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Dynamics, Analysis, Applications

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Edited by

Albert Fathi
Georgia Institute of Technology

Philip J. Morrison
University of Texas at Austin

Tere M-Seara
Universitat Politécnica de Catalunya

Sergei Tabachnikov
Pennsylvania State University

CAMBRIDGE
UNIVERSITY PRESS

Albert Fathi
afathi30@gatech.edu

Philip J. Morrison
morrison@physics.utexas.edu

Tere M-Seara
tere.m-seara@upc.edu

Sergei Tabachnikov
sot2@psu.edu

Silvio Levy (*Series Editor*)
levy@msp.org

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Denjoy subsystems and horseshoes

MARIE-CLAUDE ARNAUD

We introduce a notion of weak Denjoy subsystem (WDS) that generalizes the Aubry–Mather–Cantor sets to diffeomorphisms of manifolds. We explain how a rotation number can be associated to such a WDS. Then we build in any horseshoe a continuous one parameter family of such WDS that is indexed by its rotation number. Looking at the inverse problem in the setting of Aubry–Mather theory, we also prove that for a generic conservative twist map of the annulus, the majority of the Aubry–Mather sets are contained in some horseshoe that is associated to a Aubry–Mather set with a rational rotation number.

1. Introduction and main results

All the dynamicists know the famous Poincaré sentence about periodic orbits:

> *Ce qui nous rend ces solutions périodiques si précieuses, c'est qu'elles sont, pour ainsi dire, la seule brèche par où nous puissions essayer de pénétrer dans une place jusqu'ici réputée inabordable.*

But a periodic orbit for a dynamical system $f : X \to X$ is simply a finite invariant subset and the dynamics restricted to this set cannot be very complicated. What is more interesting is the dynamics close to such a periodic orbit, that may give rise to various rich phenomena. For example, for a symplectic diffeomorphism of a surface, two kinds of restricted dynamics to invariant Cantor sets can exist close to the periodic orbits, that are:

- Horseshoes close to hyperbolic periodic points (see [27]);[1] since the work of Katok in [16], they are known to be the evidence of positive topological entropy. Moreover, they contain a dense set of periodic points.

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[1] We will define them precisely later in the article.

- Aperiodic Aubry–Mather sets close to elliptic periodic points (see [3; 8; 22]); they are known to have zero topological entropy and contain no periodic points.

Although we will later focus on some specific horseshoes, we give here a general definition of horseshoe.

Definition. Let $f : M \to M$ be a surface diffeomorphism. A *horseshoe for f* is a f-invariant subset $H \subset M$ such that the dynamics $f_{|H}$ is C^0 conjugate to the one of a nontrivial transitive subshift with finite type. A horseshoe for f is a *σ_2-horseshoe* when the dynamics $f_{|H}$ is C^0 conjugate to the shift with two symbols.

Example. The first horseshoe was introduced by S. Smale in [27] close to a transversal homoclinic intersection of a hyperbolic periodic point. This horseshoe is hyperbolic. Burns and Weiss extended this in [7] to the case of topologically transversal homoclinic intersection. Le Calvez and Tal use purely topological horseshoes for 2-dimensional homeomorphisms in [20].

The category of aperiodic Aubry–Mather set was recently extended in [2] to the notion of so-called Denjoy subsystem by P. Le Calvez and the author. We recall the definition given in [2].

Definition. Let $f : M \to M$ be a C^k diffeomorphism of a manifold M. A *C^k (resp. Lipschitz) Denjoy subsystem for f* is a triplet (K, γ, h) where:

- $\gamma : \mathbb{T} \to M$ is a C^k (resp. bi-Lipschitz) embedding.
- $h : \mathbb{T} \to \mathbb{T}$ is a Denjoy example with invariant compact minimal set $K \subset \mathbb{T}$.
- $f(\gamma(K)) = \gamma(K)$.
- $\gamma \circ h_{|K} = f \circ \gamma_{|K}$.

Remarks.
- In this definition, $\gamma(\mathbb{T})$ is not necessarily invariant.
- Observe the importance of γ to fix the regularity of $\gamma(K)$.
- For $k = 0$, what we call a C^0-diffeomorphism is in fact a homeomorphism and in this case we just require that γ is a continuous embedding.
- The embedding is also useful to define a circular order on the Cantor set $\gamma(K)$.

Example. There exists different notions of Aubry–Mather sets for the exact symplectic twist maps of the annulus; see [3] and [22]. We will follow [4] and for us, an Aubry–Mather set is a well ordered compact set that contains only minimizing orbits in a variational setting; see, e.g., [3; 4]. Let us recall some results that are contained in [4] and [1] and that we will use. We fix an exact symplectic twist map f of the infinite annulus and a lift $F : \mathbb{R}^2 \to \mathbb{R}^2$. Then:

- Every Aubry–Mather set is a partial Lipschitz graph.
- Every Aubry–Mather set $\mathcal{A}$ has a rotation number $\rho(\mathcal{A}) \in \mathbb{R}$.
- For every $r \in \mathbb{R}\backslash\mathbb{Q}$, there exists a unique maximal (for $\subset$) Aubry–Mather set $\mathcal{A}_r$ with rotation number r that contains every Aubry–Mather set with the same rotation number.
- For every $r = \frac{p}{q} \in \mathbb{Q}$, there exist two Aubry–Mather set $\mathcal{A}_r^{\pm}$ with rotation number r that are maximal (for $\subset$) among the Aubry–Mather sets with the same rotation number. They are such that: $\forall x \in \tilde{\mathcal{A}}_r^{+}, \pi_1 \circ F^q(x) \geq \pi_1(x) + p$ (resp. $\forall x \in \tilde{\mathcal{A}}_r^{-}, \pi_1 \circ F^q(x) \leq \pi_1(x) + p$) where $\pi_1 : \mathbb{R}^2 \to \mathbb{R}$ is the first projection.
- If $(\mathcal{A}_n)$ is a sequence of Aubry–Mather sets such that the sequence of rotation numbers $(\rho(\mathcal{A}_n))$ converges to some $r \in \mathbb{R}$, then $\bigcup_{n\in\mathbb{N}} \mathcal{A}_n$ is relatively compact and any limit point of $(\mathcal{A}_n)$ for the Hausdorff distance is an Aubry–Mather set with rotation number r.

The Aubry–Mather sets $\mathcal{A}_r$ that have an irrational rotation number and that are not a complete graph always contain a Lipschitz Denjoy subsystem $\mathcal{C}_r$.

We noticed that an important advantage of γ is to define a circular order along $\gamma(K)$. But to do that, we only need the embedding restricted to K. That is why we introduce now a new notion, the one of *weak Denjoy subsystem* that extends the one of Denjoy subsystem. This notion is similar to the one of Denjoy set that was introduced by J. Mather in [23].

Definition. Let $f : M \to M$ be a homeomorphism of a manifold M. A *weak Denjoy subsystem for f* (in short WDS) is a triplet (K, j, h) where:

- $h : \mathbb{T} \to \mathbb{T}$ is a Denjoy example with invariant minimal set $K \subset \mathbb{T}$.
- $j : K \to M$ is a homeomorphism onto its image.
- $f(j(K)) = j(K)$.
- $j \circ h_{|K} = f \circ j$.

When j is bi-Lipschitz or a C^k embedding (in the Whitney sense), we speak of Lipschitz or C^k weak Denjoy subsystem for f. Two WDS (K_1, j_1, h_1) and (K_2, j_2, h_2) are *equivalent* if $j_1(K_1) = j_2(K_2)$.

The restriction of a Denjoy subsystem to its nonwandering set is always a WDS. On a surface, we have the reverse implication.

Proposition 1.1. *Let (K, j, h) be a WDS of a surface homeomorphism. Then there exists a C^0 Denjoy subsystem (K, γ, h) such that $\gamma_{|K} = j$.*

Remarks.
- This result is specific to the case of surfaces because it uses a classical result on extension of homeomorphisms between Cantor sets of surfaces.
- We do not know about such a result with more regularity: Lipschitz, C^1 (a kind of Whitney extension theorem for diffeomorphisms). Observe that we proved in [2] that there exists no C^2 Denjoy subsystem.

Remark. Let us recall that a *circular order relation* on a set X is a relation $\prec$ that is defined on the triplets of points of X such that:

- If $x, y, z \in X$, we have $x \prec y \prec z$ or $z \prec y \prec x$; we use the notation $[x, z]_\prec = \{y \in X; x \prec y \prec z\}$.
- If $x \neq z$, the two previous lines of inequalities are simultaneously satisfied if and only if $x = y$ or $y = z$.
- If $x \prec y \prec z$, then $y \prec z \prec x$.
- If $x \prec y \prec z$ and $x \prec z \prec t$ then $x \prec y \prec t$.

If $\prec$ is a circular order on X, the inverse order $-\prec$ is defined by

$$\forall x, y, z \in X, \quad x(-\prec)y(-\prec)z \Leftrightarrow z \prec y \prec x.$$

Notations.
- If (K, j, h) is a WDS, we denote by $\prec_K$ the circular order on $j(K)$ that is deduced from the one of $K \subset \mathbb{T}$ via the map j.
- The *graph* $\mathcal{G}(\prec_K)$ of this order relation is the set of the triplets $(a, b, c) \in (j(K))^3$ such that $j^{-1}(a) \prec j^{-1}(b) \prec j^{-1}(c)$ where $\prec$ is the usual order on $\mathbb{T}$. This graph $\mathcal{G}(\prec_K)$ is then a closed subset of $(j(K))^3$ and then of $(M)^3$. Observe that for every $a, c \in j(K)$, $\mathcal{G}(\prec_K, a, c) = \{b \in j(K); (a, b, c) \in \mathcal{G}(\prec_K)\}$ is a nonempty compact subset of M, called an *interval* of $\mathcal{G}(\prec_K)$.

Remark. We have $\mathcal{G}(\prec_K, a, a) = j(K)$ and for $a \neq c$, $\mathcal{G}(\prec_K, a, c)$ contains at least a and c. Moreover, we have $\mathcal{G}(\prec_K, a, c) = \{a, c\}$ if and only if $\{a, c\}$ is one gap of the Cantor set.[2]

The first theorem we will prove allows us to extend Poincaré's notion of rotation number to WDS, or more precisely to the classes of equivalence of WDS.

Theorem 1.2. *Let (K_1, j_1, h_1) and (K_2, j_2, h_2) be two equivalent WDS for a same homeomorphism $f : M \to M$ of a manifold M. Then*:

- *There exists a homeomorphism $h : \mathbb{T} \to \mathbb{T}$ such that $h \circ h_1 = h_2 \circ h$.*
- *We have $\prec_{K_1} = \prec_{K_2}$ or $\prec_{K_1} = -\prec_{K_2}$, hence the two orders have the same intervals.*

[2]Observe that in this case, a and c are α and ω-asymptotic under the dynamics.

Corollary 1.3. *The map ρ defined on the set of WDS with values in $\mathbb{T}/x \sim -x$ that associates to any WDS (K, γ, h) the rotation number of h modulo its sign is such that if (K_1, γ_1, h_1) and (K_2, γ_2, h_2) are equivalent, then $\rho(K_1, \gamma_1, h_1) = \rho(K_2, \gamma_2, h_2)$.*

Let us endow the set of WDS with a topology that focus on their order relation.

Notations. We endow M with a Riemannian metric d and M^3 is endowed with the natural sup distance associated to d that is denoted by d_∞. Then D (resp. D_∞) is the associated Hausdorff distance on the set of nonempty compact subsets of M (resp. M^3).

Definition. Let $f : M \to M$ be a homeomorphism of a manifold M. Let (K_i, j_i, h_i) be two weak Denjoy subsystems for f. We denote by $\mathcal{G}(\prec_{K_i}) \subset M^3$ (resp. $\mathcal{G}(- \prec_{K_i})$) the graph of $\prec_{K_i}$ (resp. $- \prec_{K_i}$).

We define a distance δ on the set of the weak Denjoy subsystems for f by the following equality.

We have

$$\delta((K_1,j_1,h_1),(K_2,j_2,h_2))$$
$$=\max\big\{D(j_1(K_1),j_2(K_2)),\min\{D_\infty(\mathcal{G}(\prec_{K_1}),\mathcal{G}(\prec_{K_2})),D_\infty(\mathcal{G}(-\prec_{K_1}),\mathcal{G}(\prec_{K_2}))\}\big\}.$$

Proposition 1.4. *The map that associates to every WDS its rotation number is continuous.*

Remark. The previous result extends a result that is well-known in the setting of well-ordered sets for twist maps.

Horseshoes and WDS are different but in general, it is believed that, up to some entropy restriction, horseshoes dynamics contain every dynamics (via symbolic dynamics).[3]

We will prove that every horseshoe contains many WDS, and even a continuous 1-parameter family (D_ρ) continuously depending on its rotation number ρ where ρ is in a nontrivial interval of $\mathbb{T}/x \sim -x$ of irrational numbers.

Theorem 1.5. *Let $f : M \to M$ be a C^k diffeomorphism and let $\mathcal{H}$ be a horseshoe for f. Then exists $N \geq 1$ and a continuous map $D : r \in (\mathbb{T}\backslash\mathbb{Q})/x \sim -x \mapsto (K_r, j_r, h_r)$ such that:*

- *$D(r) = (K_r, j_r, h_r)$ is a continuous WDS with rotation number r for f^N.*
- *$j_r(K_r) \subset \mathcal{H}$.*

Moreover, if $\mathcal{H}$ is a σ_2-horseshoe, we have $N = 1$.

[3]This is not completely correct because, for example, the dynamics of an odomoter cannot be embedded in a horseshoe even if it has zero entropy: it is an isometry and the horseshoe is expansive.

Different authors before us built embedding of Denjoy dynamics into horseshoes. The first one is certainly [12], that embeds some Denjoy dynamics into the abstract horseshoe by using Sturmian sequences (this article follows the seminal work of Hedlund and Morse in [25]). In [15], the authors build an uncountable family of Denjoy dynamics in a given horseshoe. If we analyze their construction, for every irrational rotation number, they build an uncountable family of weak Denjoy subsystems with two holes that are not conjugate together (see Markley, [21], for a characterization of conjugated Denjoy examples). In [6], Boyland used a distance different from the one we use (his distance uses the Hausdorff distance D in M and also a distance on the set of Borel probability measures) and proved that for every irrational rotation number and every integer $N \geq 1$, there is a N-dimensional topological disc of weak Denjoy subsystems having this rotation number in every horseshoe. He also explained a general method to obtain all the weak Denjoy subsystem of a horseshoe. In [5], looking for special invariant measures of the angle doubling on the circle, Bousch uses the one side shift on $\{0, 1\}^{\mathbb{N}}$ and the unique invariant measure with support in a Cantor set analogous to the one we build.

Remarks.

- The continuous WDS that we will embed in the horseshoe are WDS that have only a pair of orbits that are ω asymptotic (and then α-asymptotic because we have a Denjoy dynamics), i.e., that correspond to a Denjoy example with exactly one orbit of a wandering interval (we will say one gap).
- Observe that the shift dynamics is expansive. Hence we cannot embed in it a WDS with a infinite countable number of gaps: one of these gaps would have all its orbit with diameter less than the expansivity constant, which is impossible.
- But it is possible to embed a family of WDS with a finite number p of gaps in a $\sigma_{\sup\{2,p\}}$-horseshoe.
- A similar method to embed Cantor sets with an interval of rotation numbers was proposed by K. Hockett and P. Holmes for dissipative twist maps in [15]. Here we proved a more general statement (for WDS) and also prove a continuity result.

Corollary 1.6. *Let $f : M^{(2)} \to M^{(2)}$ be a C^k diffeomorphism of a surface and let $\mathcal{H}$ be a horseshoe for f. Then exists $N \geq 1$ and a map $D : r \in (\mathbb{T}\backslash\mathbb{Q})/x \sim -x \mapsto (K_r, \gamma_r, h_r)$ such that*:

- *$D(r) = (K_r, \gamma_r, h_r)$ is a continuous Denjoy subsystem with rotation number r for f^N.*
- *The map $W : r \in (\mathbb{T}\backslash\mathbb{Q})/x \sim -x \mapsto (K_r, \gamma_{r|K_r}, h_r)$ is continuous.*

- $\gamma_r(K_r) \subset \mathcal{H}$.

Moreover, if $\mathcal{H}$ is a σ_2-horseshoe, we have $N = 1$.

Remarks.
- We do not know how to choose continuously the embedding γ_r or at least its image. But we do not need that to describe the dynamics on $\gamma_r(K_r)$.
- In the setting of the Aubry–Mather theory, the map that associates to any Aubry–Mather set $\mathcal{A}_r$ the graph that linearly interpolates $\mathcal{A}_r$ is in fact continuous when we endow the set of functions with the C^0 distance, and we will see that the Aubry–Mather sets with an irrational rotation number are actually contained in some horseshoes in the generic case. But the Aubry–Mather set do not continuously depend on the rotation number $r \in \mathbb{R}\backslash\mathbb{Q}$, so even in the case of the Aubry–Mather sets we do not know if we can interpolate in a continuous way by a curve.

We now focus on Aubry–Mather theory and address the inverse problem: are the WDS that appear in a natural way in symplectic 2-dimensional dynamics contained in some horseshoe?

Theorem 1.7. *Let $f : \mathbb{T} \times \mathbb{R} \to \mathbb{T} \times \mathbb{R}$ be an exact symplectic twist map and let $F : \mathbb{R}^2 \to \mathbb{R}^2$ be a lift of f. Assume that $\mathcal{A}_r^+$ (resp. $\mathcal{A}_r^-$) is uniformly hyperbolic for some rational number $r \in \mathbb{Q}$. Let $\mathcal{V}_r$ be a neighborhood of $\mathcal{A}_r^+$ (resp. $\mathcal{A}_r^-$). Then there exists a horseshoe $\mathcal{H}_r^+$ (resp. $\mathcal{H}_r^-$) for some f^N and $\varepsilon > 0$ such that:*

- *$\mathcal{H}_r^+$ (resp. $\mathcal{H}_r^-$) contains $\mathcal{A}_r^+$ (resp. $\mathcal{A}_r^-$) and is contained in $\mathcal{V}_r$.*
- *Every Aubry–Mather set with rotation number in $(r, r + \varepsilon)$ (resp. $(r - \varepsilon, r)$) is contained in $\mathcal{H}_r^+$ (resp. $\mathcal{H}_r^-$).*
- *Every point in $\mathcal{H}_r^+$ (resp. $\mathcal{H}_r^-$) has no conjugate points, i.e., has its orbit that is locally minimizing.*

Remarks.
- It is well known that the topological entropy of a twist map restricted to the union of all its hyperbolic Aubry–Mather sets is zero and has zero Hausdorff dimension; see [9]. Theorem 1.7 implies that for an open and dense subset of conservative twist diffeomorphisms (in any reasonable topology), there exists an invariant set $\mathcal{K}$ of points with no conjugate points such that the dynamics restricted to $\mathcal{K}$ has positive topological entropy and positive Hausdorff dimension.
- In [18], a transitive set that contains all the Aubry–Mather sets is built by P. Le Calvez. But this set is very different from the one we build here, because it contains in general orbits with conjugate points and is far from every Aubry–Mather set $\mathcal{A}_r^{\pm}$. Moreover, it is not a horseshoe.

- Observe that no WDS (K, j, h) that is contained in a hyperbolic horseshoe is C^1. Indeed, the endpoints a, b of every gap are α and ω-asymptotic and their orbits are dense in $j(K)$. But for n large enough, $f^n(a)$ and $f^n(b)$ are in the same local stable manifold and then oriented in the stable direction and $f^{-n}(a)$ and $f^{-n}(b)$ are in the same local unstable manifold and the oriented in the unstable direction. Hence, close to any point in $j(K)$, we find points such that the geodesic that joins them is either along the stable or the unstable direction. So j cannot be C^1. In the Aubry–Mather setting, it is Lipschitz.
- As we noticed before, a weak Denjoy subsystem (K, j, h) that is contained in a horseshoe has a finite number of gaps. When the horseshoe is uniformly hyperbolic with an expansivity constant equal to ε and j is k-bi-Lipschitz, it can be proved that the number of gaps is at most $\frac{k}{\varepsilon}$.

