as a perturbative calculation of the map  $r_{\varepsilon}$  since it allows us to compute the Hamiltonian of  $\mathcal{R}_0 = \frac{dr_{\varepsilon}}{d\varepsilon}|_{\varepsilon=0} \circ r_0^{-1}$ , the derivative of the map  $r_{\varepsilon}$ , once we know the unperturbed manifold and  $\mathcal{F}_0 = \frac{df_{\varepsilon}}{d\varepsilon}|_{\varepsilon=0} \circ f_0^{-1}$ .

**Remark 27.** Note that the choice of the identification  $k_{\varepsilon}$  in such a way that it is symplectic from N to  $\Lambda_{\varepsilon}$  endowed with the restrictions of the global symplectic forms is a generalization of the constructions in Section 8.1 of [27]. There, as  $\Lambda = N$  and  $k_0$  was simply the trivial inclusion, the system of coordinates on  $\Lambda_{\varepsilon}$  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  $\omega$  is a 2-form on M invariant under  $f_{\varepsilon}$ , for every  $u, v \in T_x M$  and  $n \in \mathbb{Z}$  we have

$$\omega(x)(u,v) = \omega(f_{\varepsilon}^{n}(x))(Df_{\varepsilon}^{n}(x)u, Df_{\varepsilon}^{n}(x)v).$$
(62)

Applying repeatedly (62) and taking into account the different rates of growth in Definition 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

$$\begin{pmatrix} 0 & \omega^{su} & 0\\ \hline -\omega^{su} & 0 & 0\\ \hline 0 & 0 & \omega|_{E^c} \end{pmatrix}.$$
(63)

Since  $d\omega = 0$  (respectively  $\omega = d\alpha$ ) and  $\Lambda_{\varepsilon}$  is an invariant manifold for  $f_{\varepsilon}$  we obtain that  $d_{\Lambda_{\varepsilon}}\omega|_{\Lambda_{\varepsilon}} = 0$  where  $d_{\Lambda_{\varepsilon}}$  denotes the exterior differential in  $\Lambda_{\varepsilon}$  (respectively 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  $\Lambda_{\varepsilon}$  are symplectic.

Hence, we can define a symplectic form  $\omega_{\varepsilon,N}$  on N by

$$\omega_{\varepsilon,N} = k_{\varepsilon}^*(\omega|_{\Lambda_{\varepsilon}}). \tag{64}$$

Note that  $\omega_{\varepsilon,N}$  depends on  $k_{\varepsilon}$ , which is not uniquely determined. Nevertheless, we will not include the  $k_{\varepsilon}$  in the notation unless it can lead to confusion. In Lemma 28 we will show that if

 $k_{\varepsilon}$  is chosen to satisfy (59),  $\omega_{\varepsilon,N}$  is constant. This reinforces the notion that (59) is a very natural normalization to avoid the non-uniqueness in (53).

A consequence of (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

$$\omega_{\varepsilon,N} = r_{\varepsilon}^* \omega_{\varepsilon,N}. \tag{65}$$

In other words,  $r_{\varepsilon}$  is a symplectic map with respect to the form  $\omega_{\varepsilon,N}$ .

If  $\omega$  is exact and  $f_{\varepsilon}^*$  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  $\alpha_{\varepsilon,N} = k_{\varepsilon}^* \alpha$ ,

$$r_{\varepsilon}^* \alpha_{\varepsilon,N} = \alpha_{\varepsilon,N} + d_N \left( k_{\varepsilon}^* d P^{f_{\varepsilon}} \right) \tag{66}$$

so that  $r_{\varepsilon}^*$  is also exact symplectic.

The proof of  $R_{\varepsilon} = F_{\varepsilon} \circ k_{\varepsilon}$  is only a computation:

$$d(F_{\varepsilon} \circ k_{\varepsilon}) = k_{\varepsilon}^{*} dF_{\varepsilon} = k_{\varepsilon}^{*} (i_{\mathcal{F}_{\varepsilon}} \omega_{|\Lambda_{\varepsilon}})$$
  
$$= k_{\varepsilon}^{*} (i_{\mathcal{F}_{\varepsilon}^{c}} \omega_{|\Lambda_{\varepsilon}} + i_{\mathcal{F}_{\varepsilon}^{u}} \omega_{|\Lambda_{\varepsilon}} + i_{\mathcal{F}_{\varepsilon}^{s}} \omega_{|\Lambda_{\varepsilon}})$$
  
$$= k_{\varepsilon}^{*} (i_{\mathcal{F}_{\varepsilon}^{c}} \omega_{|\Lambda_{\varepsilon}}) = i_{k_{\varepsilon}^{*}} \mathcal{F}_{\varepsilon}^{c} k_{\varepsilon}^{*} \omega_{|\Lambda_{\varepsilon}} = i_{\mathcal{R}_{\varepsilon}} \omega_{\varepsilon,N}.$$

The only thing remaining to obtain Theorem 26 is the following:

**Lemma 28.** With the notations above, if we choose  $k_{\varepsilon}$  satisfying (59) as in Theorem 24, we have that  $\omega_{\varepsilon,N}$  is independent of  $\varepsilon$ , that is

$$\omega_{\varepsilon,N} = \omega_{0,N}.$$

**Proof.** We compute  $\frac{d}{d\varepsilon}\omega_{\varepsilon,N}$  using Cartan's "magic" formula

$$\begin{aligned} \frac{d}{d\varepsilon}\omega_{\varepsilon,N} &= \frac{d}{d\varepsilon}k_{\varepsilon}^{*}\omega\\ &= k_{\varepsilon}^{*}(i_{\mathcal{K}_{\varepsilon}}\,d\omega + di_{\mathcal{K}_{\varepsilon}}\omega)\\ &= k_{\varepsilon}^{*}\,di_{\mathcal{K}_{\varepsilon}}\omega\\ &= d_{N}k_{\varepsilon}^{*}i_{\mathcal{K}_{\varepsilon}}\omega. \end{aligned}$$

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  $v \in T_x N$  is defined by

$$\big(k_{\varepsilon}^* i_{\mathcal{K}_{\varepsilon}} \omega(x)\big) v = i_{\mathcal{K}_{\varepsilon}} \omega\big(k_{\varepsilon}(x)\big) \big(dk_{\varepsilon}(x)v\big) = \omega\big(k_{\varepsilon}(x)\big) \big(\mathcal{K}_{\varepsilon}\big(k_{\varepsilon}(x)\big), dk_{\varepsilon}(x)v\big).$$

Now, we observe that, by (59)

$$\mathcal{K}_{\varepsilon} \circ (k_{\varepsilon}(x)) \in E^{s}_{k_{\varepsilon}(x)} \oplus E^{u}_{k_{\varepsilon}(x)}$$

whereas

$$dk_{\varepsilon}(x) \in E_{k_{\varepsilon}(x)}^{c}$$
.

By (63) we obtain the desired result and, hence concludes the proof of Theorem 26.  $\Box$ 

# 5. Perturbative formulas for the scattering map

In this section we are going to study a  $C^r$  family of symplectic diffeomorphisms  $f_{\varepsilon} : M \to M$ , where  $f_0$  has a normally hyperbolic invariant manifold  $\Lambda$  such that  $\omega_{|\Lambda}$  is non-degenerate and has also a homoclinic channel  $\Gamma$  verifying Definition 3, so that, there exists a scattering map  $\sigma_0 = \sigma^{\Gamma} : H^- \to H^+$  as in (10).