A remarkable result of P. Le Calvez asserts that general Aubry–Mather sets of general exact symplectic twist diffeomorphisms are uniformly hyperbolic; see[19]. Joint with Theorem 1.7, this implies the following corollary.

Corollary 1.8. *There exists a dense G_δ subset $\mathcal{G}$ of the set of C^k exact symplectic twist diffeomorphisms (for $k \geq 1$) such that for every $f \in \mathcal{G}$, there exist an open and dense subset $U(f)$ of $\mathbb{R}$ and a sequence $(r_n)_{n\in\mathbb{N}}$ in $U(f) \cap \mathbb{Q}$ such that every minimizing Aubry–Mather set with rotation number in $U(f)$ is hyperbolic and contained in a horseshoe associated to a minimizing hyperbolic Aubry–Mather set whose rotation number is r_n.*

Remark. Observe that in [11], Goroff gives an example where the union of all the Aubry–Mather sets is uniformly hyperbolic.

An open problem is the possible extension of Theorem 1.7 in a relaxed setting. Hence we rise the following questions.

Question (A. Fathi). Without assuming hyperbolicity, are the Aubry–Mather sets that are Cantor contained in some (nonhyperbolic) horseshoe?

Another question concerns the dynamics that are not necessarily twist diffeomorphisms.

Question. For a (possibly generic) symplectic diffeomorphism, is any WDS contained in some horseshoe?

It is possible to build C^1 or C^2 examples that have WDS that are not contained in horseshoes (examples that have a C^1 invariant curve on which the dynamics is Denjoy, see [14]), but our question concerns higher differentiability.

1A. ***Notations.*** For any hyperbolic periodic point x of a C^1 diffeomorphism, we denote by $W^s(x, f)$ or $W^s(x)$ (resp. $W^u(x, f)$ or $W^u(x)$) its stable (resp. unstable) submanifold and by $W^s_{\text{loc}}(x, f)$ or $W^s_{\text{loc}}(x)$ (resp. $W^u_{\text{loc}}(x, f)$ or $W^u_{\text{loc}}(x)$) its local stable (resp. unstable) submanifold. We adopt exactly the same notations for not necessarily periodic points that belong to some hyperbolic set.

Also we mention that the annulus is $\mathbb{A} = \mathbb{T} \times \mathbb{R}$, that its tangent space is $\mathbb{A} \times \mathbb{R}^2$ and that the tangent space at every point is endowed with its usual Euclidean norm. Moreover, we use the notation $\pi_1 : \mathbb{A} \to \mathbb{T}$ for the first projection as well as its lift $\pi_1 : \mathbb{R}^2 \to \mathbb{R}$.

2. Proof of Proposition 1.1

We assume that (K, j, h) is a weak Denjoy subsystem of a surface homeomorphism. If we embed $\mathbb{T}$ in $\mathbb{R}^2$, then K is a Cantor set that is a subset of $\mathbb{R}^2$.

The main argument of the proof is a result that is contained in Chapter 13 of [24].

Theorem. *Every homeomorphism between two Cantor subsets of $\mathbb{R}^2$ can be extended so as to give a homeomorphism of $\mathbb{R}^2$ onto itself.*

Corollary 2.1. *Let C be a Cantor subset that is contained in a topological open disc D. For every $\delta > 0$, there exists a finite number of disjoint topological discs $D_1, \dots, D_n$ with diameter less than δ such that*

$$C \subset \bigcup_{1 \le i \le n} D_k \subset \bigcup_{1 \le i \le n} \bar{D}_k \subset D.$$

Let us prove the corollary. If C is a Cantor set that is contained in an open disc D, there exists a homeomorphism $h : D \to \mathbb{R}^2$ such that $h(C)$ is the triadic Cantor set $C_0 \subset \mathbb{R} \times \{0\}$. We can decrease slightly D in such a way that $C \subset D' \subset \bar{D}' \subset D$ and h is restricted to the closed topological disc $\bar{D}'$. For every $\varepsilon > 0$, there exists a covering of C_0 by a finite number of topological discs $d_1, \dots, d_n$ that are contained in $h(D')$ and have diameter less than ε; indeed, this result is well known for the triadic subset in the real line and we just have to choose ε less than the distance between C_0 and $\mathbb{R}^2 \backslash h(D')$ and thicken the intervals into topological discs. Because h^{-1} is uniformly continuous, we deduce that for every $\varepsilon > 0$, there exists a finite covering of C by a finite number of disjoint discs that are contained in D' and have diameter less than ε. □

There exists $\eta > 0$ (that is less than the radius of injectivity of the Riemannian metric on $j(K)$) such that every set with diameter less than η that intersects $j(K) = C$ is contained in some topological disc. As $C = j(K)$ is a Cantor set, it is (uniformly) homeomorphic to the triadic Cantor set. Hence, there exists a closed partition of C into a finite number of sets $C_1, \dots, C_p$ that are open an closed in C and have diameter less than η. As the diameter of every C_j is less than η, there exists a topological disc B_j that contains the Cantor set C_j. We introduce the notation $\delta = \min\{\min\{d(C_i, C_j); i \neq j\}, \eta\}$. Then we can apply Corollary 2.1: there exists a finite number of disjoint topological discs $D_1^j, \dots, D_{n_j}^j$ with diameter less than $\frac{\delta}{2}$ such that $C_j \subset \bigcup_{1\leq k\leq n_j} D_k^j \subset \bigcup_{1\leq k\leq n} \overline{D}_k^j \subset B_j$. For every $i \neq j$, D_k^j intersects C_j and has diameter less than $d(C_i, C_j)/2$. We deduce that if $(j, k) \neq (j', k')$, then $D_k^j \cap D_{k'}^{j'} = \varnothing$. We have found a covering of C by disjoint discs. We can join them to obtain a topological disc D in M that contains C. There exists a homeomorphism $\Phi : D \to \mathbb{R}^2$.

Then the Cantor subset $\Phi \circ j(K)$ of $\mathbb{R}^2$ is homeomorphic to the Cantor subset K of $\mathbb{R}^2$.

We deduce that there exists a homeomorphism $\psi : \mathbb{R}^2 \to \mathbb{R}^2$ that extends the homeomorphism $\Phi \circ j : K \to \Phi \circ j(K)$.[4] Then $\gamma = \Phi^{-1} \circ \psi : \mathbb{T} \to D \subset M$ is a simple continuous curve and (K, γ, h) is a Denjoy subsystem that extends (K, j, h).

3. Proof of Theorem 1.2 and Corollary 1.3

3A. ***Proof of the first point of Theorem 1.2 and of Corollary 1.3.*** Let (X, d) be a metric space. We associate to any continuous dynamical system $F : X \to X$ an equivalence relation $\mathcal{R}_F$ that is defined by

$$x\mathcal{R}_F y \Leftrightarrow \lim_{k\to+\infty} d(F^k x, F^k y) = 0.$$

Observe that if $H : X \to Y$ is a homeomorphism and if X is compact, then we have

$$x\mathcal{R}_F y \Leftrightarrow H(x)\mathcal{R}_{H\circ F\circ H^{-1}} H(y).$$

Hence $X/\mathcal{R}_F$ is compact if and only if $Y/\mathcal{R}_{H\circ F\circ H^{-1}}$ is compact. We denote by $p_F : X \to X/\mathcal{R}_F$ the projection.

Because of Poincaré classification of circle homeomorphisms (see for example [17]), for every orientation preserving homeomorphism h of the circle with an irrational rotation number, we have $\mathcal{R}_h = \mathcal{R}_{h^{-1}}$. Moreover, for such an orientation preserving homeomorphism of the circle with irrational rotation number, the relation is closed and it is also true for the restriction to any invariant compact subset. In this case, the quotient space, that corresponds to a closed equivalence relation on a compact space, is also compact. We then consider a semiconjugation k between the orientation preserving homeomorphism h of the

[4]Observe that this is specific to the 2-dimensional setting and that there exists some homeomorphisms between two Cantor subsets of $\mathbb{R}^3$ that cannot be extended to a homeomorphism of $\mathbb{R}^3$, see Theorem 5 of chapter 18 of [24].

circle with irrational rotation number and a rotation R_α, i.e., k is nondecreasing continuous map onto the circle such that

$$k \circ h = R_\alpha \circ k.$$

Then $k : \mathbb{T} \to \mathbb{T}$ is continuous and we have

$$\forall x, y \in \mathbb{T}, \quad k(x) = k(y) \Leftrightarrow x\mathcal{R}_h y.$$

We denote by K_h the unique nonempty minimal h-invariant compact subset (then K_h is $\mathbb{T}$ or a Cantor subset) and we denote by G_h the set of points of K_h that are $\mathcal{R}_h$ related to another point of $\mathbb{T}$. In other words, G_h is the union of the endpoints of the gaps of the set K_h. Then there exists a unique map $\bar{k} : K_h/\mathcal{R}_h \to \mathbb{T}$ such that $\bar{k} \circ p_h = k$. The definition of the quotient topology implies that $\bar{k}$ is continuous and it is then a homeomorphism from $K_h/\mathcal{R}_h$ to $\mathbb{T}$. Moreover, there exists a unique map $\bar{h} : K_h/\mathcal{R}_h \to K_h/\mathcal{R}_h$ that is the quotient dynamics and that satisfies

$$\bar{h} \circ p_h = p_h \circ h;$$

we have then

$$\bar{k} \circ \bar{h} = R_\alpha \circ \bar{k},$$

i.e., $\bar{k}$ is a conjugation between $\bar{h}$ and R_α.

Let us consider two WDS (K_1, j_1, h_1) and (K_2, j_2, h_2) for the same homeomorphism $f : M \to M$ of a manifold M such that $C = j_1(K_1) = j_2(K_2)$. Let k_i be a semiconjugation between h_i and a rotation R_{a_i}, i.e.,

$$k_i \circ h_i = R_{a_i} \circ k_i.$$

As $f_{|C} = j_i \circ h_i \circ j_i^{-1}$, then $C/\mathcal{R}_f$ is homeomorphic to $K_i/\mathcal{R}_{h_i}$ and so to $\mathbb{T}$. We denote by $p : C \to C/\mathcal{R}_f$ the projection and by $\bar{f} : C/\mathcal{R}_f \to C/\mathcal{R}_f$ the reduced dynamics; see Figure 1.

Then the map $k_i \circ j_i^{-1} : C \to \mathbb{T}$ is a continuous surjection such that

$$k_i \circ j_i^{-1}(x) = k_i \circ j_i^{-1}(y) \Leftrightarrow p(x) = p(y).$$

Hence, there exists a unique homeomorphism $\ell_i : C/\mathcal{R}_f \to \mathbb{T}$ such $\ell_i \circ p = k_i \circ j_i^{-1}$. We have then for all $\bar{x} = p(x) \in C/\mathcal{R}_f$

$$\begin{aligned}
R_{a_i} \circ \ell_i(\bar{x}) &= R_{a_i} \circ k_i \circ j_i^{-1}(x) \\
&= k_i \circ h_i \circ j_i^{-1}(x) \\
&= k_i \circ j_i^{-1} \circ (j_i \circ h_i \circ j_i^{-1})(x) \\
&= k_i \circ j_i^{-1} \circ f(x) \\
&= \ell_i(\bar{f}(\bar{x})).
\end{aligned}$$

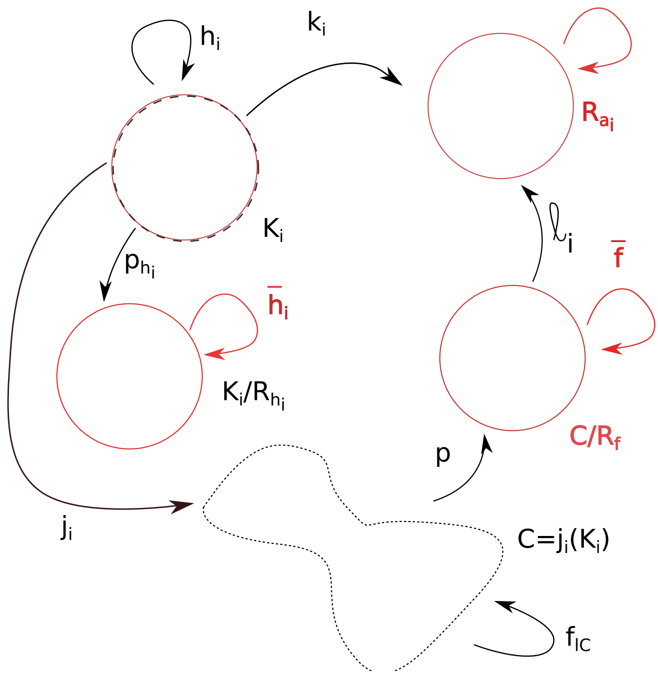


Figure 1. Two WDS, (K_1, j_1, h_1) and (K_2, j_2, h_2) for the same homeomorphism $f : M \to M$ of a manifold M such that $C = j_1(K_1) = j_2(K_2)$.

We deduce that

$$R_{a_1} = \ell_1 \circ \bar{f} \circ \ell_1^{-1} = (\ell_1 \circ \ell_2^{-1}) \circ R_{a_2} \circ (\ell_1 \circ \ell_2^{-1})^{-1}.$$

As R_{a_1} and R_{a_2} are conjugate, we have $a_1 = \pm a_2$. More precisely, $a_1 = a_2$ when the conjugation preserves the orientation (and then is $(x \mapsto x + C)$) and $a_1 = -a_2$ when the conjugation reverses the orientation (and then is $(x \mapsto C - x)$). This gives Corollary 1.3 but doesn't end the proof of the first point of Theorem 1.2.

To finish the proof of this point, let us observe that

$$j_1(G_{h_1} \cap K_1) = j_2(G_{h_2} \cap K_2) = \{x \in C; \exists y \in C; y \neq x, y\mathcal{R}_f x\}$$

is the set of the endpoints of the gaps of $f_{|C}$ (gaps are pairs of points that are ω-asymptotic). We denote this set by C_0.

Thus we have $k_i(G_{h_i}) = k_i \circ j_i^{-1}(C_0) = \ell_i \circ p(C_0)$. We deduce that $k_1(G_{h_1}) = \ell_1 \circ \ell_2^{-1}(k_2(G_{h_2}))$. As $\ell_1 \circ \ell_2^{-1}$ is either a translation $x \mapsto x + C$ or a symmetry $x \mapsto C - x$, there exists $C \in \mathbb{R}$ such that either $k_1(G_{h_1}) = C + k_2(G_{h_2})$ or

$k_1(G_{h_1}) = C - k_2(G_{h_2})$. In other words, the image by k_1 of the union of the gaps of K_{h_1} is the image by a translation or a symmetry of the image by k_2 of the union of the gaps of K_{h_2}. As explained in [13] and [21], this is equivalent to the fact that h_1 and h_2 are conjugated.

3B. ***Proof of the second point of Theorem 1.2.*** For the second point, we know that $j_i : K_i \to C$ defines the order $\prec_{K_i}$. If we identify points that are ω-asymptotic, we obtain a reduced order relation $\bar{\prec}_{K_i}$ on $K_i/\mathcal{R}_{h_i}$ and $C/\mathcal{R}_f$ and $\bar{j}_i : K_i/\mathcal{R}_{h_i} \to C/\mathcal{R}_f$ is an order preserving homeomorphism. As there are only two possible orientations on the circle, we deduce for the two reduced order relations on $C/\mathcal{R}_f$ that either they are equal or they are reverse. To deduce the result for the nonreduced relation, we have just to note that there is only one way to define the closed order relation $\prec_{K_i}$ on C whose reduced relation is $\bar{\prec}_{K_i}$.

4. Proof of Proposition 1.4

Let us begin by explaining some results on the symbolic dynamics of WDS. If (K, j, h) is a WDS for f, we can encode the dynamics in the following noninjective way.[5] Let $x_0 \in j(K)$ be a point of $j(K)$. We consider the interval I_0 of $j(K)$ of the points $y \in j(K)$ such that x_0, y and $f(x_0)$ are in this order for $\prec_K$. We decide that $x_0 \in I_0$ but $f(x_0) \notin I_0$. We denote by $I_1 = j(K)\backslash I_0$ the complement of I_0 in $j(K)$. Then we consider the map that associates to every point $x \in j(K)$ its *itinerary*

$$\mathcal{I}(x) = (n_k(x))_{k\in\mathbb{Z}}$$

where $f^k(x) \in I_{n_k(x)}$. When x_0 is the right end of a gap (a gap is the image by j of the two endpoints of a wandering interval of h) of $j(K)$, I_0 and I_1 are closed and open in $j(K)$ and then $\mathcal{I}$ is continuous.[6]

We assume that x_0 is indeed the right end of a gap of $j(K)$ and we denote by $\mathcal{K}$ the set $\mathcal{I}(K)$. As the Denjoy example is semiconjugate to the rotation with angle $\alpha = \rho(h)$, $\mathcal{I}(x_0)$ is nothing else than the Sturmian sequence that is associated to the rotation R_α, i.e., (see [10]) $n_k(x) = 0$ if and only if $k\alpha \in [0, \alpha)$.

Let us now consider a WDS (K_1, j_1, h_1) that is close to (K, j, h) for the topology that we defined before. Let (x_1, x_0) be the gap whose x_0 is the right end in $j(K)$. Then the interval $\mathcal{G}(\prec_K, x_1, x_0) = \{x_0, x_1\}$ has only two points. As $\mathcal{G}(\prec_{K_1})$ is close to $\mathcal{G}(\prec_K)$ for the Hausdorff distance, there exists two points $y_1, y_0 \in j(K_1)$ that are close to x_1, x_0 and such that $\mathcal{G}(\prec_{K_1}, y_1, y_0)$ is contained

[5]Observe that this is not necessarily the encoding that is given by the subshift of finite type on the horseshoe when this WDS is contained in some horseshoe.

[6]We will prove in Section 5 that when h is a Denjoy example with one gap, then $\mathcal{I}$ is in fact a homeomorphism on its image.

in a neighborhood of $\mathcal{G}(\prec_K, x_1, x_0)$. As we know that $y_1, y_0 \in \mathcal{G}(\prec_{K_1}, y_1, y_0)$, that y_0 is close to x_0 and that y_1 is close to x_1, this implies that $\mathcal{G}(\prec_{K_1}, y_1, y_0)$ is close to $\mathcal{G}(\prec_K, x_1, x_0)$ for the Hausdorff distance. Then we write

$$\mathcal{G}(\prec_{K_1}, y_1, y_0) = \mathcal{G}_0 \cup \mathcal{G}_1$$

where the points of $\mathcal{G}_0$ are close to x_0 and the points of $\mathcal{G}_1$ are close to x_1. Observe that $\mathcal{G}(\prec_{K_1}, y_1, y_0)$ is an interval for $\prec_{K_1}$, where $\prec_{K_1}$ define a (noncircular) total order. Hence we can define $z_1 = \sup \mathcal{G}_1$ and $z_0 = \inf \mathcal{G}_0$. Then $\{z_1, z_0\}$ is a gap of K_1 that is close to $\{x_1, x_0\}$ for the Hausdorff topology. We then associate to z_1 its itinerary exactly as we did for x_1. Let us fix $N \geq 1$. Then if (K_1, j_1, h_1) is close enough to (K, j, h), the two itineraries between $-N$ and N match. But these itineraries determine the first terms of the continued fraction of the two rotations numbers of h_1, h (see [10]). Because they coincide up to the order N, we deduce that $\rho(h_1)$ is close to $\rho(h)$ and then that the rotation number map is continuous.

5. Proof of Theorem 1.5 and Corollary 1.6

5A. *Proof of Theorem 1.5.* We will use the following notions.

Definition. A *n-cylinder* in Σ_2 is a set of sequences $(u_k)_{k\in\mathbb{Z}} \in \{0, 1\}^{\mathbb{Z}}$ such that $u_{-n} = \delta_{-n}; \dots, u_0 = \delta_0; \dots; u_n = \delta_n$ where the δ_is are fixed in $\{0, 1\}$. Defining $d((u_k)_{k\in\mathbb{Z}}, (v_k)_{k\in\mathbb{Z}}) = \max_{k\in\mathbb{Z}} |u_k - v_k|/(|k| + 1)$, observe that a n-cylinder is exactly a closed ball with radius $1/(n + 2)$. A n-word of u is a sequence of n successive terms of u.

Let $f : M \to M$ be a C^k diffeomorphism and let $\mathcal{H}$ be a horseshoe for f. Then there exists a transitive subshift with finite type $\sigma_A : \mathcal{K} \to \mathcal{K}$ that is defined on some shift invariant compact subset $\mathcal{K}$ of Σ_p such that $f_{|\mathcal{H}}$ is C^0 conjugate to σ_A. Then there exists a σ_A-invariant compact subset $\mathcal{K}_0 \subset \mathcal{K}$ and $N \geq 1$ such that $\sigma^N_{A|\mathcal{K}_0}$ is C^0 conjugate to σ_2. Hence we just need to prove the theorem for a σ_2-horseshoe to deduce the general statement. We assume that $f_{|\mathcal{H}} = k \circ \sigma_2 \circ k^{-1}$.

Let $h_\alpha : \mathbb{T} \to \mathbb{T}$ be a Denjoy example with minimal Cantor set C_α such that:

- $\mathbb{T} \backslash C_\alpha$ is the orbit of one interval $I_\alpha = (a_\alpha, b_\alpha)$.
- The rotation number of h is α.

We consider two disjoint segments $I_0(\alpha)$ and $I_1(\alpha)$ in $\mathbb{T}$ such that:

- One endpoint of $I_j(\alpha)$ is in I_α and the other one is in $h_\alpha(I_\alpha)$.
- $I_0(\alpha)$ joins I_α to $h_\alpha(I_\alpha)$ in the direct sense.

Let $k_\alpha : \mathbb{T} \to \mathbb{T}$ be a semiconjugation between h_α and R_α, i.e., $k_\alpha \circ h_\alpha = R_\alpha \circ k_\alpha$. Then, the intervals $I_0(\alpha)$ and $I_1(\alpha)$ are mapped on intervals $K_0 = [0, \alpha]$ and

$K_1 = [\alpha, 1]$. As α is irrational, if $(n_k)_{k\in\mathbb{Z}} \in \Sigma_2$ is any sequence of 0 and 1, there exists at most one $\theta \in \mathbb{T}$ such that, for every $k \in \mathbb{Z}$, we have $\theta + k\alpha \in K_{n_k}$. Let us now consider two points $\theta_1 \neq \theta_2$ in C_α such that for every $k \in \mathbb{Z}$, $h_\alpha^k(\theta_1)$ and $h_\alpha^k(\theta_2)$ belong to a same interval $I_{n_k}(\alpha)$. Then for every $k \in \mathbb{Z}$, the points $k_\alpha \circ h_\alpha^k(\theta_1) = k_\alpha(\theta_1) + k\alpha$ and $k_\alpha \circ h_\alpha^k(\theta_2) = k_\alpha(\theta_2) + k\alpha$ belong to the same interval K_{n_k} and so $k_\alpha(\theta_1) = k_\alpha(\theta_2)$, i.e., θ_1 and θ_2 are the two endpoints of some gap of the Cantor set C_α. So there exists $k \in \mathbb{Z}$ such that $h_\alpha^k(\theta_1)$ and $h_\alpha^k(\theta_2)$ are the two endpoints of I_α for example $I_\alpha = (h_\alpha^k(\theta_1), h_\alpha^k(\theta_2))$. But this implies that $h_\alpha^k(\theta_1) \in I_1(\alpha)$ and $h_\alpha^k(\theta_2) \in I_0(\alpha)$ and this contradicts that for every $k \in \mathbb{Z}$, $h_\alpha^k(\theta_1)$ and $h_\alpha^k(\theta_2)$ belong to a same interval $I_{n_k}(\alpha)$. So we have proved that if we use the notation for $\theta \in C_\alpha$ that $h_\alpha^k(\theta) \in I_{n_k(\theta)}$, then the map $\ell_\alpha : C_\alpha \to \Sigma_2$ defined by $\ell_\alpha(\theta) = (n_k(\theta))_{k\in\mathbb{Z}}$ is injective. As the $I_k(\alpha) \cap C_\alpha$ are open (and closed) in C_α, this map is also continuous and then is a homeomorphism onto its image. This provides a homeomorphism from C_α onto $\ell_\alpha(C_\alpha) \subset \Sigma_2$ such that

$$\forall \theta \in C_\alpha, \ell_\alpha \circ h_\alpha(\theta) = \sigma_2 \circ \ell_\alpha(\theta).$$

The WDS with rotation number $\alpha \in \left[0, \frac{1}{2}\right) \backslash \mathbb{Q}$ that we consider is then $(C_\alpha, j_\alpha = k \circ \ell_\alpha, h_\alpha)$.

Observe that $\ell_\alpha(b_\alpha) = (n_k(b_\alpha))_{k\in\mathbb{Z}}$ is the Sturmian sequence that is associated to the rotation R_α. Let us recall that if $u = (u_k)_{k\in\mathbb{Z}}$ is a Sturmian sequence, then for every $n \geq 1$, there are exactly $n + 1$ n-words in u. As $h_{\alpha|C_\alpha}$ is minimal, the orbit of $\ell_\alpha(b_\alpha)$ under σ_2 is dense in $\ell_\alpha(C_\alpha)$. Now let us fix $\alpha_0 \in [0, 1/2) \backslash \mathbb{Q}$ and $n \geq 1$. There exists $N \geq 1$ such that all the m-words in $\ell_{\alpha_0}(b_{\alpha_0})$ with $m \leq 2n + 1$ are contained in $(n_k(b_{\alpha_0}))_{k\in[-N,N]}$. If α is close enough to α_0, $(n_k(b_\alpha))_{k\in[-N,N]}$ is equal to $(n_k(b_{\alpha_0}))_{k\in[-N,N]}$. As $\ell_\alpha(b_\alpha) = (n_k(b_\alpha))_{k\in\mathbb{Z}}$ is Sturmian, this implies that all the m-words in $\ell_\alpha(b_\alpha)$ with $m \leq 2n+1$ are contained in $(n_k(b_\alpha))_{k\in[-N,N]} = (n_k(b_{\alpha_0}))_{k\in[-N,N]}$, which means that the distance between the σ_2 orbits of $\ell_\alpha(b_\alpha)$ and $\ell(b_{\alpha_0})$ is less than $1/(n + 2)$. This implies that $\ell_\alpha(C_\alpha)$ is $\frac{1}{n}$-close to $\ell_{\alpha_0}(C_{\alpha_0})$. Hence $j_\alpha(C_\alpha) = k(\ell_\alpha(C_\alpha))$ is close to $j_{\alpha_0}(C_{\alpha_0}) = k(\ell_{\alpha_0}(C_{\alpha_0}))$.

Now we want to prove that $\mathcal{G}(\prec_{C_\alpha})$ is close to $\mathcal{G}(\prec_{C_{\alpha_0}})$. In a equivalent way, we can work in Σ_2 instead of $\mathcal{H}$ and assume that the graphs of $\mathcal{G}(\prec_{C_\alpha})$ and $\mathcal{G}(\prec_{C_{\alpha_0}})$ are in $(\Sigma_2)^3$. Then the intersection of the n cylinder $C(\delta_{-n}, \dots, \delta_0, \dots, \delta_n) = \{(u_k)_{k\in\mathbb{Z}}; \forall k \in [-n, n], u_k = \delta_k\}$ with $\ell_\alpha(C_\alpha)$ is an interval for the order $\prec_{C_\alpha}$, that is before encoding the intersection of intervals $\bigcap_{k=-n}^{k=n} h_\alpha^{-k}(I_{\delta_k})$. This interval is nonempty if and only if $(\delta_i)_{i\in[-n,n]}$ is a $(2n+1)$-word of the Sturmian sequence $(n_k(b_{\alpha_0}))_{k\in\mathbb{Z}}$ for α_0. Now let us fix $n \geq 1$. There exists $N \geq 1$ such that all the admissible $(2n + 1)$-words of $(n_k(b_{\alpha_0}))_{k\in\mathbb{Z}}$ are contained in the sequence $(n_k(b_{\alpha_0}))_{k\in[-N,N]}$. There exists a neighborhood V of α_0 in $\mathbb{T}$ such that, for every $\alpha \in V$, we have:

- $\forall k \in [-N, N]$, $n_k(b_\alpha) = n_k(b_{\alpha_0})$.
- The intervals
$$C(n_{k-n}(b_\alpha), \dots, n_k(b_\alpha), \dots, n_{k+n}(b_\alpha)) \cap \ell_\alpha(C_\alpha)$$
and
$$C(n_{k-n}(b_{\alpha_0}), \dots, n_k(b_{\alpha_0}), \dots, n_{k+n}(b_{\alpha_0})) \cap \ell_\alpha(C_{\alpha_0})$$
for $n - N \le k \le N - n$ (that are $\frac{1}{n}$-close to each other) are in the same order, for $\prec_{K_\alpha}$ for the first ones and for $\prec_{K_{\alpha_0}}$ for the second ones, because it is the order of this intervals for the two rotations.

We deduce that $\mathcal{G}(\prec_{C_\alpha})$ is $\frac{1}{n}$-close to $\mathcal{G}(\prec_{C_{\alpha_0}})$.

5B. ***Proof of Corollary 1.6.*** It is a corollary of Proposition 1.1 and Theorem 1.5.

6. Proof of Theorem 1.7 and Corollary 1.8

Definition. Let $f : \mathbb{A} \to \mathbb{A}$ be a diffeomorphism. Then f is an exact symplectic twist map if:

- The diffeomorphism f is isotopic to identity.
- If $\lambda = \pi_2 d\pi_1$ is the Liouville 1-form on $\mathbb{A}$, then $f^*\lambda - \lambda$ is exact.
- If $F : \mathbb{R}^2 \to \mathbb{R}^2$ is a lift of f, for every $x \in \mathbb{R}$, the map $y \in \mathbb{R} \mapsto \pi_1 \circ f(x, y)$ is a C^1 diffeomorphism onto $\mathbb{R}$.

6A. ***Proof of Theorem 1.7.*** We assume that $f : \mathbb{T} \times \mathbb{R} \to \mathbb{T} \times \mathbb{R}$ is an exact symplectic twist map and that $F : \mathbb{R}^2 \to \mathbb{R}^2$ is one of its lifts. We assume that $\mathcal{A}_r^+$ is uniformly hyperbolic for some rational number $r \in \mathbb{Q}$. We want to prove that there exists a horseshoe $\mathcal{H}_r^+$ for some f^n and $\varepsilon > 0$ such that:

- $\mathcal{H}_r^+$ contains $\mathcal{A}_r^+$.
- Every Aubry–Mather set with rotation number in $(r, r + \varepsilon)$ is contained in $\mathcal{H}_r^+$.
- Every point in $\mathcal{H}_r^+$ has no conjugate points, i.e., has its orbit that is locally minimizing.

We write $r = \frac{p}{q}$ as an irreducible fraction. As $\mathcal{A}_r^+$ is a compact uniformly hyperbolic set, it has a finite number of q-periodic points. We denote them by $x_1, \dots, x_n$ in the usual cyclic order along $\mathbb{T}$ (for the first projection). Then $\mathcal{A}_r^+$ is the union of these periodic points and some heteroclinic orbits between these heteroclinic points; see, e.g., [4]. Moreover, such heteroclinic orbit for f^q that is contained in $\mathcal{A}_r^+$ can only connect an x_k to x_{k+1} (with $x_{n+1} = x_1$). If two heteroclinic orbits in $\mathcal{A}_r^+$ connect the same x_k to x_{k+1}, we can choose an order on the union of these two orbits $(y_j)_{j\in\mathbb{Z}}$ and $(z_j)_{j\in\mathbb{Z}}$ for f^q such that

$$x_k < \cdots < y_{j-1} < z_{j-1} < y_j < z_j < y_{j+1} < z_{j+1} < \cdots < x_{k+1}.$$

Let $\varepsilon > 0$ be an expansivity constant for $f^q_{|\mathcal{A}_r^+}$ and let K be a Lipschitz constant of the Aubry–Mather set $\mathcal{A}_r^+$ as a graph. Then for some j we have $d(y_j, z_j) \geq \varepsilon$. Hence the distance between the projections of y_j, z_j on the first factor is more than $\varepsilon/(1+K)$ for some j. Of course we can use the same argument for any finite set of heteroclinic orbits $(y_j^1)_{j\in\mathbb{Z}}, \dots, (y_j^N)_{j\in\mathbb{Z}}$ connecting x_k to x_{k+1} in $\mathcal{A}_r^+$. We have

$$x_k \cdots < y_{j-1}^1 < \cdots < y_{j-1}^N < y_j^1 < \cdots < y_j^N < \cdots < x_{k+1},$$

and we find N integers $j_1, \dots, j_N$ such that (with the convention $y_j^{N+1} = y_{j+1}^1$)

$$\forall i \in \{0, N\},\, d(y_{j_i}^i, y_{j_i}^{i+1}) \geq \varepsilon.$$

Then the intervals $(\pi_1(y_{j_1}^1), \pi_1(y_{j_1}^2)), \dots, (\pi_1(y_{j_N}^N), \pi_1(y_{j_N}^{N+1}))$ are disjoint intervals in $\mathbb{T}$ with length larger or equal to $\varepsilon/(K+1)$. This implies that $N \leq (K+1)/\varepsilon$. Hence $\mathcal{A}_r^+$ is a hyperbolic set that is the union of periodic orbits and of a *finite* number of heteroclinic orbits. Moreover, there always exists at least a heteroclinic connection in $\mathcal{A}_r^+$ between two adjacent periodic points in $\mathcal{A}_r^+$ (see [4]). Hence $\mathcal{A}_r^+$ is a cycle of transverse heteroclinic intersections with period q (see definition in the Appendix).

We introduce the notation $p : \mathbb{R}^2 \to \mathbb{T} \times \mathbb{R}$ for the usual projection. When $E \subset \mathbb{T} \times \mathbb{R}$, we denote by $\tilde{E} = p^{-1}(E)$ its lift.

Let us fix a neighborhood $\mathcal{N}$ of $\mathcal{A}_r^+$. Then $\mathcal{A}_r^- \backslash \mathcal{N}$ is finite because $\mathcal{A}_r^-$ is the union of $\mathcal{A}_r^- \cap \mathcal{A}_r^+$ and the union of a finite number of orbits that are homoclinic to $\mathcal{A}_r^- \cap \mathcal{A}_r^+$. For every $x \in \tilde{\mathcal{A}}_r^- \backslash \tilde{\mathcal{N}}$, we have $\pi_1 \circ F^q(x) < \pi_1(x) + p$. Then $\varepsilon = \min\{\pi_1(x) + p - \pi_1 \circ F^q(x);\, x \in \tilde{\mathcal{A}}_r^- \backslash \tilde{\mathcal{N}}\}$ is a positive number. We introduce the open set

$$\mathcal{U} = p\Big(\big\{x \in \mathbb{R}^2;\, \pi_1(x) + p - \pi_1 \circ F^q(x) > \tfrac{\varepsilon}{2}\big\}\Big)$$

that contains $\mathcal{A}_r^- \backslash \mathcal{N}$. Then $\mathcal{N} \cup \mathcal{U}$ is a neighborhood of $\mathcal{A}_r^+ \cup \mathcal{A}_r^-$. As the rotation number map is continuous and as the union of minimizing orbits is closed, there exists $\eta > 0$ such that every Aubry–Mather set with rotation number in $(r - \eta, r + \eta)$ is in $\mathcal{N} \cup \mathcal{U}$. If moreover $\mathcal{A}$ is an Aubry–Mather set with rotation number in $(r, r + \eta)$, then we have

$$\forall x \in \tilde{\mathcal{A}}, \quad \pi_1 \circ F^q(x) > \pi_1(x) + p.$$

Hence $\mathcal{A} \cap \mathcal{U} = \varnothing$ and thus $\mathcal{A} \subset \mathcal{N}$. We have the proved that there exists $\eta > 0$ such that every Aubry–Mather set with rotation number in $(r, r+\eta)$ is contained in $\mathcal{N}$.

We then use Section A3 of the Appendix. There exists $N \geq 1$ and a neighborhood $\mathcal{N}$ of the cycle of transverse heteroclinic intersections with period q $\mathcal{A}_r^+$, such that the maximal f^{qN} invariant set contained in $\mathcal{N}$ is a horseshoe $\mathcal{H}_r^+$ for f^{qN} (see Definition). This horseshoe then satisfies the two first points of Theorem 1.7.

Moreover, observe that along $\mathcal{A}_r^+$, there exists a Df invariant field of half-lines (the half Green bundles g_+ of G_+, see [1]) transverse to the vertical fiber, that is a subset of the unstable bundle along $\mathcal{A}_r^+$. By continuity of the unstable bundle along any hyperbolic set, we can extend g_+ to the whole $\mathcal{H}_r^+$ into a field of half-line that are contained in the unstable bundle. If $\mathcal{N}$ is small enough, this field as well as its first qN images by Df is also transverse to the vertical. This implies the last point of Theorem 1.7.

6B. ***Proof of Corollary 1.8.*** We use the results of P. Le Calvez that are in [19]. We consider the G_δ subset $\mathcal{G}$ of the set of C^k symplectic twist diffeomorphisms f whose elements satisfy the following conditions:

- If x is a periodic point for f with smallest period q, none of the eigenvalues of $Df^q(x)$ is a root of unity.
- All the heteroclinic intersections between invariant manifolds of hyperbolic periodic points are transverse.

It is proved in [19] that all the Aubry–Mather sets that have a rational rotation number are hyperbolic. By Theorem 1.7, for every $r \in \mathbb{Q}$, there exists an open interval $(r - \varepsilon_r, r + \varepsilon_r)$ such that every Aubry–Mather set with rotation number in this interval is contained in the horseshoe $\mathcal{H}_r^+$ or the horseshoe $\mathcal{H}_r^-$. This gives the conclusion of the corollary for

$$U(f) = \bigcup_{r \in \mathbb{Q}} (r - \varepsilon_r, r + \varepsilon_r).$$

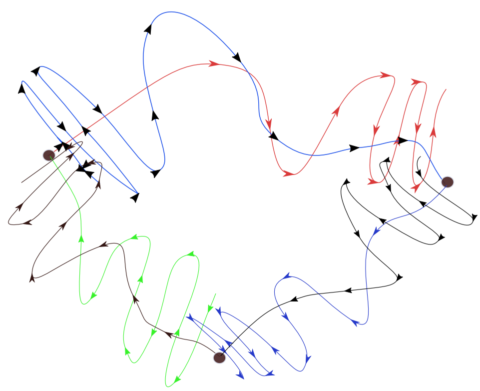
Appendix: On horseshoes

In this section, we will be interested in some horseshoes that are related to the heteroclinic intersections. Generally, authors look at what happens close to one homoclinic point associated to a periodic point (in [7], the authors also consider heteroclinic connections for two fixed points). But to apply our results to Aubry–Mather sets, we will need to study the horseshoes that can be built by using a (circular) family of periodic points and heteroclinic intersections. Let us explain this now.