Then, if  $\varepsilon$  is small enough, the theory of normally hyperbolic invariant manifolds (see Theorem 23) and the persistence of conditions (5), (6) ensures that there exist a normally hyperbolic invariant manifold  $\Lambda_{\varepsilon}$  and a homoclinic channel  $\Gamma_{\varepsilon}$  and then it is possible to consider the scattering map  $\sigma_{\varepsilon} := \sigma_{\varepsilon}^{\Gamma_{\varepsilon}} : H_{\varepsilon}^{-} \to H_{\varepsilon}^{+}$  defined in some domain  $H_{\varepsilon}^{-} \subset \Lambda_{\varepsilon}$  close to  $H^{-}$ .

**Remark 29.** Note that, from Definition 3, 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  $\Gamma$ .

A situation that has been considered very often in the literature is a family of maps indexed by  $\varepsilon$  such that for  $\varepsilon = 0$  the stable and unstable manifolds of  $\Lambda$  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 [27] it is shown that, under appropriate conditions, for  $0 < |\varepsilon| \ll 1$ , one can find transversal intersections along a manifold  $\Gamma_{\varepsilon}$ . Furthermore, it is possible to show that the manifold  $\Gamma_{\varepsilon}$  extends smoothly in  $\varepsilon$  across  $\varepsilon = 0$ . Another method is in [35]. In this case, it also follows that the scattering map extends also smoothly across  $\varepsilon = 0$ .

Of course, the limiting manifold  $\Gamma_0$  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  $\varepsilon$ .

By Theorem 8, the scattering map  $\sigma_{\varepsilon}$  defined in (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  $\sigma_{\varepsilon}$  is contained in  $\Lambda_{\varepsilon}$ . Since  $\Lambda_{\varepsilon}$  is a submanifold of positive codimension, it could happen that  $\Lambda_{\varepsilon}$  is disjoint from  $\Lambda_{\varepsilon'}$  when  $\varepsilon \neq \varepsilon'$ , hence there is no common domain for all  $\sigma_{\varepsilon}$ , 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 Theorems 24 and 26 that there is a unique symplectic parameterization  $k_{\varepsilon}$  between the reference manifold N and the normally hyperbolic invariant manifold  $\Lambda_{\varepsilon}$ . So, we consider

$$s_{\varepsilon} = k_{\varepsilon}^{-1} \circ \sigma_{\varepsilon} \circ k_{\varepsilon} : (k_{\varepsilon})^{-1} (H_{\varepsilon}^{-}) \subset N \to (k_{\varepsilon})^{-1} (H_{\varepsilon}^{+}) \subset N.$$

Hence, our goal in this section is to give formulas for the Hamiltonian function  $S_{\varepsilon}$  which generates the deformation  $S_{\varepsilon}$  of the scattering map  $s_{\varepsilon}$ .

The main result of this section is Theorem 31, which contains formula (67) which expresses the Hamiltonian  $S_{\varepsilon}$  of the deformation of the scattering map  $s_{\varepsilon}$  in terms of the orbit appearing in the connection, and the Hamiltonian  $F_{\varepsilon}$  of the change of the map  $f_{\varepsilon}$ . We note that the formula and the calculation leading to it are coordinate independent.

In Section 5.2 we derive formula (72) which expresses the primitive  $P^{s_{\varepsilon}}$  of the deformation of the scattering map  $s_{\varepsilon}$  in terms of the primitive  $P^{f_{\varepsilon}}$  of the change of the map in the case that  $f_{\varepsilon}$  is exact symplectic.

An analogous result to Theorem 31 for the case of Hamiltonian flows is provided in Theorem 32. The proofs of Theorems 31 and 32 are given respectively in Sections 5.1 and 5.3, and some heuristic considerations relating the proofs of Theorems 31 and 12 are given in Section 5.4.

**Remark 30.** From the point of view of applications it is very natural to study the Hamiltonian  $S_{\varepsilon}$ . In [22,25–27] 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  $s_{\varepsilon}$ . 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 26 we computed the Hamiltonian  $R_{\varepsilon}$  for  $r_{\varepsilon}$  so that, the combination of formula (61) for  $R_{\varepsilon}$  and formula (67) for  $S_{\varepsilon}$  will provide the desired comparison. In the above papers one can find calculations up to first order in  $\varepsilon$  which agree with the ones presented here. See Section 6 for a detailed comparison in the case of geodesic flows.

The main result of this section is

**Theorem 31.** Let  $f_{\varepsilon}: M \to M$  be a  $C^{r}$  family of symplectic diffeomorphisms where  $f_{0}$  has a normally hyperbolic invariant manifold  $\Lambda$  such that  $\omega_{|\Lambda}$  is non-degenerate and also has a homoclinic channel  $\Gamma$  verifying Definition 3, so that there exists a scattering map  $\sigma_{0} = \sigma^{\Gamma}: H^{-} \to H^{+}$  as in (10).

Assume also that the parameterization  $k_{\varepsilon}$  of the perturbed normally hyperbolic invariant manifold  $\Lambda_{\varepsilon}$  verifies (59), and denote  $s_{\varepsilon} = k_{\varepsilon}^{-1} \circ \sigma_{\varepsilon} \circ k_{\varepsilon}$ , where  $\sigma_{\varepsilon}$  is the perturbed scattering map associated to the perturbed homoclinic channel  $\Gamma_{\varepsilon}$ . Then, denoting  $\Gamma_{\varepsilon}^{N} = f_{\varepsilon}^{N}(\Gamma_{\varepsilon})$ , the Hamiltonian for  $s_{\varepsilon}$  is given by

$$S_{\varepsilon} = \lim_{N_{\pm} \to +\infty} \sum_{j=0}^{N_{-}-1} F_{\varepsilon} \circ f_{\varepsilon}^{-j} \circ (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}})^{-1} \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ f_{\varepsilon}^{-j} \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon}$$
$$+ \sum_{j=1}^{N_{+}} F_{\varepsilon} \circ f_{\varepsilon}^{j} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ f_{\varepsilon}^{j} \circ k_{\varepsilon}$$
$$= \lim_{N_{\pm} \to +\infty} \sum_{j=0}^{N_{-}-1} F_{\varepsilon} \circ f_{\varepsilon}^{-j} \circ (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} \circ s_{\varepsilon}^{-1} - F_{\varepsilon} \circ k_{\varepsilon} \circ r_{\varepsilon}^{-j} \circ s_{\varepsilon}^{-1}$$
$$+ \sum_{j=1}^{N_{+}} F_{\varepsilon} \circ f_{\varepsilon}^{j} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ k_{\varepsilon} \circ r_{\varepsilon}^{j}.$$
(67)

In the case that our family of maps  $f_{\varepsilon}$  correspond to the time T flow of a Hamiltonian vector field  $\mathcal{H}_{\varepsilon}$  of Hamiltonian  $H_{\varepsilon}$  we can adapt the previous result to obtain a formula for the Hamiltonian  $S_{\varepsilon}$  of the scattering map  $s_{\varepsilon} = s^{\Gamma, \mathcal{H}_{\varepsilon}}$ , that was shown in (15) that is independent of T.

Concretely, we have the following

**Theorem 32.** 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  $\Lambda_{\varepsilon}$  and that its parameterization verifies (59). Denoting by  $S_{\varepsilon}$  the Hamiltonian generating the deformation of  $s_{\varepsilon}$ , it is given by

$$S_{\varepsilon} = \lim_{T_{\pm} \to \infty} \int_{-T_{-}}^{0} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ \left(\Omega_{\varepsilon^{-}}^{\Gamma_{\varepsilon}}\right)^{-1} \circ (\sigma_{\varepsilon})^{-1} \circ k_{\varepsilon} - \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ (\sigma_{\varepsilon})^{-1} \circ k_{\varepsilon} + \int_{0}^{T_{+}} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ (\sigma_{\varepsilon})^{-1} \circ k_{\varepsilon} - \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \circ k_{\varepsilon}.$$
(68)

**Remark 33.** We call attention to the similarities between the formulas (67) and (68) and the formulas (28) and (29). In Appendix A, 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 5.4.

It is important to note that the sums and the integrals in (67) and (68) converge uniformly together with several of their derivatives. The argument, which is given in Theorem 14, is the same as in the discussion of Theorem 12.

Formula (67) is closely related to the following formula, which is true for any  $N_-, N_+ \in \mathbb{N}$ :

$$s_{\varepsilon} = k_{\varepsilon}^{-1} \circ f_{\varepsilon}^{-N_{+}} \circ \Omega_{\varepsilon+}^{\Gamma_{\varepsilon}^{N_{+}}} \circ f_{\varepsilon}^{N_{+}+N_{-}} (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}^{-N_{-}}})^{-1} \circ f_{\varepsilon}^{-N_{-}} \circ k_{\varepsilon}.$$

$$(69)$$

The formula (69) is a direct consequence of the formula (31).

Formulas (67) and (68) are analogous to formula (A.3) in quantum mechanics in Appendix A.

## 5.1. Proof of Theorem 31

The proof will be based on studying (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  $\Gamma_{\varepsilon}$  and then, their domains depend on  $\varepsilon$ .

As it turns out, it is possible to introduce identification maps for all the  $\Gamma_{\varepsilon}^{n}$  with  $\Gamma_{0}^{n}$ , so that the calculation can be referred to the  $\Gamma_{0}^{n}$ '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  $\varepsilon$ . This will allow us to consider the maps in (69) as defined in open sets of the whole manifold M and not only in  $\Gamma_{\varepsilon}^n$ . Then, applying Proposition 19 we will obtain a formula for finite  $N_{\pm}$ . When we take limits as  $N_{\pm} \to \infty$ , we will obtain the desired formula (67). In particular, the terms corresponding to the wave operators  $\Omega_{\varepsilon\pm}^{\Gamma_{\varepsilon}^n}$  will disappear in the limit as  $N_{\pm} \to \infty$ .

We start the proof by establishing a technical extension result that we will use to extend  $\Omega_{\epsilon\pm}^{\Gamma_{\epsilon}}$ .

Recall that, by the  $\lambda$ -lemma, the manifolds  $\Gamma_{\varepsilon}^{n}$  are getting  $C^{\ell-1}$  close to  $\Lambda_{\varepsilon}$  when  $n \to \pm \infty$ . 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  $\rho$  centered at any  $x \in N$ .

We denote  $N_{\rho} = \{y \in M \mid \text{dist}(y, N) < \rho\}.$ 

**Proposition 34.** Let  $(M, \omega)$  be a symplectic manifold. Let N,  $\Gamma_{\varepsilon}^{n} \subset M$  be symplectic submanifolds. Assume that:

- (a) There exist  $C^r$  families of maps  $h_{\varepsilon}^n : N \to \Gamma_{\varepsilon}^n$  such that  $\|h_{\varepsilon}^n\|_{C^r(N)} \leq \delta$ . (The  $C^r$ -norm is understood in all the variables including  $\varepsilon$ .)
- (b)  $h_{\varepsilon}^{n}$  are symplectic from N to  $\Gamma_{\varepsilon}^{n}$ .
- (c)  $\|\partial_{\varepsilon}h_{\varepsilon}^{n}\|_{C^{r-1}(N)} \to 0$ , when  $n \to \infty$  (as  $n \to -\infty$ ).

Then, it is possible to find  $\hat{h}^n_{\varepsilon} : \hat{N}_{\rho} \to M$  such that:

- (i)  $\hat{h}^n_{\varepsilon}|_N = h^n_{\varepsilon}$ ,
- (ii)  $\|\hat{h}_{\varepsilon}^{n}\|_{C^{r}(\hat{N}_{\varepsilon})} \leq 2\delta$ ,
- (iii)  $\|\partial_{\varepsilon}\hat{h}^{n}_{\varepsilon}\|_{C^{r-1}(\hat{N}_{o})} \to 0$ , when  $n \to \infty$  (or  $n \to -\infty$ ),
- (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  $h_{\varepsilon}^n$  to some families  $\tilde{h}_{\varepsilon}^n$  satisfying (i)–(iii) using e.g. the identifications given by the exponential mapping and the Levi-Civita connection

$$\tilde{h}^n_{\varepsilon}(\exp_x(v)) = \exp_{h^n_{\varepsilon}(x)}(\tilde{v})$$

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

$$\left\|\left(\tilde{h}_{\varepsilon}^{n}\right)^{*}\omega-\omega\right\|_{C^{\ell-2}(\hat{N}_{\rho})}=\mathcal{O}(\rho).$$

Now, we can apply the global Darboux theorem with dependence on parameters [2] to find families of diffeomorphisms  $g_{\varepsilon}^{n}$  such that

$$(g_{\varepsilon}^{n})_{*}(\tilde{h}_{\varepsilon}^{n})_{*}\omega = \omega.$$

The desired diffeomorphism is  $\hat{h}_{\varepsilon}^{n} = g_{\varepsilon}^{n} \circ \tilde{h}_{\varepsilon}^{n}$ .  $\Box$ 

Denoting  $h_{\varepsilon\pm}^n = (\Omega_{\varepsilon\pm}^{\Gamma_{\varepsilon}^n})^{-1} \circ k_{\varepsilon}$  we know, by Lemma 9, Theorem 26 and the  $\lambda$ -lemma applied to the normally hyperbolic invariant manifold  $\Lambda_{\varepsilon}$ , that the diffeomorphisms  $h_{\varepsilon,\pm}^n$  verify the hypotheses of Proposition 34. Therefore, we obtain extensions  $\hat{h}_{\varepsilon\pm}^n$  and  $(\hat{h}_{\varepsilon\pm}^n)^{-1}$  of their inverses.

Using this notation and (54), formula (69) reads:

$$\begin{split} s_{\varepsilon} &= r_{\varepsilon}^{-N_{+}} \circ (k_{\varepsilon})^{-1} \circ \Omega_{\varepsilon+}^{r_{\varepsilon}^{N_{+}}} \circ f_{\varepsilon}^{N_{+}+N_{-}} \big( \Omega_{\varepsilon-}^{r_{\varepsilon}^{-N_{-}}} \big)^{-1} \circ k_{\varepsilon} \circ r_{\varepsilon}^{-N_{-}} \\ &= r_{\varepsilon}^{-N_{+}} \circ \big( h_{\varepsilon+}^{N_{+}} \big)^{-1} \circ f_{\varepsilon}^{N_{+}+N_{-}} h_{\varepsilon-}^{-N_{-}} \circ r_{\varepsilon}^{-N_{-}}. \end{split}$$

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  $s_{\varepsilon}: N \to N$  defined by

$$s_{\varepsilon} = r_{\varepsilon}^{-N_{+}} \circ \left(\hat{h}_{\varepsilon+}^{N_{+}}\right)^{-1} \circ f_{\varepsilon}^{N_{+}+N_{-}} \circ \hat{h}_{\varepsilon-}^{-N_{-}} \circ r_{\varepsilon}^{-N_{-}}.$$
(70)

Applying repeatedly Proposition 19 to formula (70), we obtain that the Hamiltonian of  $s_{\varepsilon}$  is

$$S_{\varepsilon} = -(R_{\varepsilon} \circ r_{\varepsilon}^{N_{+}} + \dots + R_{\varepsilon} \circ r_{\varepsilon}) - H_{\varepsilon+}^{N_{+}} \circ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}} + (F_{\varepsilon} + F_{\varepsilon} \circ f_{\varepsilon}^{-1} + \dots + F_{\varepsilon} \circ f_{\varepsilon}^{-N_{+}-N_{-}+1}) \circ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}} + H_{\varepsilon-}^{-N_{-}} \circ f_{\varepsilon}^{-N_{-}-N_{+}} \circ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}} - (R_{\varepsilon} \circ r_{\varepsilon}^{N_{-}} + \dots + R_{\varepsilon} \circ r_{\varepsilon}) \circ (\hat{h}_{\varepsilon-}^{-N_{-}})^{-1} \circ f_{\varepsilon}^{-N_{-}-N_{+}} \circ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}}.$$