A1. *Introduction to heteroclinic horseshoes.* We will consider heteroclinic cycles. For a diffeomorphism $f : M \to M$ of a surface, we will call a q-periodic point x a *saddle* if the two eigenvalues λ, μ of $Df^q(x)$ are positive and such that $\mu < 1 < \lambda$.

Definition. Let $f : M \to M$ be a surface diffeomorphism. A *cycle of transverse heteroclinic intersections with period* 1 is determined by:

- A finite cyclically ordered set of saddle hyperbolic fixed points $x_{n+1} = x_1, \dots, x_n$ with an orientation on each submanifold $W^s(x_i)$ and $W^u(x_i)$.
- For every $k \in [1, n]$ a nonzero finite number n_k of transverse heteroclinic points $y_1^k, \dots, y_{n_k}^k$ in $W^u(x_k, f) \cap W^s(x_{k+1}, f)$ such that $x_k, y_1^k, \dots, y_{n_k}^k$ are in this order along $W^u(x_k, f)$ and $y_1^k, \dots, y_{n_k}^k, x_{k+1}$ also along $W^s(x_{k+1}, f)$.[7] Moreover, they define different orbits:



Definition. Let $f : M \to M$ be a surface diffeomorphism and let $q \geq 1$ be an integer. A *cycle of transverse heteroclinic intersections with period* q is determined by:

- A finite cyclically ordered set of saddle hyperbolic q-periodic points $x_{nq+1} = x_1, \dots, x_{nq}$ such that this order is preserved by f with an orientation on each submanifold $W^s(x_i)$ and $W^u(x_i)$; we assume that every set $\{x_i, x_{i+n}, \dots x_{i+(q-1)n}\}$ is an orbit.
- For every $k \in [1, qn]$ a nonzero finite number n_k of transverse heteroclinic points $y_1^k, \dots, y_{n_k}^k$ in $W^u(x_k, f) \cap W^s(x_{k+1}, f)$ such that $x_k, y_1^k, \dots, y_{n_k}^k$ are in this order along $W^u(x_k, f)$ and $y_1^k, \dots, y_{n_k}^k, x_{k+1}$ also along $W^s(x_{k+1}, f)$.[8] Moreover, they define different orbits.

[7] This implies that the y_i^k are all on a same branch of $W^u(x_k, f)$ and $W^s(x_{k+1}, f)$.
[8] This implies that the y_i^k are all on a same branch of $W^u(x_k, f)$ and $W^s(x_{k+1}, f)$.

- We also assume $n_{k+n} = n_k$, that x_k and x_{n+k} are on a same orbit and that y_j^k and y_j^{n+k} are on the same orbit.

Notation. Now we consider a cycle of transverse heteroclinic intersections $\mathcal{H}$ with period q for f that is given by the x_k and the y_j^k as before. We denote by $K(\mathcal{H})$ the union of the orbits of the x_k and the y_j^k.

Remark. Observe that $K(\mathcal{H})$ is a f-invariant compact set that is uniformly hyperbolic. We denote by E the tangent bundle TM. By [28], we can translate the hyperbolicity condition by using some cones. This is an open condition and we can extend these cones to a compact neighborhood $\mathcal{V}$ of $K(\mathcal{H})$ such that:

- There exists a continuous splitting $E = E^1 \oplus E^2$ on $\mathcal{V}$ that coincides with $E = E^s \oplus E^u$ on $K(\mathcal{H})$ and two norms $|\cdot|_i$ on E^i such that
$$C_x = \{v = v_1 + v_2, v_1 \in E_x^1, v_2 \in E_x^2, |v_1|_{1,x} \le |v_2|_{2,x}\};$$
the family $(C_x)_{x\in\mathcal{V}}$ is the associated cone field; the dual cone field is the family $(C_x^*)_{x\in\mathcal{V}}$ defined by $C_x^* = E_x \setminus \operatorname{int} C_x$.
- For some constant $c > 1$, we have for every $x \in \mathcal{V}$, $v_1 \in E_x^1$ and $v_2 \in E_x^2$
$$c^{-1}\|v_1 + v_2\| \le \max\{|v_1|_{1,x}, |v_2|_{2,x}\} \le c\|v_1 + v_2\|_x.$$
- There exists an integer $m \ge 1$ and a constant $\mu > 1$ so that:
  (1) For $x \in \mathcal{V}$, $Df(C_x) \subset \widetilde{C}_{\mu,f(x)}$ where
$$\widetilde{C}_{\lambda,x} = \{v = v_1 + v_2 \in E_x; \mu|v_1|_{1,x} \le |v_2|_{2,x}\}.$$
  (2) For $x \in \mathcal{V}$, for $v \in C_x$, $\|Df^m(v)\|_{f^m(x)} \ge \mu.\|v\|_x$.
  (3) For $x \in \mathcal{V}$, for $v \in C_x^*$, $\|Df^{-m}(v)\|_{f^{-m}(x)} \ge \mu.\|v\|_x$.

We define
$$\mathcal{K}(\mathcal{V}) = \bigcap_{k\in\mathbb{Z}} f^k(\mathcal{V}).$$
Then $\mathcal{K}(\mathcal{V})$ is compact and hyperbolic. Let $\varepsilon > 0$ be a constant of expansivity, i.e., such that
$$\forall x, y \in \mathcal{K}(\mathcal{V}), (\forall k \in \mathbb{Z}, d(f^k x, f^k y) < \varepsilon) \Rightarrow x = y.$$

Choosing possibly a smaller neighborhood, we can assume that the diameter of every connected component of $\mathcal{V}$ is smaller than ε, and also that $\mathcal{V}$ has a finite number N of connected components that all meet $K(\mathcal{V})$.

We denote by $\mathcal{C}_1, \dots, \mathcal{C}_N$ the connected components of $\mathcal{V}$ and define the itinerary function $H : \mathcal{K}(\mathcal{V}) \to \Sigma_N$ by $f^k(x) \in \mathcal{C}_{H(x)_k}$. Hence the k-th component of $H(x)$ corresponds to the connected component of $\mathcal{V}$ that contains $f^k x$. Then

H is continuous. Because of the expansiveness property, H is injective, so H is a homeomorphism from $\mathcal{K}(\mathcal{V})$ onto $H(\mathcal{K}(\mathcal{V})) \subset \Sigma_N$ such that

$$\forall x \in \mathcal{K}(\mathcal{V}), \quad \sigma \circ H(x) = H \circ f(x).$$

But in fact, we are looking for dynamics that are actually conjugate to a transitive subshift of finite type. In order to build such dynamics, we will be more precise for the choice of $\mathcal{V}$ in Section A3.

A2. *Rectangles partition.* Here we explain how a good family of rectangles, called a rectangles partition, is useful to build a locally maximal invariant hyperbolic sets. We introduce geometric Markov partition, that are reminiscent from the Markov partition and that are studied in [26], but as we didn't find the exact setting that we use elsewhere, we give some details.

We assume that $f : M \to M$ is a C^1 diffeomorphism and that $\mathcal{V} \subset M$ is an open set endowed with two continuous families of open symmetric cones, the unstable one $x \in \mathcal{V} \mapsto C^u(x) \subset T_x M$ and the stable one $x \in \mathcal{V} \mapsto C^s(x) \subset T_x M$ such that, if we denote the closure of a set A by $\bar{A}$, we have for a constant $\lambda \in (0, 1)$:

- $\forall x \in \mathcal{V} \cap f^{-1}(\mathcal{V})$, $Df(\overline{C^u}(x)) \subset C^u(f(x))$ and $Df(C^s(x)) \supset \overline{C^s}(f(x))$.
- $\forall x \in \mathcal{V}$, $\forall v \in C^u(x)$, $\|Df(x)v\| \geq \frac{1}{\lambda}\|v\|$ and $\forall x \in \mathcal{V}$, $\forall v \in C^s(x)$,
$$\|Df(x)v\| \leq \lambda \|v\|.$$
- $\forall x \in \mathcal{V}$, $C^u(x) \cap C^s(x) = \{\vec{0}\}$.

Definition.
- A C^1-embedding $\gamma : [a, b] \to \mathcal{V}$ define a *unstable* (*resp. stable*) *curve* if $\forall t \in [a, b]$, $\gamma'(t) \in C^u(\gamma(t))$ (resp. $\forall t \in [a, b]$, $\gamma'(t) \in C^s(\gamma(t))$).
- A *rectangle* R is given by an embedding $\Phi_R : [0, 1]^2 \to R \subset \mathcal{V}$ such that for every $t \in [0, 1]$, $\Phi_R(\{t\} \times [0, 1])$ (resp. $\Phi_R([0, 1] \times \{t\})$) defines a stable (resp. unstable) curve.
- Then the *stable* (*resp. unstable*) boundary of R is $\partial^s R = \Phi_R(\{0, 1\} \times [0, 1])$ (resp. $\partial^u R = \Phi_R([0, 1] \times \{0, 1\})$.
- A rectangle R' is a *stable* (*resp. unstable*) *subrectangle* of a rectangle R if $R' \subset R$ and $\partial^u R' \subset \partial^u R$ (resp. $\partial^s R' \subset \partial^s R$).

Remarks.
(1) Observe that a stable curve is always transversal to an unstable curve, and that when their mutual intersection with some rectangle is nonempty, then it is a point.
(2) To a given rectangle R, we can associate different embeddings Φ_R and then different stable and unstable foliations $\mathcal{F}^s(R)$ and $\mathcal{F}^s(R)$.
(3) The stable and unstable boundaries are independent from the embedding.

(4) When $\gamma \subset \mathcal{V}$ is a unstable (stable) curve, every connected component of $f(\gamma) \cap \mathcal{V}$ (resp. $f^{-1}(\gamma) \cap \mathcal{V}$) is also an unstable (resp. stable) curve.

Let us now introduce the notion of rectangles partition that we will use.

Definition. A *rectangles partition* is a finite set $\{\mathcal{R}_1, \dots, \mathcal{R}_m\}$ of disjoint rectangles of $\mathcal{V}$ such that, if we use the notation $\mathcal{R}_{jk} = f(\mathcal{R}_j) \cap \mathcal{R}_k$, we have:

- For every $j, k \in \{1, \dots, m\}$, either $\mathcal{R}_{jk} = \varnothing$ or $\mathcal{R}_{jk}$ is an unstable subrectangle of $\mathcal{R}_k$. When $\mathcal{R}_{jk} \neq \varnothing$, we use the notation
$$\mathcal{R}_j \xrightarrow{f} \mathcal{R}_k,$$
and we say that we have a *transition* from $\mathcal{R}_j$ to $\mathcal{R}_k$.
- When $\mathcal{R}_{jk} \neq \varnothing$, then $f(\partial^u \mathcal{R}_j) \cap \partial^u \mathcal{R}_k = \varnothing$ and $f(\partial^s \mathcal{R}_j) \cap \partial^s \mathcal{R}_k = \varnothing$.

An *admissible sequence* is then $(i_k)_{k\in\mathbb{Z}} \in \{1, \dots, m\}^{\mathbb{Z}} = \Sigma_m$ such that
$$\forall k \in \mathbb{Z}, \mathcal{R}_{i_k} \xrightarrow{f} \mathcal{R}_{i_{k+1}}.$$

Remark. Observe that $\mathcal{R}_j \xrightarrow{f} \mathcal{R}_k$ if and only if $\mathcal{R}_k \xrightarrow{f^{-1}} \mathcal{R}_j$ (the stable boundary for f^{-1} is then the unstable one for f).

Notation. We denote by $\Lambda(\mathcal{R}_1, \dots, \mathcal{R}_m)$ the maximal invariant set that is contained in $\mathcal{R}_1 \cup \dots \cup \mathcal{R}_m$, i.e.,
$$\Lambda(\mathcal{R}_1, \dots, \mathcal{R}_m) = \bigcap_{k\in\mathbb{Z}} f^k(\mathcal{R}_1 \cup \dots \cup \mathcal{R}_m).$$

Observe that this set is hyperbolic. Hence there exist a stable and an unstable submanifold at every of its points. We even have the following result.

Proposition A.1. *If $x \in \Lambda(\mathcal{R}_1, \dots, \mathcal{R}_m) \cap \mathcal{R}_{i_0}$, then the connected component of $W^s(x) \cap \mathcal{R}_{i_0}$ (resp. $W^u(x) \cap \mathcal{R}_{i_0}$) that contains x is a stable (resp. unstable) curve that joins the two connected components of $\partial^u \mathcal{R}_{i_0}$ (resp. $\partial^s \mathcal{R}_{i_0}$).*

Proof. As $\Lambda(\mathcal{R}_1, \dots, \mathcal{R}_m)$ is hyperbolic, there exists $\varepsilon > 0$ such that for every $x \in \Lambda(\mathcal{R}_1, \dots, \mathcal{R}_m)$, the length of every branch of $W^s(x)$ is greater than ε. We denote by $\mathcal{M} > 0$ a lower bound of the length of the stable curves contained in one $\mathcal{R}_{j_0}$ that join the two components of $\partial^u \mathcal{R}_{j_0}$. Then we choose $N \geq 1$ such that $\frac{\varepsilon}{\lambda^N} > \mathcal{M}$. Then if j_0 is such that $f^N(x) \in \mathcal{R}_{j_0}$, the curve $f^{-N}(W^s(f^N(x)) \cap \mathcal{R}_{j_0})$ is contained in $W^s(x)$ and crosses the two connected components of $\partial^u \mathcal{R}_{i_0}$. This gives the wanted result. □

Different versions of the following proposition exist in different settings. We will provide a proof for the convenience of the reader.

Proposition A.2. *Let $\{\mathcal{R}_1, \dots, \mathcal{R}_m\}$ be a rectangle partition for f in $\mathcal{V}$. Let $(i_k)_{k\in\mathbb{Z}} \in \Sigma_m$ be a sequence. The two following assertions are equivalent*:

- *$(i_k)_{k\in\mathbb{Z}}$ is an admissible sequence.*
- *There exists a unique point $x \in \mathcal{R}_{i_0}$ such that*

$$\forall k \in \mathbb{Z}, \quad f(x) \in \mathcal{R}_{i_k}.$$

Proof. We just prove the direct implication, the only one that is nontrivial. Hence we assume that $(i_k)_{k\in\mathbb{Z}}$ is an admissible sequence.

We begin by proving the existence of x. For every $n \in \mathbb{N}$, we introduce the notation

$$D_n^s = \bigcap_{k=0}^{n} f^{-k}(\mathcal{R}_{i_k}) \quad \text{and} \quad D_n^u = \bigcap_{k=0}^{n} f^{k}(\mathcal{R}_{i_{-k}}).$$

Then $(D_n^u)_{n\in\mathbb{N}}$ (resp. $(D_n^s)_{n\in\mathbb{N}}$) is a decreasing sequence of unstable (resp. stable) rectangles of $\mathcal{R}_{i_0}$. Hence $(K_n)_{n\in\mathbb{N}} = (D_n^u \cap D_n^s)_{n\in\mathbb{N}}$ is a decreasing sequence of nonempty compact subsets of $\mathcal{R}_{i_0}$. Their intersection contains at least one point x, and this point satisfies

$$\forall k \in \mathbb{Z}, \quad f^k(x) \in \mathcal{R}_{i_k}.$$

We now want to prove the unicity of x. We introduce the notation

$$D_\infty^u = \bigcap_{n\in\mathbb{N}} D_n^u \quad \text{and} \quad D_\infty^s = \bigcap_{n\in\mathbb{N}} D_n^s.$$

Lemma A.3. *The set D_∞^u (resp. D_∞^s) is an unstable curve that joins the two connected components of $\partial^s R_{i_0}$ (resp. $\partial^u R_{i_0}$). More precisely, if $\{x\} = D_\infty^u \cap D_\infty^s$, then $D_\infty^u \subset W^u(x)$ and $D_\infty^s \subset W^s(x)$.*

Let us prove Lemma A.3. We just prove the result for D_∞^s. As every D_n^s is a stable rectangle, D_∞^s is a connected compact set that joins the two connected components of $\partial^u R_{i_0}$. To prove that it is a (at least continuous) curve, we just need to prove that it intersects every leaf of the unstable foliation $\mathcal{F}^u(\mathcal{R}_{i_0})$ of $\mathcal{R}_{i_0}$ at most once. So let $\mathcal{L}^u$ be an unstable leaf of $\mathcal{R}_{i_0}$ and let x, y be two points of $D_\infty^s \cap \mathcal{L}^u$. We denote by $\mathcal{L}^u[x, y]$ the arc of $\mathcal{L}^u$ that has for endpoints x and y. Observe that $\mathcal{L}^u[x, y] \subset \mathcal{R}_{i_0}$ Then for every $n \in \mathbb{N}$, the connected component $\mathcal{L}_n$ of $f^n(\mathcal{L}^u) \cap \mathcal{R}_{i_n}$ that contains $f^n(\mathcal{L}^u[x, y])$ is an unstable curve of $\mathcal{R}_{i_n}$.[9] Let $\mathcal{B}$ a common upper bound of the lengths of the unstable leaves that are contained in some rectangle of the Markov partition (observe that these curves are uniformly Lipschitz graphs in the charts $\Phi_{\mathcal{R}_i}$). Then we have length$(\mathcal{L}_n) \leq \mathcal{B}$ and we

[9] Observe that the endpoints of this curve are indeed in $\mathcal{R}_{i_n}$ and hence by the point (4) of the remark, $f^n(\mathcal{L}^u[x, y]) \subset \mathcal{R}_{i_n}$.

deduce $\forall n \in \mathbb{N}$, $\text{length}(\mathcal{L}^u[x, y]) = \text{length}(f^{-n}(\mathcal{L}_n)) \leq \lambda^n \mathcal{B}$. So $x = y$ and D^s_∞ intersects every unstable leaf at most once, and so exactly once because D^s_∞ is a connected set that joins the two connected components of $\partial^u R_{i_0}$.

Moreover, observe that D^s_∞ contains the connected component C^s of $W^s(x) \cap \mathcal{R}_{i_0}$ that contains x. This implies that $D^s_\infty = C^s$ is a smooth stable curve (see Proposition A.1). $\square$

A3. ***Precise construction of heteroclinic horseshoes.*** We use the same notations as in Section A1.

Remark. As explained before, we want to build an invariant set that is close (for the Hausdorff distance) to $K(\mathcal{H})$. That is why we need to use all the heteroclinic intersections that are in $K(\mathcal{H})$ in our construction. Another approach could be to use the transitivity of the relation $\mathcal{R}$ defined on q-periodic points by: $x\mathcal{R}y$ if $W^s(x, f)$ and $W^u(y, f)$ have a transverse heteroclinic intersection. This implies that every periodic point in $K(\mathcal{H})$ has a homoclinic intersection and thus we could use directly Smale's method (see [27]) to build a homoclinic horseshoe. Unfortunately, a neighborhood of this homoclinic orbit is not necessarily a neighborhood of the whole $K(\mathcal{H})$ and so this horseshoe is in general not close to $K(\mathcal{H})$ for the Hausdorff distance, so doesn't give us what we want.

Theorem A.4. *There exists $N \geq 1$ and a neighborhood $\mathcal{N}$ of the cycle $K(\mathcal{H})$ of transverse heteroclinic intersections with period q, such that the maximal f^{qN} invariant set contained in $\mathcal{N}$ is a horseshoe Λ for f^{qN} (see Definition).*

As $K(\mathcal{H})$ is (uniformly) hyperbolic, we can chose a neighborhood $\mathcal{V}$ of $K(\mathcal{H})$, a constant $\lambda \in (0, 1)$ and two continuous families of open symmetric cones (see Section A1) the unstable one $x \in \mathcal{V} \mapsto C^u(x) \subset T_xM$ and the stable one $x \in \mathcal{V} \mapsto C^s(x) \subset T_xM$ such that, if we denote the closure of a set A by $\bar{A}$, we have:

- $\forall x \in \mathcal{V} \cap f^{-1}(\mathcal{V})$, $Df(\overline{C^u}(x)) \subset C^u(f(x))$ and $Df(C^s(x)) \supset \overline{C^s}(f(x))$.
- $\forall x \in \mathcal{V}$, $\forall v \in C^u(x)$, $\|Df(x)v\| \geq \frac{1}{\lambda}\|v\|$ and $\forall x \in \mathcal{V}$, $\forall v \in C^s(x)$,
$$\|Df(x)v\| \leq \lambda\|v\|.$$
- $\forall x \in \mathcal{V}$, $C^u(x) \cap C^s(x) = \{\vec{0}\}$.

Notation. For every x_k, we denote by $B^s(x_k)$ the branch of $W^s(x_k)$ that contains the y_i^{k-1}s and by $B^u(x_k)$ the branch of $W^u(x_k)$ that contains the y_i^ks. Then we choose a small (curved) rectangle R_k with two sides on $B^s(x_k)$ and $B^u(x_k)$; see Figure 2.

We denote by δ_k^u and δ_k^s the size of R_k along $B^u(x_k)$ and $B^s(x_k)$.

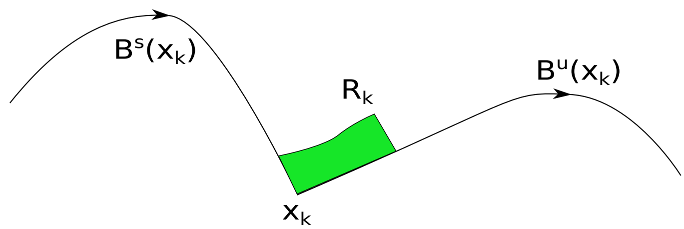


Figure 2. A small (curved) rectangle R_k with two sides on $B^s(x_k)$ and $B^u(x_k)$.tw.

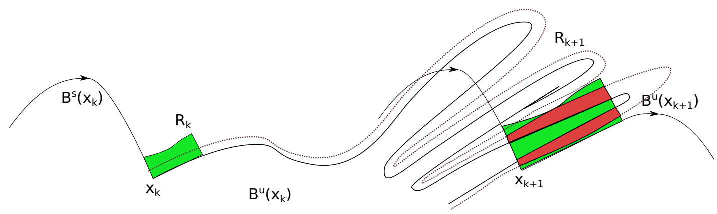


Figure 3. The subrectangles of R_{k+1} which are connected components of $f^{qN_k}(R_k) \cap R_{k+1}$ that meets $W^s_{\mathrm{loc}}(x_{k+1})$ at some point of the orbit of y^k_i.

Then we look at the Poincaré map for f^q from R_k onto R_{k+1}. Adjusting the quantities δ^u and δ^s, we can find some N_k such that $f^{qN_k}(R_k) \cap R_{k+1}$ contains the union of a finite numbers of unstable rectangles. There are two cases:

- When $n = q = 1$, there are $n_0 + 1$ rectangles: R^0_0 that contains x_0 and R^1_0, R^2_0, ..., $R^{n_0}_0$ such that R^i_0 is a connected component of $f^{qN_0}(R_0) \cap R_0$ that meets $W^s_{\mathrm{loc}}(x_0)$ at some point of the orbit of y^0_i.
- When $nq > 1$, there are n_k unstable subrectangles of R_{k+1} that we denote by R^1_{k+1}, R^2_{k+1}, ..., $R^{n_k}_{k+1}$ such that R^i_{k+1} is a connected component of $f^{qN_k}(R_k) \cap R_{k+1}$ that meets $W^s_{\mathrm{loc}}(x_{k+1})$ at some point of the orbit of y^k_i;[10] see Figure 3.

[10]Observe that $f^{qN_k}(R_k) \cap R_{k+1}$ can have other connected components, for example connected components that correspond to other heteroclinic intersections. We just work with some chosen heteroclinic points.

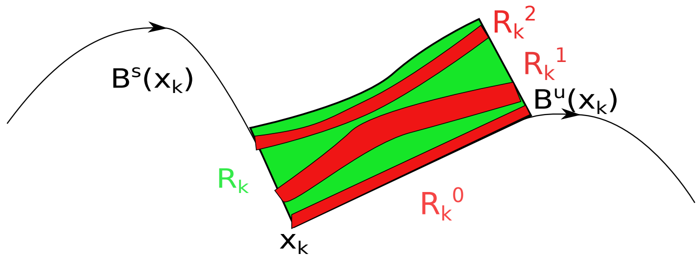


Figure 4. The connected component of $R_k \cap f^{qN}(R_k)$ that contains x_k.

When we decrease δ_k^u or δ_{k+1}^s, then N_k increases and when we decrease δ_k^s or δ_{k+1}^u, then N_k doesn't change. Hence, if we possibly decrease the δ_k^u's, we can assume that all the N_k are equal to some constant integer that we denote by N. Let us denote by R_k^0 the connected component of $R_k \cap f^{qN}(R_k)$ that contains x_k and let us prove that it is disjoint from the R_k^i for $1 \le i \le n_k$. There are two cases:

- There is only one fixed point in the heteroclinic cycle, i.e., $q = n = 1$; in this case the rectangles R_1^i are different connected components of $R_1 \cap f^N(R_1)$ and so they are disjoint.
- If not, as the different R_k are disjoint, in particular $f^{qN}(R_k)$ and $f^{qN}(R_{k-1})$ are disjoint and every unstable rectangle that is contained in $R_k \cap f^{qN}(R_k)$ is disjoint from $\bigcup_{i=1}^{n_{k-1}} R_k^i$; see Figure 4.

We introduce the notation $\mathcal{T}_k = \bigcup_{i=0}^{n_k} R_k^i$ and consider now the f^{qN}-invariant set

$$\Lambda = \bigcap_{j\in\mathbb{Z}} f^{jqN}\left(\bigcup_{k=1}^{qn} \mathcal{T}_k\right).$$

Then the R_k^js with $1 \le k \le nq$ and $0 \le j \le n_k$ define a rectangle partition for $f_{|\mathcal{V}}^{qN}$ and the following transitions occur:[11]

- $\forall i \in [0, n_k]$, $R_k^i \xrightarrow{f^{qN}} R_k^0$.
- $\forall i \in [0, n_k], \forall j \in [1, n_{k+1}]$, $R_k^i \xrightarrow{f^{qN}} R_{k+1}^j$.

We denote by A the associated matrix. Observe that for every R_k^i, R_h^j, then R_k^i can be connected to R_h^j by a succession of such transitions. We deduce from Proposition A.2 that $f_{|\Lambda}^{Nq}$ is conjugate to the subshift associated to A, that is

[11] We do not know if other transitions occur.

transitive. In particular, $f^{Nq}_{|\Lambda}$ is mixing, has an infinity of periodic points and has positive topological entropy.

Remarks. • If we decrease the constants δ^u_k and δ^s_k, then we increase N but this is not a problem because we just add some iterations of f^q that are close to the periodic orbits where we know exactly how the dynamics looks like. An advantage is that decreasing sufficiently these constants, we can be sure that $\bigcup_{j=0}^{qN} f^j\big(\bigcup_{k=1}^{qn} \mathcal{T}_k\big)$ is contained in a small neighborhood of the heteroclinic cycle $K(\mathcal{H})$. So in this case, the Hausdorff distance between $K(\mathcal{H})$ and the invariant set $\bigcup_{j=1}^{qN} f^j(\Lambda)$ is also as small as we want.

• Being defined by a rectangle partition, the set Λ is a locally maximal invariant set by f^{qN}.

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marie-claude.arnaud@math.univ-paris-diderot.fr

Université de Paris, CNRS, Institut de Mathématiques de Jussieu-Paris Rive Gauche, Paris, France

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Impact Hamiltonian systems and polygonal billiards

L. BECKER, S. ELLIOTT, B. FIRESTER, S. GONEN COHEN, MICHAL PNUELI AND VERED ROM-KEDAR

The dynamics of a beam held on a horizontal frame by springs and bouncing off a step is described by a separable two degrees of freedom Hamiltonian system with impacts that respect, point wise, the separability symmetry. The energy in each degree of freedom is preserved, and the motion along each level set is conjugated, via action angle coordinates, to a geodesic flow on a flat two-dimensional surface in the four dimensional phase space. Yet, for a range of energies, these surfaces are not the simple Liouville–Arnold tori — these are compact orientable surfaces of genus two, thus the motion on them is not conjugated to simple rotations. Namely, even though energy is not transferred between the two degrees of freedom, the impact system is quasiintegrable and is not of the Liouville–Arnold type. In fact, for each level set in this range, the motion is conjugated to the well studied and highly nontrivial dynamics of directional motion in L-shaped billiards, where the billiard area and shape as well as the direction of motion vary continuously on isoenergetic level sets. Return maps to Poincaré section of the flow are shown to be conjugated, on each level set, to interval exchange maps which are computed, up to quadratures, in the general nonlinear case and explicitly for the case of two linear oscillators bouncing off a step. It is established that for any such oscillator-step system there exist step locations for which some of the level sets exhibit motion which is neither periodic nor ergodic. Changing the impact surface by introducing additional steps, staircases, strips and blocks from which the particle is reflected, leads to isoenergy surfaces that are foliated by families of genus k level set surfaces, where the number and order of families of genus k depend on the energy.

1. Introduction

Quasiintegrable dynamics appear in nonconvex billiards with boundary consisting of horizontal and vertical segments [3; 31; 32] and in nonconvex billiards created

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by segments belonging to confocal quadrics [7; 8; 13]. The resulting dynamics are related to deep mathematical theories on interval exchange maps (IEM), on directed motion on translation surfaces, on genericity of curves in the space of affine lattices, on the Teichmüller geometry of moduli space and even on some results in number theory; see [5; 13; 26]. We show that this fascinating collection of interrelated mathematical fields are also related to the rich research area of Hamiltonian impact systems (HIS). Thus, these theories are related to a large variety of physically realizable models. We present this connection in the simplest possible setting and in the discussion we comment on some future synergetic directions.

In [7; 31] the two known integrable billiards in the plane, rectangles and ellipses, are modified by considering nonconvex boundaries consisting of segments that respect the symmetries of the integrable billiard dynamics. The resulting tables, *nibbled rectangles* [3] — domains defined by segments of horizontal and vertical boundaries (the simplest nontrivial geometries are slitted rectangle and L-shaped billiards, see, e.g., Figure 2) and *nibbled ellipses* [7; 8; 11; 13] — domains defined by segments of confocal quadrics, display fascinating dynamical properties. The nibbled rectangles are rational polygons and are thus analyzed by constructing, by reflections along the horizontal and vertical segments, a flat surface (possibly with singularities). Then, the directional billiard flow on the nibbled rectangle is conjugated to the geodesic flow on the glued flat surface. The genus of the flat surface is computable depending only on the number and type of corners; see [3]. The return map to a transverse section of the surface is an IEM, and thus, the dynamics on the flat surface and the properties of the IEM are related. The dynamics on a given surface depend on the direction of motion. For a flat torus, the dynamics satisfy the Veech dichotomy: depending on the direction, either the motion is periodic or uniquely ergodic. The higher genus surfaces that are produced by the nibbled rectangles do not necessarily satisfy this condition; For the tables that do not produce lattice surfaces, there can be directions of motion for which the dynamics are uniquely ergodic, directions of motion such that a band of periodic trajectories coexists with a band of trajectories that are dense on some set in the associated flat surface, and there can be also directions which are ergodic but not uniquely ergodic. Characterizing the measure of these sets of directions for a given billiard, the measure of parameters on which such behavior occurs for a given family of billiards, and defining proper statistical properties of the dynamics for such directions are delicate problems which are under current study, see e.g., [3; 5; 11; 13; 16; 25].

In [7; 8; 11; 13] it was discovered that the above tools may be applied to the study of the dynamics in nibbled ellipses. Since reflections from confocal quadrics preserve the same integral of motion, for any fixed integral of motion a conjugacy to a directional motion on a glued flat surface is found, and, thus, an IEM can be constructed. Notably, each constant of motion (namely, each caustic) in a nibbled elliptic table defines a directional flow on a different flat surface while the direction of motion is fixed [13]. Recently it was established that under some conditions on the nibbled ellipse the family of directional flow on the resulting surfaces corresponds to a generic curve in the corresponding moduli space [11; 13]. We show here that a rich class of HIS produces families of directional flow on flat surfaces, where both the direction and the geometry of the surfaces vary piecewise smoothly. While the question of conditions for genericity of the flow on isoenergetic surfaces remains open, the tools developed in [11; 13] appear relevant; see [12].

The field of Hamiltonian impact systems (HIS), which corresponds to a smooth conservative motion in a domain D with elastic impacts from its boundaries, combines two types of dynamical systems — the nontrivial, possibly chaotic, smooth motion associated with Hamiltonian flows [2], and, the dynamics resulting from elastic impacts, which have been extensively studied mainly in the context of billiards [19]. The combination of these two fields is natural from a modeling point of view, as, in many systems, there is a smooth bounded interaction component (e.g., attraction between atoms) and short range repulsion (e.g., atomic repulsion between atoms) giving rise to steep potentials that may be approximated, as a singular perturbation, by elastic reflections [17; 19; 20; 22]. Analysis of nonintegrable HIS includes local analysis near periodic orbits of the HIS [4; 9; 17], analysis near homoclinic orbits of the HIS [20], studies of the impact dynamics in some adiabatic limits [14; 15], persistence of KAM tori of motion along convex boundaries [30], and even establishment of hyperbolic behavior for some specific type of systems of particles [27; 28].

A class of HIS systems which is amenable to analysis under various perturbation is the Liouville integrable Hamiltonian impact systems (LIHIS) — these are integrable Hamiltonian systems with impact surfaces which respect the integrability symmetries and for which the motion on almost all level sets is rotational.

Definition 1.1. An HIS with compact level sets defined on a domain D belonging to a smooth manifold with piecewise smooth boundary is a Liouville-integrable HIS (LIHIS) if:

Resp F All the integrals of motion of the smooth Liouville-integrable Hamiltonian flow are preserved under impacts.

Resp θ The motion on any connected component of a regular level set, namely, on components in the allowed region of motion on which the differentials of the constants of motion are independent, is conjugated to a directed motion on a torus.

For smooth systems (hereafter, by smooth we mean C^∞-functions as in the Arnold–Liouville theorem, though, all results are probably correct also for C^r, $r \geqslant 2$ potentials) the Resp θ condition follows from the Resp F condition by the Arnold–Liouville theorem [1], and in some works HIS satisfying the Resp F conditions are called integrable [27]. Examples for LIHIS are mechanical separable Hamiltonians (i.e., $H(q, p) = \sum_{i=1}^{N}(p_i^2/(2m) + V_i(q_i)))$ with compact level sets undergoing impacts from a perpendicular wall — an impact surface which is an infinite $N-1$-dimensional plane in the configuration space with a normal aligned along one of the q_i axes; see [22; 23] for the $N = 2$ case.[1] Then, elastic impacts with the wall send $p_i \to -p_i$, and both the Resp F and Resp θ conditions are satisfied on regular level sets (as, in the (q_i, p_i) plane one can define action angle coordinates [14] and all other degrees of freedom are not affected; see [23]). As argued in [23], it is expected that separable systems with impact surfaces that consist of several such perpendicular walls are also LIHIS (e.g., a billiard in a rectangular box). This class of LIHIS enriches the number of integrable impact systems from merely two families for billiards (ellipsoidal billiards [6] and rectangular boxes) to the huge class of all integrable separable Hamiltonian systems with perpendicular walls (and possibly to other integrable Hamiltonian systems with properly defined impact surfaces). Moreover in [22; 23] it is establish that under some nondegeneracy assumptions on V_i, perturbations of such 2 degrees of freedom LIHIS by small smooth coupling terms and/or small smooth deformation of the walls are amenable to perturbation analysis (in particular to impact-KAM theory [22; 23]). The extension of these ideas to HIS with quadratic potentials in elliptic billiards [10; 24] is yet to be developed.

Now consider separable Hamiltonians impacting from surfaces in the configuration space that are composed of several finite or semiinfinite planar plates, all of which are perpendicular to one of the q_i-axes. Then, elastic impacts are of the same form, $p_i \to -p_i$, so the Resp F condition is still satisfied. The HIS flow resides on the intersection of the level set $\{(q, p) \mid H_i(q_i, p_i) = e_i, i = 1, \dots, N\}$ with the billiard phase-space domain (i.e., with $(q, p) \in D \times \mathbb{R}^n$), and the boundary created by the impact surfaces is glued according to the elastic impact rule. For regular level sets of the smooth system these glued level sets are N dimensional surfaces. Nonetheless, as shown next, in some cases the Resp θ condition is not satisfied. We call such systems quasiintegrable HIS (QIHIS), as we show that their dynamics is conjugated, on some of the level sets, to the directional motion on quasiintegrable billiards.

[1] Separable systems means hereafter decoupled systems — product systems of $N-1$ degrees of freedom mechanical Hamiltonians. The more general class of separable systems defined in [21] is not analyzed here.

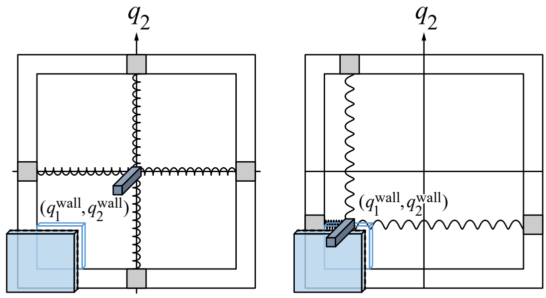

Figure 1. A mechanical model for the Hamiltonian-step system (equations (1) and (3)). (a) A rigid beam is confined between rigid horizontal and vertical springs hinged to supports that slide with no friction along a frame. (b) Two aligned rigid steps are placed in front and on the back of the frame, so when the beam hits these barriers an elastic impact occurs.

To simplify the presentation we consider one of the simplest possible QIHIS: two uncoupled oscillators that impact from a single right step in the configuration space, see Figure 1 for a physical realization of such a system; a springy beam is held on a horizontal frame and reflects from a step. The springs are connected to slider blocks that slide with no friction along a rectangular frame of ducts, and the step-walls, marked by a dotted line are out of the frame plane so that the slider blocks slide freely under the step walls and do not collide with them. The beam hits the step walls and bounces off them (always parallel to the out of plane axis). The springs are rigid to bending (can extend only in one direction) and are uncoupled. Thus, as the beam bounces off the step-walls elastically, it retains its vertical and horizontal energies (e_1, e_2). Without the step, the system is a classical integrable system — all orbits belonging to a given level set (e_1, e_2) satisfy the Veech dichotomy: either all orbits are dense and cover the torus of angle variables uniformly (equidistributed) or all orbits on this torus are closed. This behavior also implies that the return map to a transverse section of this torus is a rotation, and the rotation number on the prescribed level set determines which of the two options occurs. We show that this basic property is changed in the step-system. In particular, we identify a range of isoenergy level set surfaces that are of genus two and thus the return maps to a transverse section on such surfaces is, generally, a 5-IEM. This implies, for example, that an observable which depends on the oscillators phases (e.g., observable depending on the location of the beam) can have very delicate statistical properties [16; 25].