As the parameterization for the invariant manifold verifies normalization (59), we know that the Hamiltonian of the restricted map  $r_{\varepsilon}$  is given in formula (61) by  $R_{\varepsilon} = F_{\varepsilon} \circ k_{\varepsilon}$ . Since  $S_{\varepsilon}$  is defined in *N*, we have that  $\hat{h}_{\varepsilon\pm}^n = h_{\varepsilon\pm}^n = (\Omega_{\varepsilon\pm}^{\Gamma_{\varepsilon}^n})^{-1} \circ k_{\varepsilon}$ , and using also formula (9) for the wave operators  $\Omega_{\varepsilon\pm}^{\Gamma_{\varepsilon}^n}$  and (54), we can easily obtain that

$$\begin{aligned} R_{\varepsilon} \circ r_{\varepsilon}^{n} &= F_{\varepsilon} \circ k_{\varepsilon} \circ r_{\varepsilon}^{n} = F_{\varepsilon} \circ f_{\varepsilon}^{n} \circ k_{\varepsilon}, \\ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}} &= \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}^{N_{+}}}\right)^{-1} \circ k_{\varepsilon} \circ r_{\varepsilon}^{N_{+}} = \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}^{N_{+}}}\right)^{-1} \circ f_{\varepsilon}^{N_{+}} \circ k_{\varepsilon} \\ &= f_{\varepsilon}^{N_{+}} \circ \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}}\right)^{-1} \circ k_{\varepsilon}, \end{aligned}$$

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$$\begin{split} f_{\varepsilon}^{-N_{-}-N_{+}} \circ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}} &= f_{\varepsilon}^{-N_{-}-N_{+}} \circ f_{\varepsilon}^{N_{+}} \circ \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}}\right)^{-1} \circ k_{\varepsilon} \\ &= f_{\varepsilon}^{-N_{-}} \circ \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}}\right)^{-1} \circ k_{\varepsilon}, \\ \left(\hat{h}_{\varepsilon-}^{-N_{-}}\right)^{-1} \circ f_{\varepsilon}^{-N_{-}-N_{+}} \circ \hat{h}_{\varepsilon+}^{N_{+}} \circ r_{\varepsilon}^{N_{+}} &= k_{\varepsilon}^{-1} \circ \Omega_{\varepsilon-}^{\Gamma_{\varepsilon}^{-N_{-}}} \circ f_{\varepsilon}^{-N_{-}} \circ \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}}\right)^{-1} \circ k_{\varepsilon} \\ &= (k_{\varepsilon})^{-1} \circ f_{\varepsilon}^{-N_{-}} \circ \Omega_{\varepsilon-}^{\Gamma_{\varepsilon}} \circ \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}}\right)^{-1} \circ k_{\varepsilon} \\ &= (k_{\varepsilon})^{-1} \circ f_{\varepsilon}^{-N_{-}} \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon}. \end{split}$$

And we obtain the following formula, for any  $N_{\pm}$ 

$$\begin{split} S_{\varepsilon} &= \sum_{j=1}^{N_{+}} F_{\varepsilon} \circ f_{\varepsilon}^{j} \circ \left( \Omega_{\varepsilon+}^{\Gamma_{\varepsilon}} \right)^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ f_{\varepsilon}^{j} \circ k_{\varepsilon} \\ &+ \sum_{j=0}^{N_{-}-1} F_{\varepsilon} \circ f_{\varepsilon}^{-j} \circ \left( \Omega_{\varepsilon-}^{\Gamma_{\varepsilon}} \right)^{-1} \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon} - F_{\varepsilon} \circ f_{\varepsilon}^{j} \circ \sigma_{\varepsilon}^{-1} \circ k_{\varepsilon} \\ &- H_{\varepsilon+}^{N_{+}} \circ f_{\varepsilon}^{N_{+}} \circ \left( \Omega_{\varepsilon+}^{\Gamma_{\varepsilon}} \right)^{-1} \circ k_{\varepsilon} + H_{\varepsilon-}^{-N_{-}} \circ f_{\varepsilon}^{-N_{-}} \circ \left( \Omega_{\varepsilon+}^{\Gamma_{\varepsilon}} \right)^{-1} \circ k_{\varepsilon}. \end{split}$$

Now we observe that, by property (iii) in Proposition 34, 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  $N_{\pm} \to \infty$  we obtain the desired formula (67).

The second expression for the Hamiltonian in formula (67) is a simple consequence of the fact that  $\sigma_{\varepsilon} \circ k_{\varepsilon} = k_{\varepsilon} \circ s_{\varepsilon}$  and that  $f_{\varepsilon} \circ k_{\varepsilon} = k_{\varepsilon} \circ r_{\varepsilon}$ .

## 5.2. The primitive function of the scattering map $s_{\varepsilon}$

In Theorems 12 and 13 we have obtained formulas for the primitive  $P^{\sigma}$  of a scattering map  $\sigma$  on a normally hyperbolic invariant manifold for an 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 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 [27] 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  $s_{\varepsilon}$ , which is the expression of the scattering map in the reference manifold.

The primitive function of the inner map  $r_{\varepsilon}$  is very easy from the properties of restriction. Recall that, since  $k_{\varepsilon}^* \alpha_{\Lambda_{\varepsilon}} = \alpha_N$  (see Theorem 26), we have that  $P^{k_{\varepsilon}} = 0$ . Therefore, using the formula (25) for the primitive of compositions, we have:

$$P^{r_{\varepsilon}} = P^{f_{\varepsilon}} \circ k_{\varepsilon}. \tag{71}$$

Proceeding as in Theorems 12 and 13 we obtain the primitive for  $s_{\varepsilon}$ , using (70) instead of (31). This gives, in the case of families of maps  $f_{\varepsilon}$ :

$$P^{s_{\varepsilon}} = \lim_{N_{\pm} \to \infty} \sum_{j=0}^{N_{\pm}-1} P^{f_{\varepsilon}} \circ f_{\varepsilon}^{j} \circ \left(\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}}\right)^{-1} \circ s_{\varepsilon} \circ k_{\varepsilon} - P^{f_{\varepsilon}} \circ f_{\varepsilon}^{j} \circ s_{\varepsilon} \circ k_{\varepsilon}$$
$$+ \sum_{j=1}^{N_{\pm}} P^{f_{\varepsilon}} \circ f_{\varepsilon}^{-j} \circ \left(\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}}\right)^{-1} \circ k_{\varepsilon} - P^{f_{\varepsilon}} \circ f_{\varepsilon}^{-j} \circ k_{\varepsilon}$$
(72)

and in the case of a family of flows  $\Phi_{t,\varepsilon}$ :

$$P^{s_{\varepsilon}} = \lim_{T_{\pm} \to \infty} \int_{-T_{-}}^{0} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ (\Omega_{-\varepsilon}^{\Gamma_{\varepsilon}})^{-1} \circ k_{\varepsilon} - (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ k_{\varepsilon}$$
$$+ \int_{0}^{T_{+}} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}})^{-1} \circ s_{\varepsilon} \circ k_{\varepsilon} - (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon}) \circ \Phi_{t,\varepsilon} \circ s_{\varepsilon} \circ k_{\varepsilon}.$$
(73)