The paper is ordered as follows: in Section 2 we define the step-system and state the main results: Theorem 2.2 which conjugates the step dynamics to the quasiintegrable dynamics of directed motion on a compact orientable surfaces of genus two and to L-shaped billiards, Corllary 2.3 which concludes that the energy surface has nontrivial foliation, Corllary 2.4 which concludes that including additional steps, staircases, strips and rectangular scatterers can be similarly analyzed, Theorem 2.5 which concludes that Poincaré return maps of the Hamiltonian impact step flow are conjugated, on each level set, to an IEM and Theorem 2.6 which summarizes the results for the case of linear oscillators with impacts from a step. In Section 3 we prove our main results — that the motion in this system, on each level set, is conjugated to either a billiard flow, in a specific direction, on a rectangular domain, or to a billiard flow, in a specific direction, on an L-shaped billiard. Moreover, we prove that beyond a prescribed energy, the shape of the billiard on isoenergy surfaces changes from rectangular to continuously varying L-shaped billiards, back to rectangular domain, namely, that the topology of the invariant level set surfaces changes on isoenergy surfaces from genus one surfaces to genus two surfaces and back to genus one surfaces. In Section 4 we define and compute (up to quadratures) the corresponding Poincaré return maps for the level-set dynamics (Theorems 4.1 and 4.2), thus proving Theorem 2.5. Section 5 is devoted to establishing some specific properties of the resulting IEM, in particular, showing that typically there are many isolated level sets at which one of the intervals lengths vanishes. Section 6 applies these main results to linear oscillators, where the IEM are explicitly found, thus proving Theorem 2.6. We end with a discussion in which we list several natural extensions of this work and some open problems.

2. The step-system: setup and main results

Consider an autonomous smooth separable Hamiltonian corresponding to a particle motion in $\mathbb{R}^2$:

$$H = H_1(q_1, p_1) + H_2(q_2, p_2) = \frac{p_1^2}{2m} + V_1(q_1) + \frac{p_2^2}{2m} + V_2(q_2) \tag{1}$$

where we assume for simplicity of presentation that the potentials $V_i(q)$ have a single simple minimum and are concave — they monotonically increasing to infinity as $|q - q_{i,\min}|$ increases (other interesting cases will be studies elsewhere). With no loss of generality, take the particle mass to be $m = 1$ and the potentials minima to be at $q_{i,\min} = 0$ with $V_i(0) = 0$. For positive i-energies $e_i = H_i(q_i(t), p_i(t)) > 0, i = 1, 2$, the particle oscillates with frequencies $(\omega_1(e_1), \omega_2(e_2))$ in the box $[q_1^{\min}(e_1), q_1^{\max}(e_1)] \times [q_2^{\min}(e_2), q_2^{\max}(e_2)]$ of the configuration space, where $q_i^{\min}(e_i)$ and $q_i^{\max}(e_i)$ denote the minimal and maximal value of $q_i(t)$ on the level set e_i (so $V_i(q_i^{\min}(e_i)) = V_i(q_i^{\max}(e_i)) = e_i$). Since $q_{i,\min} = 0$, for all positive e_i, $q_i^{\min}(e_i) < 0 < q_i^{\max}(e_i)$ and the level sets are nested $\frac{d}{de_i} q_i^{\max}(e_i) > 0$, $\frac{d}{de_i} q_i^{\min}(e_i) < 0$). Denote by $(\theta_i(t) = \omega_i(e_i)t + \theta_i(0), I_i(e_i))$ the action-angle coordinates of the 1 degrees of freedom Hamiltonian $H_i(q_i, p_i) = H_i(I_i)$ (for one degrees of freedom systems with concave potential these always exist and are unique up to a shift in the angle coordinate [2]). A mechanical example of such a system is the beam held in a frame between two sets of uncoupled springs hinged on sliding, frictionless blocks (see Figure 1). The simplest case to consider is of linear oscillators (LO), namely, the case of quadratic potentials:

$$V_i^{\mathrm{LO}}(q_i) = \tfrac{1}{2}\omega_i^2 q_i^2, \quad i = 1, 2. \tag{2}$$

We formulate below the main results (Theorem 2.2, Corollaries 2.3 and 2.4 and Theorem 2.5) for nonlinear oscillators and dedicate Theorem 2.6 and Section 6 to the LO case.

Now, introduce a step S in the configuration space (see Figure 1):

$$S = \{(q_1, q_2) \mid q_1 < q_1^{\mathrm{wall}} \text{ and } q_2 < q_2^{\mathrm{wall}}\}, \quad q_1^{\mathrm{wall}} \cdot q_2^{\mathrm{wall}} \neq 0, \tag{3}$$

and assume the particle bounces off elastically from this step (we require, to avoid degeneracies, that the step is located away from the two axes), yet see [29] for a recent study on the quantized system that uses this singular case in an essential way. At the right wall of the step (hereafter, the 1-boundary), where $q_1 = q_1^{\mathrm{wall}}$ and $q_2 < q_2^{\mathrm{wall}}$, the horizontal momentum is switched $(q_1, q_2, p_1, p_2) \to (q_1, q_2, -p_1, p_2)$ whereas at the step upper wall (the 2-boundary), where $q_1 < q_1^{\mathrm{wall}}$ and $q_2 = q_2^{\mathrm{wall}}$, the vertical momentum changes sign $(q_1, q_2, p_1, p_2) \to (q_1, q_2, p_1, -p_2)$. When the particle hits the corner of the step the system is not defined and the trajectory stops. The flow is discontinuous at impacts, is smooth elsewhere, and the vertical and horizontal energies, e_i, are conserved by the impacts. We call this HIS the step system. Denote the step energies by

$$h_i^{\mathrm{step}} = V_i(q_i^{\mathrm{wall}}), \quad h^{\mathrm{step}} = h_1^{\mathrm{step}} + h_2^{\mathrm{step}}, \tag{4}$$

the step-family of level sets by:

$$\mathcal{R}^c(h) = \{(e_1, e_2) \mid e_1 \in (h_1^{\mathrm{step}}, h - h_2^{\mathrm{step}}), e_2 = h - e_1\}, \quad \text{defined for } h > h^{\mathrm{step}}, \tag{5}$$

by $T_i(e_i) = 2\pi/\omega_i(e_i)$ the period of the smooth oscillators, by

$$\Theta_2^{\mathrm{smooth}} = \Theta_2^{\mathrm{smooth}}(e_1, h) = 2\pi \frac{T_1(e_1)}{T_2(h - e_1)} \tag{6}$$

the rotation number of θ_2 on the level set $(e_1, e_2 = h - e_1)$, and by $\tilde{T}_i(e_i; q_i^{\mathrm{wall}})$ the period of the impact system when it is reflected from a wall at $q_i = q_i^{\mathrm{wall}}$ (namely, $\tilde{T}_i(e_i; q_i^{\mathrm{wall}}) = 2\int_{q_i^{\mathrm{wall}}}^{q_i^{\max}(e_i)} dq/(\sqrt{2(e_i - V_i(q_i))})$). Finally, let

$$\theta_i^{\mathrm{wall}}(e_i; q_i^{\mathrm{wall}}) = \pi \frac{\tilde{T}_i(e_i; q_i^{\mathrm{wall}})}{T_i(e_i)}. \tag{7}$$

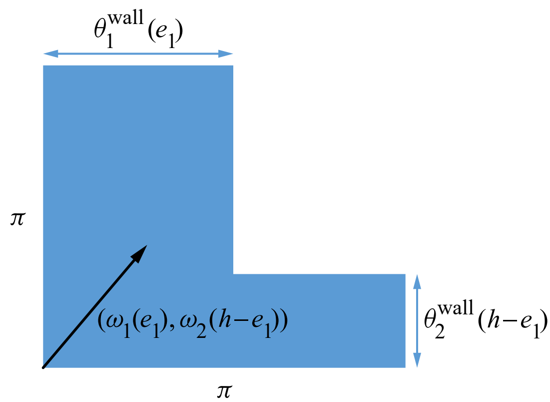

Figure 2. The directional flow on the L shaped billiard $L(\pi, \pi, \theta_1^{\text{wall}}(e_1; q_1^{\text{wall}}), \theta_2^{\text{wall}}(h - e_1; q_2^{\text{wall}}))$.

We will show later that by proper setting of the angle coordinate of the ith oscillator, $\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}})$ is the angle variable phase at the wall (see Lemma 3.4). Depending on the properties of V_i and on the sign of q_i^{wall}, the functions $\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}})$ may be monotone or not in e_i (for the LO case they are monotone, see below).

Definition 2.1. *The step system* is the two degrees of freedom HIS defined by the smooth Hamiltonian of the mechanical form (1) defined on $(q_1, q_2) \in \mathbb{R}^2 \setminus S$, with elastic reflections at the step S (equation (3)) boundaries. Each of the potentials $V_i(q_i)$ in (1) is smooth, has a single minimum at the origin and is concave: $q_i V_i'(q_i) > 0$ for all $q_i \neq 0$.

Our main results are (see Figure 2) as follows.

Theorem 2.2. *The step system is not Liouville-integrable HIS; For all $h > h^{\text{step}}$, the flow on level sets belonging to the step family, $\mathcal{R}^c(h)$, is topologically conjugate to the $(\omega_1(e_1), \omega_2(h - e_1))$- directional billiard flow on the L shaped billiard $L(\pi, \pi, \theta_1^{\text{wall}}(e_1; q_1^{\text{wall}}), \theta_2^{\text{wall}}(h - e_1; q_2^{\text{wall}}))$ whereas the step flow for the isoenergy level sets belonging to the complement of $\mathcal{R}^c(h)$ is topologically conjugate to a directional billiard flow on a rectangular billiard. For all $h > h^{\text{step}}$ both families have positive measure.*

Corllary 2.3. *For all $h > h^{\text{step}}$ the foliation of the isoenergy surface to level sets with increasing e_1 value has two singularities at which the level sets topology changes: at $e_1 = h_1^{\text{step}}$ the topology changes from a genus one surface to a genus two surface whereas at $e_1 = h - h_2^{\text{step}}$ the topology changes back to a genus one surface.*

Corllary 2.4. *By adding more steps, staircases, strips and rectangular barriers it is possible to create impact systems with level sets with any given genus ≥ 1*

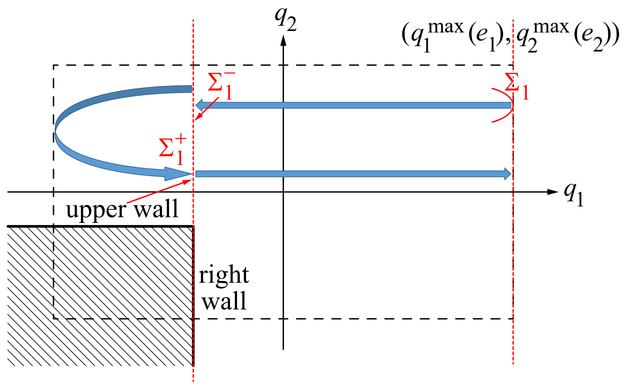

Figure 3. The return map geometry in configuration space.

and any number of disconnected components. The corresponding isoenergy surfaces are foliated by a finite number of families of level sets with equigenus and equinumber of components.

Theorem 2.5. *The return map of the step system to the section* $\Sigma_1 = \{(q, p) \mid p_1 = 0, \dot{p}_1 < 0\}$ *for each isoenergetic level set in* $\mathcal{R}^c(h)$ *is conjugated to an interval exchange map of three intervals on a circle. Restricting the angle to a natural fixed fundamental interval, for almost all level sets in* $\mathcal{R}^c(h)$*, the map becomes a five-interval exchange map* (5*-IEM*)*. The return map to the section* Σ_1 *for isoenergy level sets in the complement to* $\mathcal{R}^c(h)$ *is a rotation on a circle, namely a* 2*-IEM.*

In Section 4, explicit formulae (up to quadratures) for the return map at the isoenergy level sets $(e_1, h - e_1)$ are derived (for concreteness we consider the return map to Σ_1 - the analogous computations for the return map to Σ_2 amounts to replacing $1 \leftrightarrow 2$ in all definitions, and the same conclusions apply). These computations show that the numerical properties of three functions of e_1 (the functions $\theta_2^{\text{wall}}(h - e_1)$, $\Theta_2(e_1, h)$, $\chi_2(e_1, h)$ defined by equations (7), (23) and (26)) determine the 5-IEM. In Section 5 we discuss some properties of these functions and establish that there are isolated strongly resonant level sets at which orbits of different periods coexist, level sets for which periodic and quasiperiodic motion coexist, and, isolated level sets in $\mathcal{R}^c(h)$ at which the IEM reduces to a rotation (at these values the level set surface is a lattice surface). We believe all the other level sets have minimal dynamics and almost all of them have uniquely ergodic dynamics. Proving this conjecture, namely the genericity of the isoenergy curve of directional L-shaped billiard flows as in [11; 13], is beyond the scope of this paper. The recent paper [12] implies such results for the case $q_i^{\text{wall}} < 0$, $i = 1, 2$.

For the linear oscillator step system, the period of the smooth motion does not depend on the energy, namely, $T_i(e_i) = 2\pi/w_i$, and $q_i^{\max}(e_i) = -q_i^{\min}(e_i) = \sqrt{2e_i}/\omega_i$, hence all the functions which determine the dynamics are explicit:

$$h^{\text{step,LO}} = \tfrac{1}{2}(\omega_1^2(q_1^{\text{wall}})^2 + \omega_2^2(q_2^{\text{wall}})^2), \tag{8}$$

$$\theta_i^{\text{wall,LO}}(e_i; q_i^{\text{wall}}) = \arccos\frac{\omega_i q_i^{\text{wall}}}{\sqrt{2e_i}} \in (0, \pi), \tag{9}$$

$$\Theta_2^{\text{LO}}(e_1) = 2\frac{\omega_2}{\omega_1}\arccos\omega_1 q_1^{\text{wall}}/\sqrt{2e_1}, \tag{10}$$

$$\chi_2^{\text{LO}}(e_1, h) = \frac{\omega_2}{\omega_1}\frac{(\pi - \arccos\omega_1 q_1^{\text{wall}}/\sqrt{2e_1})}{\arccos\omega_2 q_2^{\text{wall}}/\sqrt{2(h-e_1)}}. \tag{11}$$

Theorem 2.6. *For $h > h^{\text{step,LO}}$, the flow of the linear-oscillators-step system on each level set in $\mathcal{R}^c(h)$ is topologically conjugated to the directional billiard flow in the fixed direction (ω_1, ω_2) on the L-shaped billiard*

$$L(\pi, \pi, \theta_1^{\text{wall,LO}}(e_1; q_1^{\text{wall}}), \theta_2^{\text{wall,LO}}(h - e_1; q_2^{\text{wall}})).$$

The L arms widths depend smoothly and monotonically on their arguments, and are of opposite monotonicity if and only if $q_1^{\text{wall}} q_2^{\text{wall}} > 0$. The return map to the section Σ_1 is an IEM of the form (31) *with*

$$(\theta_2^{\text{wall}}, \Theta_2, \chi_2) = (\theta_2^{\text{wall,LO}}(h - e_1; q_2^{\text{wall}}), \Theta_2^{\text{LO}}(e_1), \chi_2^{\text{LO}}(e_1, h))$$

of equations (9), (10) *and* (11).

The proof and other properties of the step LO are presented in Section 6.

3. The flow on level sets and the corresponding flat surfaces

In this section we prove Theorem 2.2. The main observation is that in terms of the smooth action angle coordinates, for the proper range of energies (the region $\mathcal{R}^c(h)$), impacts from the step correspond to a rectangular hole in the angle coordinates. Folding the torus according to the direction of motion in the configuration space leads to the motion in an L-shaped billiard with prescribed direction of motion and prescribed dimensions (up to quadratures). The rotational motion in the complimentary regions to $\mathcal{R}^c(h)$ follows from realizing that in these regions, for each level set, either there are no impacts at all or all impacts occur with only one side of the step.

Proof of Theorem 2.2. We first divide the level sets to three different classes according to the different types of impacts that may occur in each of them (Lemmas 3.1–3.3). We then introduce the action-angle coordinates for the smooth system, fold them to the proper billiard table (an L-shaped table for level

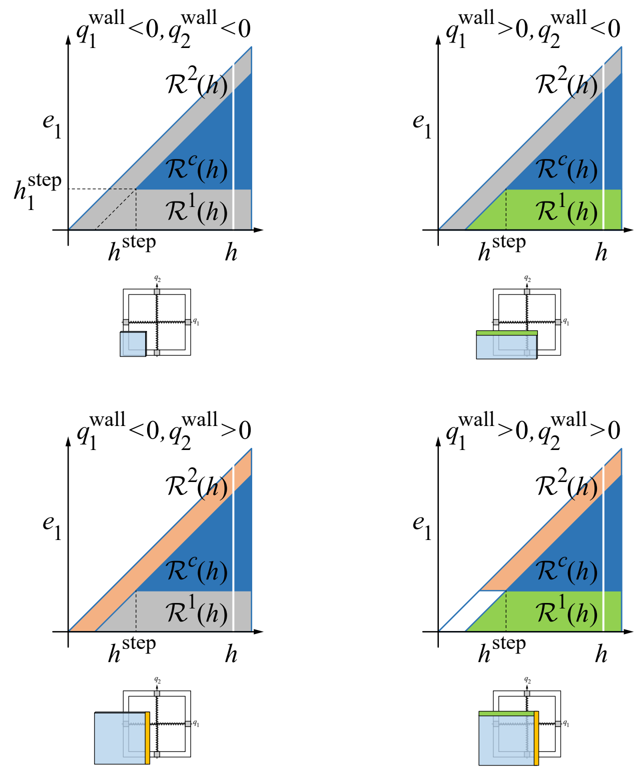

Figure 4. Impact-energy momentum bifurcation diagram for the four relative positions of the step. The region where motion is allowed and no impacts occur (gray), the region where impacts occur at both sides of the step (blue) and the regions where impacts occur only at the upper (green) or right (orange) sides of the step are shown (see Lemmas 3.1–3.3).

sets in $\mathcal{R}^c(h)$ and a rectangular table for the other level sets), and establish that the impacts from the step in the flow are mapped to impacts from the corresponding boundaries of the billiard table.

Delineating the energy level sets according to the impacts character. In the next few lemmas we detail how the collisions with the step depend on both the energy in each direction and on the location of the step. This classification, which is summarized by Figure 4 and its implications are shown in Figure 5, determines to which billiard table the flow on the level set is conjugated. Let

$$\mathcal{R}(h) = \{(e_1, e_2) \mid e_{1,2} > 0, e_1 + e_2 = h\}, \tag{12}$$

denote the open segment of allowed level set energy values on the isoenergy surface h (the white line in Figure 4) and by $\overline{\mathcal{R}}(h)$ the corresponding closed

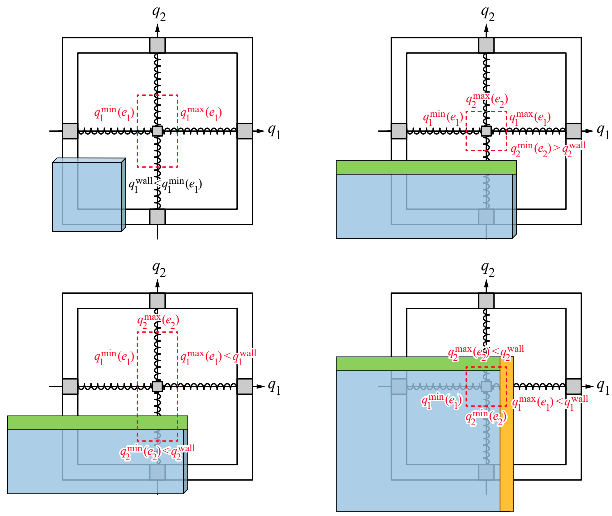

Figure 5. The level sets projection to the configuration space (dashed red box) for level sets in $\mathcal{R}^1$ (see Lemmas 3.1 and 3.2): (a) (top left) No impacts, $q_{1,2}^{\text{wall}} < 0$, $(e_1, e_2) \in \mathcal{R}^1$. (b) (top right) No impacts, $q_1^{\text{wall}} > 0$, $q_2^{\text{wall}} < 0$, $(e_1, e_2) \in \mathcal{R}^1 \cap \mathcal{R}^2$. (c) (bottom left) Impacts only with the 2-boundary (upper boundary), $q_1^{\text{wall}} > 0$, $q_2^{\text{wall}} < 0$, $(e_1, e_2) \in \mathcal{R}^1 \setminus \mathcal{R}^2$. (d) (bottom right) No motion for this level set, $q_1^{\text{wall}} > 0$, $q_2^{\text{wall}} > 0$, $(e_1, e_2) \in \mathcal{R}^1 \cap \mathcal{R}^2$.

interval. For all $h > h^{\text{step}}$, the isoenergy step-collision set, $\mathcal{R}^c(h)$, is an open segment in the interior of $\mathcal{R}(h)$. Define the two isoenergy complementary closed segments

$$\bar{\mathcal{R}}^i(h) = \{(e_1, e_2) \mid 0 \leqslant e_i \leqslant \min\{h, h_i^{\text{step}}\}, e_{\bar{i}} = h - e_i\}, \tag{13}$$

(with interior open segments, $\mathcal{R}^i(h)$), where, hereafter, we denote by $\bar{i}$ the complement degrees of freedom to i (namely $\bar{1} = 2, \bar{2} = 1$). Figure 4 shows these sets in the energy-momentum diagram for different locations of the walls.

Lemma 3.1. *All trajectories belonging to level sets in $\mathcal{R}^i(h)$ do not hit the i-boundary. For $0 < h < h^{\text{step}}$, $\mathcal{R}(h) = \mathcal{R}^1(h) \cup \mathcal{R}^2(h)$ and the segment $\bar{\mathcal{R}}^1(h) \cap \bar{\mathcal{R}}^2(h)$ is nonempty. For all $h > h^{\text{step}}$, $\bar{\mathcal{R}}(h) = \bar{\mathcal{R}}^1(h) \cup \mathcal{R}^c(h) \cup \bar{\mathcal{R}}^2(h)$ and these three segments are nonempty and disjoint.*

Proof. Since the potentials are concave the level sets are nested. Level sets in the interior of $\mathcal{R}^i(h)$ satisfy $e_i < h_i^{\text{step}}$, hence, for all t, the trajectories satisfy: $q_i(t; e_i) \in [q_i^{\min}(e_i), q_i^{\max}(e_i)] \subset (q_i^{\min}(h_i^{\text{step}}), q_i^{\max}(h_i^{\text{step}}))$. By definition, $q_i^{\text{wall}} \in \{q_i^{\min}(h_i^{\text{step}}), q_i^{\max}(h_i^{\text{step}})\}$ so such trajectories do not cross the line $q_i = q_i^{\text{wall}}$ and the step ith boundary cannot be impacted. The rest of the lemma follows from the definitions of $\mathcal{R}(h)$, $\mathcal{R}^{1,2}(h)$, $\mathcal{R}^c(h)$, equations (5), (12) and (13); see also Figure 4. □

Figure 5 demonstrates that in accordance with Lemma 3.1, level sets that belong to $\mathcal{R}^1(h)$ do not impact the 1-boundary (the right side of the step). Next we establish when such level sets impact the 2-boundary (the upper side of the step).

Lemma 3.2. *If* $q_i^{\text{wall}} < 0$, *trajectories associated with level sets in* $\mathcal{R}^i(h)$ *do not hit the step. If* $q_i^{\text{wall}} > 0$, *the dynamics in* $\mathcal{R}^i(h)$ *is further divided to the following two cases*:

For level sets in $\mathcal{R}^i(h)\backslash\overline{\mathcal{R}}^{\bar{i}}(h)$: *Trajectories hit the* $\bar{i}$*-boundary only, and the impacts are transverse.*

For level sets in $\mathcal{R}^1(h)\cap\mathcal{R}^2(h)$: *Trajectories do not hit the step if* $q_{\bar{i}}^{\text{wall}} < 0$ *and are not in the allowed region of motion if* $q_{\bar{i}}^{\text{wall}} > 0$.

Proof. If (e_1, e_2) belong to $\mathcal{R}^i(h)$ then $e_i < h_i^{\text{step}}$ (see (13)). If additionally, $q_i^{\text{wall}} < 0$, then $q_i^{\min}(e_i) > q_i^{\text{wall}}$, so the oscillation in the ith direction do not reach the wall, independently of the oscillation amplitude in the $\bar{i}$ direction (see Figure 5(a)).

If $q_i^{\text{wall}} > 0$, then $q_i^{\max}(e_i) < q_i^{\text{wall}}$, so, while impacts cannot occur with the i boundary, transverse impacts with the $\bar{i}$ boundary occur when$e_{\bar{i}} > h_{\bar{i}}^{\text{step}}$, namely when $(e_1, e_2) \in \mathcal{R}^i(h)\backslash\overline{\mathcal{R}}^{\bar{i}}(h)$ (see Figure 5(b)).

If $q_i^{\text{wall}} > 0$ and $e_{\bar{i}} < h_{\bar{i}}^{\text{step}}$, so $(e_1, e_2) \in \mathcal{R}^1(h)\cap\mathcal{R}^2(h)$, the $\bar{i}$ boundary cannot be crossed. If, additionally, $q_{\bar{i}}^{\text{wall}} < 0$, then $e_{\bar{i}} < h_{\bar{i}}^{\text{step}}$ implies that $q_{\bar{i}}^{\min}(e_{\bar{i}}) > q_{\bar{i}}^{\text{wall}}$ and the oscillations are in the allowed region of motion and do not hit the step (see Figure 5(c)), whereas if $q_{\bar{i}}^{\text{wall}} > 0$ then $q_{\bar{i}}^{\max}(e_{\bar{i}}) < q_{\bar{i}}^{\text{wall}}$ and the motion is "behind the step" namely it is not in the allowed region of motion (see Figure 5(d)). □

Lemma 3.3. *Each level set in the step collision set*, $\mathcal{R}^c(h)$, *includes trajectories which impact transversely the* 1*-boundary and trajectories which impact transversely the* 2*-boundary.*

Proof. Consider $(e_1, e_2) \in \mathcal{R}^c(h)$. Then, the projection of the level sets to the configuration space include the step position, namely, $q_i^{\min}(e_i) < q_i^{\text{wall}} < q_i^{\max}(e_i)$, $i = 1, 2$. Denote hereafter the smooth Hamiltonian flow by $\varphi_t^{\text{smooth}}(z)$ where $z = (q_1, q_2, p_1, p_2)$. The open, one dimensional set of i.c.,

$$Z_1 = \{z \,|\, z = (q_1^{\text{wall}}, q_2, -\sqrt{2(e_1 - h_1^{\text{step}})}, \pm\sqrt{2(e_2 - V_2(q_2))}), q_2 \in (q_2^{\min}(e_2), q_2^{\text{wall}})\}$$

is nonempty and belongs, by construction, to the level set (e_1, e_2). Its projection to the configuration space belongs to the right, 1-boundary of the step. Hence, for sufficiently small t, the set $\varphi_{-t}(Z_1)$ is within the allowed region of motion, belongs to the level set $(e_1, e_2) \in \mathcal{R}^c(h)$, and consists of i.c., which impact at time t the 1-boundary of the step transversely, with horizontal velocity $-\sqrt{2(e_1 - h_1^{\text{step}})}$. Similarly, defining

$$Z_2 = \big\{z \mid z = \big(q_1, q_2^{\text{wall}}, \pm\sqrt{2(e_1 - V_1(q_1))}, -\sqrt{2(e_2 - h_2^{\text{step}})}\big), q_1 \in (q_1^{\min}(e_1), q_1^{\text{wall}})\big\},$$

the set $\varphi_{-t}(Z_2)$ is within the allowed region of motion for sufficiently small t and consists of i.c., belonging to the level set $(e_1, e_2) \in \mathcal{R}^c(h)$ which impact at time t the 2-boundary of the step transversely, with vertical velocity $-\sqrt{2(e_2 - h_2^{\text{step}})}$. □

While, for most cases ("nonresonant"), each trajectory belonging to level sets $(e_1, e_2) \in \mathcal{R}^c(h)$ hits both boundaries of the step many times, in some resonant cases, it is possible to have families of trajectories belonging to level sets $(e_1, e_2) \in \mathcal{R}^c(h)$ that hit only one of the step boundaries or even avoid collisions (resonant trajectories belonging to the interval J_K of (31) with $K = 0$, see Section 4 for more details).

Action angle coordinates and transverse sections. The action angle coordinates of the 1 degrees of freedom Hamiltonian, $H_i(q_i, p_i)$, $(I_i, \theta_i(t) = \omega_i(I_i)t + \theta_i(0))$, are uniquely defined up to a shift in the angle. Since, by our assumptions, $H_i(I_i) = e_i$ is invertible, e_i or I_i may be used to label level sets (to simplify notation, we hereafter consider the frequencies as functions of the energies, e_i). By the monotonicity of $V_i(q_i)|_{q_i \neq 0}$, for all energy surfaces $h = e_1 + e_2 > 0$, each energy surface contains a family of invariant tori on which rotations occur, and its boundary consists of the two invariant circles that correspond to the normal modes — the oscillatory motion of only one oscillator with the other one at rest ($e_1 = 0$, $e_2 = h$ and $e_1 = h$, $e_2 = 0$).

For $e_i > 0$, denote by Σ_i the three dimensional transverse section $\{p_i = 0, \dot{p}_i < 0\}$, and we set the phases of the action-angle coordinates to vanish on these sections (so $\theta_i = 0 \pmod{2\pi}$ on Σ_i):

$$\Sigma_i : \{(q_i, q_{\bar{i}}, p_i, p_{\bar{i}}) \mid p_i = 0, \dot{p}_i < 0\} = \{(\theta_i, \theta_{\bar{i}}, I_i, I_{\bar{i}}) \mid \theta_i = 0, I_i > 0\}. \quad (14)$$

By the symmetry of the mechanical Hamiltonian, with this choice of the phases, $p_i(t) > 0$ for $\theta_i(t) \in (-\pi, 0) \bmod 2\pi)$ and similarly $p_i(t) < 0$ for $\theta_i(t) \in (0, \pi) \bmod 2\pi)$, namely $\operatorname{sign}(p_i(t)) = \operatorname{sign}(\dot{q}_i(t)) = -\operatorname{sign}(\theta_i(t) \bmod 2\pi)$. For p_i which is bounded away from zero, the smooth flow is smoothly conjugate, through the action angle transformation, to the directional motion on the flat torus in the direction $(\omega_1(e_1), \omega_2(e_2))$. The directed motion on the torus is conjugated, by standard folding, to the directed billiard motion on the square $(\psi_1, \psi_2) \in [-\pi, 0] \times [-\pi, 0]$ (see Figure 6). For this specific folding and for the

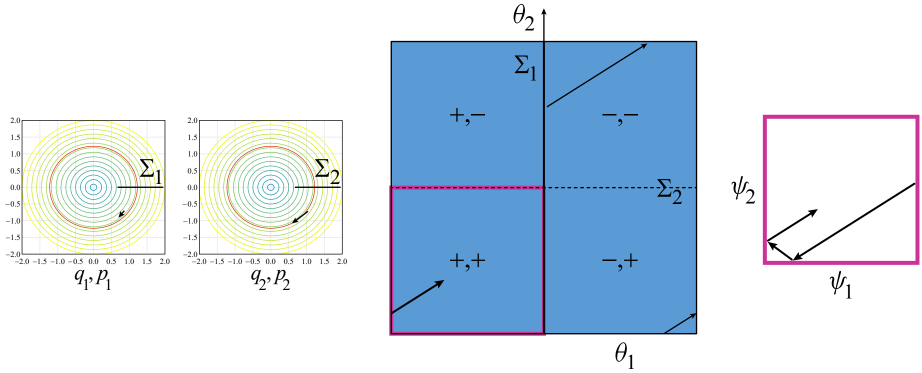

Figure 6. Folding the smooth flow to a billiard, the motion on a level set is conjugated via action angle coordinated to the directional motion on the angles-torus. The motion is conjugated to the directional billiard motion on the left lower square. The direction of motion in this billiard is in the same quadrant as the direction of motion in the configuration space; see equation (15).

choice of the angle phase (14), the direction of time is preserved along trajectories of the smooth flow and the billiard

$$\operatorname{sign}(p_i(t)) = \operatorname{sign}(\dot{q}_i(t)) = \operatorname{sign}(\dot{\psi}_i(t)) \tag{15}$$

namely, the directed billiard in the square (hereafter called the ψ-billiard) and the smooth flow on the level set (e_1, e_2) are topologically conjugated, see Figure 6. By reflections and time reversal, the flow is also conjugated to the billiard on the positive quadrant.

We use the same construction of conjugacy for the impact system. Let

$$\Sigma_i^{\pm} = \{(q, p) \mid q_i = q_i^{\text{wall}}, \pm p_i > 0\}, \tag{16}$$

and let $t_{\Sigma_i^- \to \Sigma_i^+} = T_i(e_i^{\text{wall}}) - \tilde{T}_i(e_i; q_i^{\text{wall}})$, $t_{\Sigma_i^+ \to \Sigma_i} = t_{\Sigma_i \to \Sigma_i^-} = \frac{1}{2}\tilde{T}_i(e_i; q_i^{\text{wall}})$ denote the respective travel times between the sections.

Lemma 3.4. *The sections $\Sigma_i^{\pm}$ are impacted/crossed transversely by the step-flow if and only if $e_i > h_i^{\text{step}}$. For all, i.c., belonging to a level set $e_i > h_i^{\text{step}}$, with the angle coordinate convention* (14), *the angle θ_i at the section Σ_i^- is $\theta_i^{\text{wall}}(e_i)$:*

$$\begin{aligned}
\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}) &= \omega_i(e_i) t_{\Sigma_i \to \Sigma_i^-} \\
&= \omega_i(e_i) \int_{q_i^{\text{wall}}}^{q_i^{\max}(e_i)} \frac{dq}{\sqrt{2(e_i - V_i(q_i))}} \\
&= \pi \frac{\tilde{T}_i(e_i; q_i^{\text{wall}})}{T_i(e_i; q_i^{\text{wall}})},
\end{aligned} \tag{17}$$

and a reflection from the step at q_i^{wall} *sends the angle* $\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}})$ *to*

$$2\pi - \theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}) = -\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}) \bmod 2\pi.$$

Proof. Since the level sets of H_i are nested, for $e_i < h_i^{\text{step}}$ the e_i level set is strictly interior to the h_i^{step} level set, and hence the sections $\Sigma_i^{\pm}$ are not reached by the flow. Conversely, for $e_i > h_i^{\text{step}}$, the sections $\Sigma_i^{\pm}$ are crossed by the level set, and, by the mechanical form of the Hamiltonian H_i, on these sections $p_i^2 = 2(e_i - V(q_i^{\text{wall}})) > 0$ so they are crossed transversely. The formula for $\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}})$ follows from the definition of action-angle coordinates and the convention (14). By the symmetry $p_i \to -p_i$ of mechanical Hamiltonian function it follows that the reflection from the step at q_i^{wall} sends the wall angle coordinate θ_i^{wall} to $2\pi - \theta_i^{\text{wall}}(e_i) = -\theta_i^{\text{wall}}(e_i) \bmod 2\pi$. □

Notice that, as summarized in Table 1,

$$\lim_{e_i \searrow h_i^{\text{step}}} \theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}) = \begin{cases} \pi & \text{for } q_i^{\text{wall}} < 0, \\ 0 & \text{for } q_i^{\text{wall}} > 0. \end{cases} \tag{18}$$

and

$$\lim_{e_i \to \infty} \theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}) = \theta_i^{\text{wall},\infty}, \tag{19}$$

where, for symmetric potentials, $\theta_i^{\text{wall},\infty} = \frac{\pi}{2}$.

Combining the classification of level sets according to their impacts with the boundaries (Lemmas 3.1–3.3) with the action-angle representation of the flow and the impacts on a given level set (Lemma 3.4), we establish the topological conjugacy between the impact flow on a given level set and its corresponding flat surface and billiard table. To this aim, it is convenient to define

$$\begin{aligned} &\hat{\theta}_i^{\text{wall}}(e_i, e_{\bar{i}}; q_i^{\text{wall}}, q_{\bar{i}}^{\text{wall}}) \\ &\quad = \begin{cases} \varnothing & \text{if } q_{1,2}^{\text{wall}} > 0 \wedge e_{1,2} < h_{1,2}^{\text{step}} \\ \theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}) & \text{if } e_i \geq h_i^{\text{step}} \wedge (e_{\bar{i}} \geq h_{\bar{i}}^{\text{step}} \vee q_{\bar{i}}^{\text{wall}} > 0), \\ \pi & \text{otherwise.} \end{cases} \end{aligned} \tag{20}$$

By Lemmas 3.1–3.3,

$$\hat{\theta}_i^{\text{wall}}(e_i, e_{\bar{i}}; q_i^{\text{wall}}, q_{\bar{i}}^{\text{wall}}) = \theta_i^{\text{wall}}(e_i; q_i^{\text{wall}})$$

for level sets for which impacts (transverse or tangent) with the i-boundary are allowed,

$$\hat{\theta}_i^{\text{wall}}(e_i, e_{\bar{i}}; q_i^{\text{wall}}, q_{\bar{i}}^{\text{wall}}) = \varnothing$$

for level sets that are not in the allowed region of motion, and

$$\hat{\theta}_i^{\text{wall}}(e_i, e_{\bar{i}}; q_i^{\text{wall}}, q_{\bar{i}}^{\text{wall}}) = \pi$$

for level sets in which impacts with the i-th boundary cannot occur.

Rotational dynamics for level sets in $\bar{\mathcal{R}}^i(h)$.

Lemma 3.5. *For level sets* (e_1, e_2) *in* $\bar{\mathcal{R}}^i(h)$ *the step-dynamics are smoothly conjugate to the directional motion* $(\omega_i(e_i), \omega_{\bar{i}}(e_{\bar{i}}))$ *on the torus*

$$\mathbb{T}_i(e_1, e_2) = \{(\theta_i, \theta_{\bar{i}}) \mid \theta_i \in [-\pi, \pi), \theta_{\bar{i}} \in [-\hat{\theta}_{\bar{i}}^{\text{wall}}, \hat{\theta}_{\bar{i}}^{\text{wall}})\}, \tag{21}$$

with $\hat{\theta}_{\bar{i}}$ *defined by* (20). *This step-dynamics are also conjugated to the* $(\pm\omega_i(e_i), \pm\omega_{\bar{i}}(e_{\bar{i}}))$ *directional billiard motion on the rectangular billiard* $(\psi_i, \psi_{\bar{i}}) \in [-\pi, 0] \times [-\hat{\theta}_{\bar{i}}^{\text{wall}}, 0]$. *In particular*, *the conjugation keeps the direction of motion*: *the signs of* $\dot{\psi}_{1,2}$ *and the sign of* $\dot{q}_{1,2}$ *coincide.*

Proof. By Lemma 3.2 the motion on level sets in $\mathcal{R}^i(h)$ is either: a) not defined (so $\hat{\theta}_{\bar{i}}^{\text{wall}} = \varnothing$), b) corresponds to reflections only from the $\bar{i}$-boundary of the step, or, c) the trajectory does not touch the step, so the motion occurs as in the nonimpact case on the torus (21) with $\hat{\theta}_{\bar{i}}^{\text{wall}} = \pi$.