There are two ways to obtain the derivative of the primitive  $P^{s_{\varepsilon}}$  with respect to  $\varepsilon$ . We can differentiate this formula (73) with respect to  $\varepsilon$  or we can apply Proposition 20 to  $s_{\varepsilon}$  to obtain the derivative of its primitive in terms of its Hamiltonian  $S_{\varepsilon}$  given in Theorem 32. Of course, both calculations 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 3.4.3) tells us that this second term vanishes. So that, for instance, in the case of flows, one obtains:

$$\left(\frac{d}{d\varepsilon}P^{s_{\varepsilon}}\right)_{|\varepsilon=0} = \lim_{T_{\pm}\to\infty} \int_{-T_{-}}^{0} \frac{d}{d\varepsilon} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon})_{|\varepsilon=0} \circ \Phi_{t,0} \circ \left(\Omega_{-}^{\Gamma}\right)^{-1} \circ k_{0}$$
$$- \frac{d}{d\varepsilon} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon})_{|\varepsilon=0} \circ \Phi_{t,0} \circ k_{0}$$
$$+ \int_{0}^{T_{+}} \frac{d}{d\varepsilon} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon})_{|\varepsilon=0} \circ \Phi_{t,0} \circ \left(\Omega_{+}^{\Gamma}\right)^{-1} \circ s_{0} \circ k_{0}$$
$$- \frac{d}{d\varepsilon} (\alpha \mathcal{H}_{\varepsilon} + H_{\varepsilon})_{|\varepsilon=0} \circ \Phi_{t,0} \circ s_{0} \circ k_{0}.$$
(74)

## 5.3. The case of flows: proof of Theorem 32

In this section we adapt formula (67) for the case of flows. First, we need to know the Hamiltonian  $F_{\varepsilon}$  of the deformation in the case that our family  $f_{\varepsilon}$  corresponds to the time T flow of a Hamiltonian vector field  $\mathcal{H}_{\varepsilon}$  of Hamiltonian  $H_{\varepsilon}$ . Concretely, we have the following

**Proposition 35.** 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

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$$F_{T,\varepsilon} = \int_{0}^{T} \frac{d}{d\varepsilon} H_{\varepsilon} \circ \Phi_{s-T,\varepsilon} \, ds.$$
(75)

**Proof.** We start from the consideration that the flow  $\Phi_{t,\varepsilon}$  verifies the corresponding differential equation

$$\frac{d}{dt}\Phi_{t,\varepsilon} = \mathcal{H}_{\varepsilon} \circ \Phi_{t,\varepsilon},$$
$$\Phi_{0,\varepsilon} = \mathrm{Id}.$$

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  $\varepsilon$  and D the derivative with respect to x. So, we have the variational equations:

$$\frac{d}{dt}\dot{\Phi}_{t,\varepsilon} = (D\mathcal{H}_{\varepsilon} \circ \Phi_{t,\varepsilon})\dot{\Phi}_{t,\varepsilon} + \dot{\mathcal{H}}_{\varepsilon} \circ \Phi_{t,\varepsilon},$$
$$\frac{d}{dt}D\Phi_{t,\varepsilon} = (D\mathcal{H}_{\varepsilon} \circ \Phi_{t,\varepsilon})D\Phi_{t,\varepsilon}.$$

The proof of (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  $\omega$ . Using the linearity of the contraction and that  $i_{\mathcal{H}_{\varepsilon}}\omega = dH_{\varepsilon}$ , we have

$$i_{\int_{0}^{t} (\Phi_{t-s,\varepsilon})_{*} \dot{\mathcal{H}}_{\varepsilon} \, ds} \omega = \int_{0}^{t} i_{(\Phi_{t-s,\varepsilon})_{*} \dot{\mathcal{H}}_{\varepsilon}} \omega \, ds = \int_{0}^{t} (\Phi_{t-s,\varepsilon})_{*} i_{\dot{\mathcal{H}}_{\varepsilon}} \omega \, ds$$
$$= \int_{0}^{t} (\Phi_{t-s,\varepsilon})_{*} \, d\dot{H}_{\varepsilon} \, ds = d \int_{0}^{t} (\Phi_{t-s,\varepsilon})_{*} \dot{H}_{\varepsilon} \, ds$$
$$= d \int_{0}^{t} \dot{H}_{\varepsilon} \circ \Phi_{s-t,\varepsilon} \, ds. \qquad \Box$$

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 2.4.1 that is independent of T. We compute the Hamiltonian  $S_{\varepsilon}$  of its deformation simply by "translating" formula (67) for this case and using the following facts:

$$F_{T,\varepsilon} \circ \Phi_{jT,\varepsilon} = \int_{0}^{T} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{s-T,\varepsilon} \circ \Phi_{jT,\varepsilon} \, ds = \int_{(j-1)T}^{jT} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \, du,$$

$$F_{T,\varepsilon} \circ \Phi_{-jT,\varepsilon} = \int_{0}^{T} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{s-T,\varepsilon} \circ \Phi_{-jT,\varepsilon} \, ds = \int_{-(j+1)T}^{-jT} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \, du,$$

$$\sum_{j=0}^{N_{-}-1} F_{T,\varepsilon} \circ \Phi_{-jT,\varepsilon} = \int_{0}^{0} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \, ds,$$

$$\sum_{j=1}^{N_{+}} F_{T,\varepsilon} \circ \Phi_{jT,\varepsilon} = \int_{0}^{TN_{+}} \frac{dH_{\varepsilon}}{d\varepsilon} \circ \Phi_{u,\varepsilon} \, ds.$$

With these expressions one easily obtains formula (68).

## 5.4. Heuristic considerations about the proof of Theorems 31 and 12

We think that it is quite remarkable that the formulas derived in Theorems 31 and 12 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 [23,24,28,46,59,66], and for the other quantities appearing in variational calculus [48]. In Appendix A 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  $\Lambda_{\varepsilon}$ , a second one going forward  $N_{-} + N_{+}$  units of time along the homoclinic trajectory in  $\Gamma_{\varepsilon}$  and a third orbit going backwards  $N_{+}$  units of time along the manifold  $\Lambda_{\varepsilon}$ .

The following heuristic argument (not a complete proof) will perhaps make reasonable why one can expect formulas such as (67) or (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 obit.
- 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 backward orbits.
- 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 Theorems 31 and 12.

## 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 [22,26].

For this particular example, we will show the existence of a homoclinic channel (see Definition 3) 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  $\Lambda$ . Nevertheless, in the perturbed case this globalization leads to monodromies so that the scattering map is not well defined in the whole  $\Lambda_{\varepsilon}$ .

We deal with an *n*-dimensional manifold M, and we will consider a  $C^r$  metric g on it (r sufficiently large).

We recall that a geodesic " $\lambda$ " is a curve " $\lambda$ ":  $\mathbb{R} \to M$ , 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 " $\lambda$ " as  $\lambda(t)$ , and we denote by  $\hat{\lambda} = \operatorname{Range}(\lambda) \subset \mathbf{S}_1 M$ .

We will assume that the metric *g* verifies:

H1: There exists a closed geodesic " $\Lambda$ " such that its corresponding periodic orbit  $\hat{\Lambda}$  under the geodesic flow is hyperbolic.

H2: There exists another geodesic " $\gamma$ " 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  $\hat{\Lambda}$ ,  $W^s_{\hat{\Lambda}}$ ,  $W^u_{\hat{\Lambda}}$ , 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

$$T_{\gamma(t)}W^s_{\hat{A}} + T_{\gamma(t)}W^u_{\hat{A}} = T_{\gamma(t)}\mathbf{S}_1M, \quad t \in \mathbb{R}.$$
(76)

Hypotheses H1, H2 are verified in great generality. We refer to [26, Section 2] for a discussion of the abundance. After the publication of [26], the paper [17] 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  $\Lambda$  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

$$\operatorname{dist}(``\Lambda''(s+a_{\pm}),``\gamma''(s)) \leqslant Ce^{-\beta_0|s|}, \quad \text{as } s \to \pm\infty.$$
(77)

Standard perturbation theory for periodic orbits of ordinary differential equations (see e.g. [16]) shows that the asymptotic phase shift  $\Delta := a_+ - a_-$  exists and is unique modulo an integer multiple of the period of " $\Lambda$ ".

We recall that the geodesic flow is Hamiltonian in  $T^*M$  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  $\Phi_t$  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 " $\lambda$ ":  $\mathbb{R} \to M$  we will denote

$$\lambda_E(t) = \left(\lambda_E^p(t), \lambda_E^q(t)\right)$$

the orbit such that  $H_0(\lambda_E(t)) = E$ , Range(" $\lambda$ ") = Range( $\lambda_E^q$ ) and " $\lambda$ "(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 " $\lambda$ ". 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

$$\left(\lambda_E^p(t), \lambda_E^q(t)\right) = \left(\sqrt{2E}\lambda_{1/2}^p(\sqrt{2E}t), \lambda_{1/2}^q(\sqrt{2E}t)\right).$$
(78)

Since  $\Lambda_{1/2}$  has period 1 (with our conventions that the geodesic " $\Lambda$ " is normalized to have length 1),  $\Lambda_E$  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 (78), of the Hamiltonian  $H_0$  whose range  $\hat{\Lambda}_E$  is hyperbolic in the energy surface

$$\Sigma_E := \{ (p,q) \in \mathbf{T}^* M, \ H_0(p,q) = E \}.$$
(79)

H2': The stable and unstable manifolds  $W_{\hat{A}_E}^{s,u}$  of  $\hat{A}_E$  are *n*-dimensional, and there exists a homoclinic orbit  $\gamma_E(t)$ . That is, the range of  $\gamma_E$  satisfies

$$\hat{\gamma}_E \subset \left(W^s_{\hat{\Lambda}_E} \setminus \hat{\Lambda}_E\right) \cap \left(W^u_{\hat{\Lambda}_E} \setminus \hat{\Lambda}_E\right).$$

Moreover, this intersection is transversal as intersection of invariant manifolds in the energy surface  $\Sigma_E$  along  $\hat{\gamma}_E$ .

As a consequence of the hyperbolicity of  $\hat{A}_{1/2}$ , we have that, analogously to (77), for some  $a_{\pm} \in \mathbb{R}$ , there exist C > 0 and an *exponential rate*  $\beta_0 > 0$ , such that

$$\operatorname{dist}(\Lambda_{1/2}(t+a_{\pm}),\gamma_{1/2}(t)) \leqslant C e^{-\beta_0|t|} \quad \text{as } t \to \pm \infty.$$
(80)

We consider any fixed value  $E_0 > 0$ , and introduce the manifold  $\Lambda = \bigcup_{E \ge E_0} \hat{\Lambda}_E$  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,  $W^s_{\Lambda}$  and  $W^u_{\Lambda}$ , are (n + 1)-dimensional manifolds diffeomorphic to  $[E_0, \infty) \times \mathbb{T}^1 \times \mathbb{R}^{n-1}$ , intersecting transversally along  $\gamma$ , defined by:

$$\gamma = \bigcup_{E \geqslant E_0} \hat{\gamma}_E \subset (W^s_A \setminus \Lambda) \cap (W^u_A \setminus \Lambda)$$

which is diffeomorphic to  $[E_0, \infty) \times \mathbb{R}$ .

By inequality (80) and the rescaling properties (78) we have:

$$\operatorname{dist}\left(\Lambda_E\left(t+\frac{\varphi_0+a_{\pm}}{\sqrt{2E}}\right), \gamma_E\left(t+\frac{\varphi_0}{\sqrt{2E}}\right)\right) \leqslant C\sqrt{2E}e^{-\beta_0\sqrt{2E}|t|} \quad \text{as } t \to \pm\infty.$$
(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 (81) the corresponding  $x_{\pm} \in \Lambda$  such that  $x \in W^s_{x_{\pm}} \cap W^u_{x_{\pm}}$  are given by

$$x_{\pm} = \Lambda_E \bigg( \frac{\varphi + a_{\pm}}{\sqrt{2E}} \bigg),$$

so that the definition (4) of the wave operators gives that  $\Omega_{\pm}(x) = x_{\pm}$ . Indeed, one can easily see that if we move  $x_{-} = \Lambda_E(\frac{\varphi+a_{-}}{\sqrt{2E}})$  around  $\hat{\Lambda}_E$  up to  $\Lambda_E(\frac{\varphi+a_{-}+1}{\sqrt{2E}}) = x_{-}$ , 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  $\Lambda_E$  is  $1/\sqrt{2E}$  periodic, if we take

$$x^n = \gamma_E\left(\frac{\varphi+n}{\sqrt{2E}}\right) = \Phi_{n/\sqrt{2E}}(x),$$



Fig. 5. Illustration of the closed geodesics.



Fig. 6.

property (81) gives

$$\Omega_{\pm}(x^n) = x_{\pm}^n = x_{\pm}$$

so that the maps  $\Omega_{|\gamma}^{\pm}: \gamma \to \Lambda$  are not global diffeomorphisms. See Figs. 5 and 6. In order to study the monodromy of these maps, for any  $t \in \mathbb{R}$ , we define

$$\Gamma^{t} = \left\{ \gamma_{E} \left( \frac{\varphi + t}{\sqrt{2E}} \right), \ |\varphi| < 1/2, \ E \geqslant E_{0} \right\}$$

which are homoclinic channels, that is

$$\Omega_{\pm}^{\Gamma^{t}}:\Gamma^{t}\to H_{\pm}^{t}=\Omega_{\pm}^{\Gamma^{t}}(\Gamma^{t})$$

are global diffeomorphisms.

As  $\Lambda_E$  is  $1/\sqrt{2E}$  periodic, the sets  $H^t_{\pm}$  can be written as  $H^t_{\pm} = \Lambda \setminus \bigcup_{E \ge E_0} \Lambda_E(\frac{1/2+t+a_{\pm}}{\sqrt{2E}})$ .

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  $(\varphi, E) \in (-1/2, 1/2) \times [E_0, \infty)$ .

The monodromy of  $(\Omega_{-})^{-1}$  is precisely an application of  $\Phi_{1}$ , the time 1 map of the geodesic flow. Since  $\Omega_{+} \circ \Phi_{1} = \Omega_{+}$  we see that  $\sigma$  has no monodromy and is globally well defined in  $\Lambda$  for the geodesic flow.

Concretely, we observe that  $\sigma^t = \sigma^{t'}$  in  $H^t_- \cap H^{t'}_-$ , and that  $\bigcup_{t \in \mathbb{R}} H^t_- = \Lambda$ , so it is possible to define globally the scattering map

$$\sigma: \Lambda \to \Lambda$$
$$x_{-} = \Lambda_{E} \left( \frac{\varphi + a_{-}}{\sqrt{2E}} \right) \mapsto x_{+} = \Lambda_{E} \left( \frac{\varphi + a_{+}}{\sqrt{2E}} \right).$$

We use now the notations of Section 4.2 for the parameterizations of  $\Lambda$  and introduce the (symplectic) system of coordinates  $(\varphi, J)$ ,  $J = \sqrt{2E}$  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:

$$s: N \to N$$
  
 $(\varphi, J) \mapsto (\varphi + \Delta, J)$  (82)

where  $\Delta = a_+ - a_-$  is called the phase shift.

**Remark 36.** 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 (78) which are a very particular feature of the geodesic flow. See [12] for an example, in the planar restricted three body problem, of an integrable scattering map which verifies the twist condition.

## 6.1. Perturbations of geodesic flows

In order to deal with the quasi-periodic perturbations of the geodesic flow of the form  $H_{\varepsilon}(p,q,t) = H_0(p,q) + \varepsilon^2 U(q, \varepsilon v t)$ , for some vector  $v \in \mathbb{R}^d$  considered in [26], we first study the product vector field of the geodesic flow  $H_0(p,q)$  on  $\mathbf{T}^* M$  and the quasi-periodic flow  $\dot{\theta} = \varepsilon v$  in  $\mathbb{T}^d$ , defined in the extended phase space  $\mathbf{T}^* M \times \mathbb{T}^d$ . In (82) we have computed the formulas for the scattering map associated to this geodesic flow, and, as we saw in Section 2.4.2, the scattering map on  $\tilde{A} = A \times \mathbb{T}^d$  is given, in the extended reference manifold  $\tilde{N} = N \times \mathbb{T}^d$ , by

$$\tilde{s}: \tilde{N} \to \tilde{N}$$
$$(J, \varphi, \theta) \mapsto (J, \varphi + \Delta, \theta).$$

If we want to make apparent the symplectic character of the scattering map, we add the extra actions A, conjugated to the angles  $\theta$ , obtaining the autonomous Hamiltonian  $H_0(p,q) + \varepsilon v \cdot A$  in the full symplectic space  $\mathbb{T}^*M \times \mathbb{R}^d \times \mathbb{T}^d$ . We have a (2d+2)-dimensional manifold  $\Lambda^* = \Lambda \times \mathbb{R}^d \times \mathbb{T}^d$  whose projection to the extended phase space  $\mathbb{T}^*M \times \mathbb{T}^d$  is  $\tilde{\Lambda}$ . Using the extended symplectic coordinates  $(J, \varphi, A, \theta)$ , the reference manifold of  $\Lambda^*$  is given by  $N^* = N \times \mathbb{R}^d \times \mathbb{T}^d$ , and its parameterization is given by

$$\begin{split} k^* \colon N^* &\to \Lambda^* \\ (J, \varphi, A, \theta) &\mapsto \left( k(J, \varphi), A, \theta \right) = \left( \Lambda_E(\varphi/\sqrt{2E}), A, \theta \right) \end{split}$$

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:

$$\begin{split} s^* \colon N^* \to N^* \\ (J, \varphi, A, \theta) \mapsto (J, \varphi + \Delta, A, \theta). \end{split}$$

Before applying perturbation theory we fix some homoclinic channel  $\Gamma_0^* = \Gamma^{t_0} \times \mathbb{R}^d \times \mathbb{T}^d$ 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  $\varepsilon^{2}$  guarantees the transversal intersection of  $W_{A_{\varepsilon}^{*}}^{s} \cap W_{A_{\varepsilon}^{*}}^{u}$  along a homoclinic channel  $\Gamma_{\varepsilon}^{*}, \varepsilon^{2}$ -close to  $\Gamma_{0}^{*}$ , for a normally hyperbolic invariant manifold  $A_{\varepsilon}^{*} \subset T^{*}M \times \mathbb{R}^{d} \times \mathbb{T}^{d}$  and the local existence of a perturbed scattering map  $\sigma_{\varepsilon}^{*}$ . Nevertheless, all the considerations about the global definition of the scattering map  $\sigma^{*}$  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  $\sigma_{\varepsilon}^{*}$  in a set  $H_{-\varepsilon}^{*}, \varepsilon^{2}$ -close to  $H_{-}^{*,t_{0}} = H_{-}^{t_{0}} \times \mathbb{R}^{d} \times \mathbb{T}^{d}$ , of relative measure  $1 - \varepsilon^{2}$  in  $\Lambda_{\varepsilon}^{*}$ .

We will now compare the perturbative calculation of the scattering map which was already done in [22] and [26] and formula (68).

**Remark 37.** In order to compare the perturbative formulas for the scattering map in [26] and the ones obtained applying the method of Section 5 we need to take into account the following fact. In the example considered here, the perturbed Hamiltonian is given by  $H_{\varepsilon}^*(p, q, \theta, A) =$  $H_0(p,q) + \varepsilon^2 V(q,\theta) + \varepsilon v \cdot A$ , so, it depends on the parameter  $\varepsilon$  in two different ways. On one side, the term  $\varepsilon^2$  in front of the potential makes the perturbation small. On the other hand, the term  $\varepsilon v \cdot A$  makes the potential slow in the angular variable  $\theta$ . So, as it was proved in [26], the perturbation theory is done with respect to the small parameter, which in this case is  $\varepsilon^2$ . So, when we apply formula (68) we will replace the parameter  $\varepsilon$  by  $\varepsilon^2$  in all the formulas.

In order to perform this comparison, we can choose the parameterization of the perturbed normally hyperbolic invariant manifold  $\Lambda_{\varepsilon}^{*}$  verifying hypothesis (59). In the notation of [26], any point in this manifold is given by

$$x_{\varepsilon}^{*} = (p, q, A, \theta) = k_{\varepsilon}^{*}(J, \varphi, B, \theta) = \left(\mathcal{F}(J, \varphi, \theta, \varepsilon^{2}), \mathcal{A}(J, \varphi, B, \theta, \varepsilon^{2}), \theta\right)$$

for some parameterizations  $\mathcal{F} = \Lambda_E(\varphi/\sqrt{2E}) + O(\varepsilon^2)$ ,  $\mathcal{A}$ , that, under assumption (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  $x_{\pm}^*(\varepsilon) = \sigma_{\varepsilon}^*(x_{\pm}^*(\varepsilon))$  and  $x_{\pm}^*(\varepsilon)$  was 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, to apply standard first order perturbation theory that

$$\varphi_{\pm} = \varphi + a_{\pm} + O(\varepsilon^{2}),$$
  

$$J_{\pm} = J + O(\varepsilon^{2}),$$
  

$$B_{\pm} = B + O(\varepsilon^{2}),$$
  

$$\theta_{\pm} = \theta,$$
(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 (77) and (80).

Now, denoting  $z^*(\varepsilon) = (\Omega_{\varepsilon+}^{\Gamma_{\varepsilon}^*})^{-1}(x_+^*(\varepsilon)) = (\Omega_{\varepsilon-}^{\Gamma_{\varepsilon}^*})^{-1}(x_-^*(\varepsilon))$  in the homoclinic channel  $\Gamma_{\varepsilon}^*$ , standard first order perturbation theory gives, by (81), that  $z^*(0) = \gamma_E(\varphi/J)$ . Using all these facts, Lemma 4.18 of [26] gives

$$A(x_{+}^{*}(\varepsilon)) - A(x_{-}^{*}(\varepsilon)) = \varepsilon^{2} \frac{\partial L}{\partial \theta}(E, \varphi, \theta) + O_{\mathcal{C}^{1}}(\varepsilon^{4}),$$
(84)

where  $L(E, \varphi, \theta)$  is the Poincaré function given by

$$L(E,\varphi,\theta) = \lim_{T_1,T_2\to\infty} \left[ -\int_{-T_1}^{T_2} dt \, \widetilde{U} \left( \gamma_E^q \left( t + \frac{\varphi}{\sqrt{2E}} \right), \theta + \varepsilon \nu t \right) \right. \\ \left. + \int_{-T_1}^{0} dt \, \widetilde{U} \left( \Lambda_E^q \left( t + \frac{\varphi + a_-}{\sqrt{2E}} \right), \theta + \varepsilon \nu t \right) \right. \\ \left. + \int_{0}^{T_2} dt \, \widetilde{U} \left( \Lambda_E^q \left( t + \frac{\varphi + a_+}{\sqrt{2E}} \right), \theta + \varepsilon \nu t \right) \right]$$
(85)

where the functions  $\overline{U}(\theta)$  and  $\widetilde{U}(q, \theta)$  are defined by:

$$\overline{U}(\theta) = \int_{0}^{1} U\left(\Lambda_{1/2}^{q}(\varphi), \theta\right) d\varphi, \qquad \widetilde{U}(q, \theta) = U(q, \theta) - \overline{U}(\theta).$$
(86)

**Remark 38.** 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  $\varphi$  increases by 1, the scattering map changes. Note that changing  $\varphi$  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. See Figs. 5 and 6.

Indeed, we are going to see that Hamiltonian  $S_0$  of formula (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  $(\Omega_{0\pm}^{\Gamma_0^*})^{-1} \circ k_0^*(J, \varphi, B, \theta) = (\gamma_E((\varphi - a_{\pm})/J), B, \theta)$ , we have

$$\begin{split} S_{0}(J,\varphi,B,\theta) &= \lim_{T_{\pm} \to \infty} \int_{-T_{-}}^{0} U \circ \Phi_{u,0} \circ \left( \mathcal{Q}_{0-}^{T_{0}^{*}} \right)^{-1} \circ \left( \sigma_{0}^{*} \right)^{-1} \circ k_{0}^{*}(J,\varphi,B,\theta) \\ &\quad - U \circ \Phi_{u,0} \circ \left( \sigma_{0}^{*} \right)^{-1} \circ k_{0}^{*}(J,\varphi,B,\theta) \\ &\quad + \int_{0}^{T_{+}} U \circ \Phi_{u,0} \circ \left( \mathcal{Q}_{0+}^{T_{0}^{*}} \right)^{-1} \circ k_{0}^{*}(J,\varphi,B,\theta) - U \circ \Phi_{u,0} \circ k_{0}^{*}(J,\varphi,B,\theta) \\ &= \lim_{T_{\pm} \to \infty} \int_{-T_{-}}^{0} U \circ \Phi_{u,0} \circ \left( \mathcal{Q}_{0+}^{T_{0}^{*}} \right)^{-1} \circ k_{0}^{*}(J,\varphi-\Delta,B,\theta) \\ &\quad - U \circ \Phi_{u,0} \circ k_{0}^{*}(J,\varphi-\Delta,B,\theta) \\ &\quad + \int_{0}^{T_{+}} U \circ \Phi_{u,0} \circ \left( \mathcal{Q}_{0+}^{T_{0}^{*}} \right)^{-1} \circ k_{0}^{*}(J,\varphi,B,\theta) - U \circ \Phi_{u,0} \circ k_{0}^{*}(J,\varphi,B,\theta) \\ &= \lim_{T_{\pm} \to \infty} \int_{-T_{-}}^{0} U \circ \Phi_{u,0} \circ \left( \mathcal{Y}_{E} ((\varphi-a_{+})/J), B, \theta \right) \\ &\quad - U \circ \Phi_{u,0} (\Lambda_{E} ((\varphi-\Delta)/J), B, \theta) \\ &\quad + \int_{0}^{T_{+}} U \circ \Phi_{u,0} \circ \left( \mathcal{Y}_{E} (u + (\varphi-a_{+})/J), \theta + \varepsilon v u \right) \\ &\quad - \int_{-T_{-}}^{0} U \left( \Lambda_{E}^{q} (u + (\varphi-\Delta)/J), \theta + \varepsilon v u \right) - \int_{0}^{T_{+}} U \left( \Lambda_{E}^{q} (u + (\varphi/J)), \theta + \varepsilon v u \right). \end{split}$$

So that, we obtain:

$$S_0(J,\varphi,B,\theta) = -L(J,\varphi-a_+,\theta). \tag{87}$$

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  $\varepsilon^2$ , 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

$$s_1^*(J,\varphi,B,\theta) = \mathcal{S}_0 \circ s_0^*(J,\varphi,B,\theta) = \mathcal{S}_0(J,\varphi+\Delta,B,\theta) = \mathcal{J}\nabla S_0(J,\varphi+\Delta,B,\theta)$$

where  $\mathcal{J}$  is the symplectic matrix.

We denote the coordinates of  $x_{-}^*$ , by  $(J, \varphi + a_{-}, B_{-}, \theta)$  as in (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 (84) provided in [26].

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 [22,26], also used in [25,27], allowed only to compute the energy component of the scattering map but it does not allow us to compute the  $\varphi$  component since  $\varphi$  is not a slow variable. The method of this paper, also gives the  $\varphi$  component of the first order expansion of the scattering map.

The applications in [22,26] 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  $P_{\varepsilon} = P^{s_{\varepsilon}^*}$  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 Eq. (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 (87).

The expression L had played an important role in the variational calculation in [48]. This is related to the variational interpretation of the scattering map discussed in Section 3.4.3.

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## Appendix A. 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 paper.

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 [36,55]. These references emphasize more the time independent scattering theory. Books which emphasize more the time dependent scattering theory are [58,63]. We should also mention the papers [31,32,42,43,53, 62] 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 [54].

We recall that the time-evolution in quantum mechanics is generated by a self-adjoint operator H. The Schrödinger equation is

$$\frac{d}{dt}U(t) = -iHU(t); \qquad U(0) = \mathrm{Id}$$

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  $\Phi_t$ . 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

$$\Omega_{\pm} = \lim_{t \to \pm \infty} U_f(-t) U_i(t).$$

(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  $\psi$  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

$$\Omega_{\pm}U_{i}(s) = \lim_{t \to \pm \infty} U_{f}(-t)U_{i}(t+s)$$
$$= \lim_{t \to \pm \infty} U_{f}(-t+s)U_{i}(t)$$
$$= U_{f}(s)\Omega_{\pm}.$$
(A.1)

The relations (A.1) are called the intertwining relations. From the dynamical point of view, (A.1) semiconjugate the free dynamics to the interacting dynamics.

This method of producing conjugacies has appeared several times in dynamical systems, e.g., [61]. The analogy with quantum mechanics is emphasized in [54].

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 [62] 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 [10, 11,50,52]. Relations of this type of algorithms for linearization can be found in [19,20].

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

$$\sigma = \lim_{T_{\pm} \to \infty} U_f(-T_+) U_i(T_+ + T_-) U_f(-T_-).$$
(A.2)

The perturbation theory for the quantum mechanical scattering can be derived very easily. We note that if

$$H_i = H_{i,0} + \varepsilon H_{i,1}(t) + O\left(\varepsilon^2\right)$$

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 (A.2) we obtain

$$\sigma = \sigma_0 + \varepsilon \lim_{T_{\pm} \to \infty} U_f(-T_+) \int_{0}^{T_+ + T_-} i H_f(s) U_i(s) U_f(-T_0).$$
(A.3)

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  $\Gamma \subset W^s_A \cap W^u_A$  considered.

One can therefore consider  $\Gamma$  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,

$$\sigma U_f(t) = U_f(t)\sigma. \tag{A.4}$$

The analogue of (A.4) and (A.1) 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

$$W_{x-}^{u} \pitchfork W_{x+}^{s} \Leftrightarrow f(W_{x-}^{u}) \pitchfork f(W_{x+}^{s}) \Leftrightarrow W_{f(x-)}^{u} \pitchfork W_{f(x+)}^{s}.$$

Unfortunately, this does not allow us to conclude that the f commutes with  $\sigma^{\Gamma}$ . Note that if the intersection alluded to in the first line occurs in a manifold  $\Gamma$ , the intersection in the last line occurs in a manifold  $f(\Gamma)$ .

This means that the analogue of (A.1) and (A.4) is

$$f \circ \Omega_{\pm}^{\Gamma} = \Omega_{\pm}^{f(\Gamma)} \circ f,$$
$$f \circ \sigma^{\Gamma} = \sigma^{f(\Gamma)} \circ f.$$

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 [22,25,27] we have, for the unperturbed system the commutation of the inner map  $f_0$  and the scattering map  $\sigma_0$ , 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 6 for more details of a perturbative computation of  $\sigma_{\varepsilon}$  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 [22,25,27].

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