The three rows of conditions in the definition (20) of $\hat{\theta}_{\bar{i}}^{\text{wall}}$ for $e_i < h_i^{\text{step}}$ coincide with the conditions listed for cases a,b,c in Lemma 3.2, so, to complete the proof we only need to show that case b) indeed corresponds to the rotation on the clipped torus (21) with $\hat{\theta}_{\bar{i}}^{\text{wall}} = \theta_{\bar{i}}^{\text{wall}}$. Indeed, by the mechanical form of $H_{\bar{i}}$, reflections only from the $\bar{i}$-boundary of the step imply that the corresponding angle coordinate is restricted to the interval $\theta_{\bar{i}}(t) \in [-\theta_{\bar{i}}^{\text{wall}}(e_{\bar{i}}; q_{\bar{i}}^{\text{wall}}), \theta_{\bar{i}}^{\text{wall}}(e_{\bar{i}}; q_{\bar{i}}^{\text{wall}})]$, where, by Lemma 3.4, the transverse impacts correspond to gluing the transverse section $\Sigma_{\bar{i}}^{\pm}|_{H_{\bar{i}}=e_{\bar{i}}}$:

$$\begin{aligned} \Sigma_i^-|_{H_i=e_i} &= \{(\theta, I) \mid I_i = I_i(e_i), \theta_i = \theta_i^{\text{wall}}(e_i)\}, \\ \Sigma_i^+|_{H_i=e_i} &= \{(\theta, I) \mid I_i = I_i(e_i), \theta_i = -\theta_i^{\text{wall}}(e_i)\}. \end{aligned} \tag{22}$$

by identifying the angles $\theta_{\bar{i}}^{\text{wall}}(e_{\bar{i}}; q_{\bar{i}}^{\text{wall}})$ and $-\theta_{\bar{i}}^{\text{wall}}(e_{\bar{i}}; q_{\bar{i}}^{\text{wall}})$. Namely, we obtain a directional motion on the torus (21), in the direction $(\omega_i(e_i), \omega_{\bar{i}}(e_{\bar{i}}))$. By folding to the rectangle $(\psi_i, \psi_{\bar{i}}) \in [-\pi, 0] \times [-\hat{\theta}_{\bar{i}}^{\text{wall}}, 0]$, the motion is conjugated to the ψ-billiard in this rectangular billiard, and (15) holds for the impact flow as well, proving the lemma for this case as well; see tables IIA, IIIIA, IIID, IIIID of Figure 7. □

The flow in the region $\mathcal{R}^c(h)$ *is conjugated to the L-shaped billiard flow.*

Lemma 3.6. *For level sets* (e_1, e_2) *in* $\mathcal{R}^c(h)$ *the step-dynamics are conjugate to the directional motion* $(\omega_1(e_1), \omega_2(e_2))$ *on SW - the swiss-cross shaped* (θ_1, θ_2)*-surface with vertical arms of width* $2\theta_1^{\text{wall}}(e_1)$ *and length* 2π, *horizontal arms of height* $2\theta_2^{\text{wall}}(e_2)$ *and width* 2π *and the flat surface is achieved by gluing of parallel opposite sides. This step-dynamics are also conjugate to the* $(\pm\omega_i(e_i), \pm\omega_{\bar{i}}(e_{\bar{i}}))$ *directional billiard motion on the L-shaped billiard* $L(\pi, \pi, \theta_1^{\text{wall}}(e_1; q_1^{\text{wall}}), \theta_2^{\text{wall}}(h - e_1; q_2^{\text{wall}}))$. *Reflecting the L-shaped billiard*

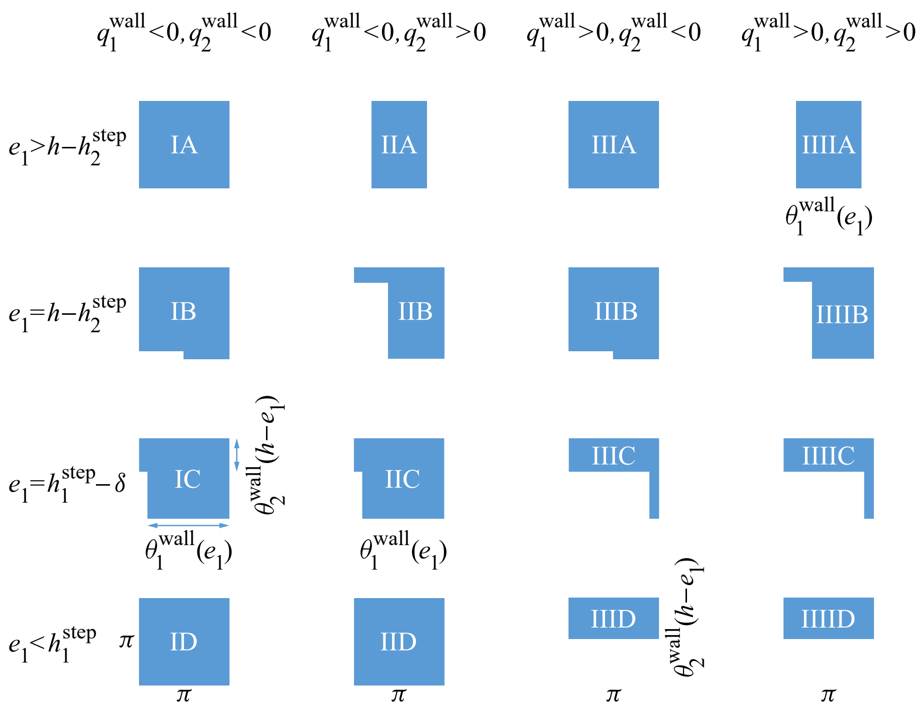

Figure 7. The isoenergy billiard geometry at the different step locations for $h > h^{\text{step}}$. The first and last rows present, respectively, the rectangular billiards for level sets in $\mathcal{R}^2(h)$ and $\mathcal{R}^1(h)$. The second and third rows present, respectively, the L-shaped billiards in $\mathcal{R}^c(h)$ just below and just above the edges of the $\mathcal{R}^c(h)$ interval (so $\delta > 0$ is small).

with respect to the θ_1-axis and the θ_2-axis provides dynamics with conjugation that keeps the direction of motion.

Proof. Recall that with the convention (14), $q_i(t; e_i) > q_i^{\text{wall}}$ if and only if the angle coordinate of the smooth flow is in the interval $(-\theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}), \theta_i^{\text{wall}}(e_i; q_i^{\text{wall}}))$. Hence, on a level set $(e_1, e_2) \in \mathcal{R}^c(h)$, the disallowed step region in the configuration space is mapped by the smooth action-angle transformation to a disallowed rectangular region in the angle variables: $(\theta_1, \theta_2) \in S_{\theta(e_1,e_2)} := [\theta_1^{\text{wall}}(e_1; q_1^{\text{wall}}), 2\pi - \theta_1^{\text{wall}}(e_1; q_1^{\text{wall}})] \times [\theta_2^{\text{wall}}(e_2; q_2^{\text{wall}}), 2\pi - \theta_2^{\text{wall}}(e_2; q_2^{\text{wall}})]$ all taken mod 2π. This rectangle cuts the four corners of the fundamental domain creating a swiss-cross surface (see Figure 8). By Lemma 3.4, the reflection rule at impact, $p_i \to -p_i$, translates to $\theta_i^{\text{wall}} \to 2\pi - \theta_i^{\text{wall}}$. Hence, the resulting flow under the step dynamics, expressed in the smooth action angle coordinates, corresponds to setting the action values to constants, $I_i(e_i)$, and letting the angles (θ_1, θ_2) increase linearly at constant speeds $(\omega_1(e_1), \omega_2(e_2))$

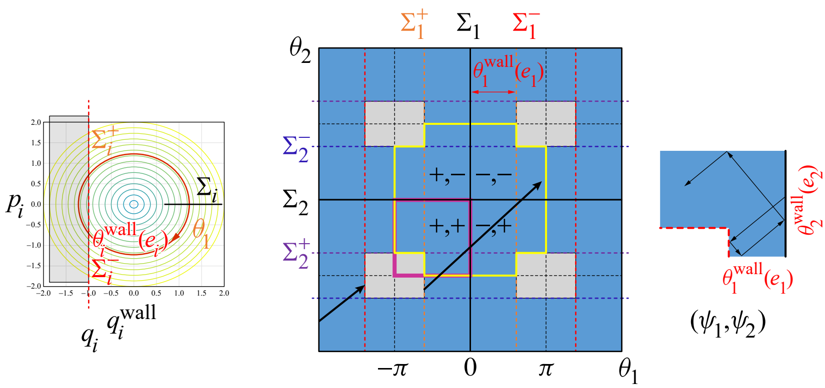

Figure 8. The step return map, the swiss-cross surface and the rotated L-shaped billiard geometry for level sets in the step region, $\mathcal{R}^c(h)$. The gray areas correspond to the step region in the angles space. The yellow outlines the boundary of SW, the Swiss-cross flat surface for which opposite parallel sides are glued.

on the torus $[0, 2\pi] \times [0, 2\pi]$, till the rectangle $S_{\theta(e_1,e_2)}$ is met. There, the gluing condition $\theta_i^{\mathrm{wall}}(e_i; q_i^{\mathrm{wall}}) \to 2\pi - \theta_i^{\mathrm{wall}}$ is applied. This is a directed flow on a "torus with a rectangular hole" namely, a compact orientable surface of genus 2. Equivalently, when shifting the torus center by $(-\pi, -\pi)$, this is a directed flow on a swiss-cross surface, see Figure 8. For all $(e_1, e_2 = h - e_1) \in \mathcal{R}^c(h)$, the dynamics under this gluing rule of the swiss-cross correspond to an unfolding of a billiard motion in the $\boldsymbol{B}(e_1) = L(\pi, \pi, \theta_1^{\mathrm{wall}}(e_1; q_1^{\mathrm{wall}}), \theta_2^{\mathrm{wall}}(h - e_1; q_2^{\mathrm{wall}}))$-shaped table [3; 32] in the directions $(\pm\omega_1(e_1), \pm\omega_2(h - e_1))$, where, as before, by the choice (14) of the angle phases, (15) holds on the L-shaped billiard that is folded onto the low-left part of the swiss-cross; see Figures 8 and 9. Thus, we have shown that the dynamics on the isoenergetic level sets in $\mathcal{R}^c(h)$ are conjugated to the family of α-directional flows on the family of L-shaped billiards, $\mathcal{B}(h) = \{\alpha(e_1) = \omega_2(h - e_1)/\omega_1(e_1), \boldsymbol{B}(e_1)\}|_{e_1 \in \mathcal{I}^c(h)}$, where $\mathcal{I}^c(h) := (h_1^{\mathrm{step}}, h - h_2^{\mathrm{step}} = h_1^{\mathrm{step}} + h - h^{\mathrm{step}})$. □

Finally, to complete the proof of Theorem 2.2, we notice that since the directed flow on a genus-2 orientable compact surface is not conjugate to a flow on a torus, and since by Lemma 3.6 the motion on the level sets $(e_1, h - e_2)$ for all $e_1 \in \mathcal{I}^c(h)$ is conjugated to such a flow, the step system is not LIHIS. The measure of the corresponding set is positive as the intersection of each level set in $\mathcal{R}^c(h)$ with the allowed region of motion has positive area and $|\mathcal{I}^c(h)| = h - h^{\mathrm{step}} > 0$. By Lemmas 3.5 the motion on the isoenergy level sets $(e_1, h - e_1)$ with $e_1 \in (0, h_1^{\mathrm{step}}) \cup (h - h_2^{\mathrm{step}}, h)$, the isoenergy complement to $\mathcal{R}^c(h)$, is conjugate to the directed flow on a torus, and this complement also

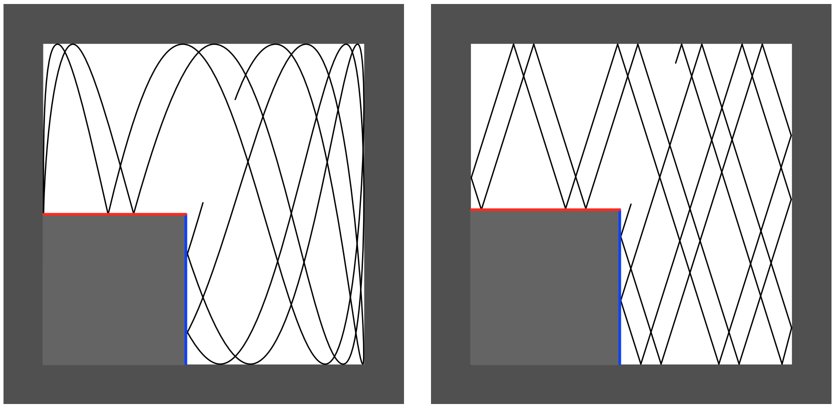

Figure 9. A simulation of the configuration space of the linear oscillators step system (left) with its corresponding matching L-shaped billiard in the angle space (right). The turning points of the flow, where $p_i = 0$, are mapped to reflections from the outer square boundaries and the elastic reflections of the flow from the step are mapped to the billiard reflections from the step.

has positive measure since, for $h > h^{\text{step}}$, the intersection of these level sets with the allowed region of motion is always of positive measure.

Each column of Figure 7 shows schematically the family of isoenergetic billiard tables obtained for the indicated positions of the step. The directional L-shaped billiard families, $\mathcal{B}(h)$, are shown in rows B and C and correspond to level sets in $\mathcal{R}^c(h)$. The widths of the arms of L-shaped tables at the edges of the segment $\mathcal{R}^c(h)$ (these depend on the signs of $q_{1,2}^{\text{wall}}$) are listed in Table 1 — note that they are distinct, namely, for all $h > h^{\text{step}}$, $\theta_i^{\text{wall}}(h_i^{\text{step}}) \neq \theta_i^{\text{wall}}(h - h_{\bar{i}}^{\text{step}})$. The rectangular billiards shown in rows A and D correspond to level sets in $\mathcal{R}^1(h)$ and $\mathcal{R}^2(h)$ respectively.

Lemma 3.4 in the above proof exposes the simple relation between reflections from vertical and horizontal boundary segments and the corresponding gluing rule in the angles variables. Corollaries 2.3 and 2.4 follow from this construction; steps (two rays meeting at a $3\pi/2$ corner) produce for sufficiently high individual energies a single hole, a staircase in the configuration space creates at sufficiently high individual energies a nibbled hole in the angles variables, a strip with handles creates, for intermediate individual energies several disconnected components and for sufficiently high individual energies two holes, and a rectangle creates for sufficiently high individual energies four holes, see Figure 10 for a demonstration. Thus, by constructing a nibbled scattering geometry which combines finite and semiinfinite horizontal and vertical segments in the configuration space, the number of holes and the number of connected components in the isoenergy

q_1^{wall}	q_2^{wall}	$\theta_1^{\text{wall}}(h_1^{\text{step}})$	$\theta_2^{\text{wall}}(h_2^{\text{step}})$
<0	<0	π	π
<0	>0	π	0
>0	<0	0	π
>0	>0	0	0

Table 1. The values of $\theta_{1,2}^{\text{wall}}$ at the two edges of $\mathcal{R}^c(h)$. The values of $\theta_2^{\text{wall}}(h-h_1^{\text{step}};q_2^{\text{wall}})$ and $\theta_1^{\text{wall}}(h-h_2^{\text{step}};q_1^{\text{wall}})$ vary accordingly with h, with limiting values $\theta_i^{\text{wall},\infty}\in(0,\pi)$; see rows B and C of Figure 7.

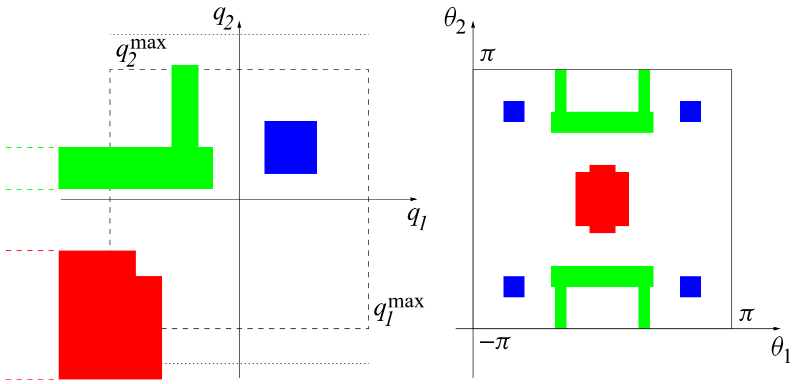

Figure 10. For the indicated level set (dashed line), a 2-step staircase (red), a strip with a handle (green) and a block (blue) in the configuration space (left figure) create, respectively, one, one and four holes in the angle-angle torus representation, and divide the torus to two disconnected components (inside and outside of the green frame). A slight increase in the vertical energy e_2 (dotted lines) makes the level set surface connected with two green holes.

level set surfaces can be manipulated. Moreover, constructing an impact energy-momentum diagram [22; 23], such as Figure 4 for the one-step system, allows to identify the critical energy values at which the topology of the energy surface changes.

4. Return maps

Proof of Theorem 2.5. In Theorem 2.2 we proved that the step dynamics on each isoenergy level set is conjugated, via the action angle transformation, to the $(\omega_1(e_1),\omega_2(h-e_1))$ directional flow on a flat surface — a glued swiss-cross for level sets in $\mathcal{R}^c(h)$ (Lemma 3.6) and a torus for level sets in the complement to $\mathcal{R}^c(h)$ (Lemma 3.5). The transverse Poincaré section Σ_1 of the step flow is conjugated to the transverse section $\theta_1 = 0$ on these surfaces via the action-angle transformation (recall (14), and notice that the assumptions on the potentials imply that $\omega_1(e_1)$ is bounded away from zero for any finite e_1), so the return map of the step flow to Σ_1 is conjugated to the return map to Σ_1 on the corresponding flat surface. The return map to Σ_1 on the flat surface is an interval exchange map on a circle: for the swiss-cross a three-interval exchange map and for the torus a rotation of a single interval; see, e.g., [32]. For a fixed fundamental interval on this circle, the return map becomes, in general, a 5-IEM for the swiss-cross case and a 2-IEM for the torus. Computations of the resulting IEMs (see Theorem 4.2) show that the lengths of the intervals of the 5-IEMs and their positions on the circle for isoenergy level sets change smoothly in the step region. In particular, conditions for having a zero length interval are expressed as an equation of smooth, nonconstant functions of e_1 which are shown to vanish at most at isolated e_1 values in the interior of $\mathcal{R}^c(h)$.

Next, we calculate $\mathcal{F}(h) = \{F = F_{(e_1,h-e_1)}\}_{e_1\in[0,h]}$, the isoenergetic family of IEMs, for the 2-IEM case (Theorem 4.1) and for the 5-IEM case (Theorem 4.2) thus completing the proof of Theorem 2.5. In Section 5 we explore some of the properties of the 5-IEM family.

Let Θ_2 denote the gain in the θ_2 phase of the return map to Σ_1 when the motion is to the right of the step:

$$\begin{aligned}\Theta_2 &= \Theta_2(e_1, h; q_{1,2}^{\text{wall}})\\ &= \frac{\hat{\theta}_1^{\text{wall}}}{\pi}\Theta_2^{\text{smooth}}\\ &= \begin{cases} 2\pi\tilde{T}_1(e_1; q_1^{\text{wall}})/T_2(h-e_1) & \text{if } \hat{\theta}_1^{\text{wall}}(e_1, h; q_{1,2}^{\text{wall}}) \neq \pi,\\ \Theta_2^{\text{smooth}}(e_1, h) & \text{if } \hat{\theta}_1^{\text{wall}}(e_1, h; q_{1,2}^{\text{wall}}) = \pi,\end{cases}\end{aligned} \tag{23}$$

where $\hat{\theta}_1^{\text{wall}}(e_1, h; q_{1,2}^{\text{wall}})$ (see equation (20)) is the effective impact angle with the side boundary of the step and $\Theta_2^{\text{smooth}}(e_1, h)$ (see equation (6)) is the rotation in θ_2 for nonimpacting trajectories. Notice that for all level sets on which motion is defined $\Theta_2 \leq \Theta_2^{\text{smooth}}$. Let

$$\Theta_2^*(e_1, h; q_{1,2}^{\text{wall}}) = 2\hat{\theta}_2^{\text{wall}}\left\{\frac{\Theta_2}{2\hat{\theta}_2^{\text{wall}}}\right\} \tag{24}$$

where $\{x\}$ denotes hereafter the fractional part of the number x. We first establish that in the complementary sets to $\mathcal{R}^c(h)$ the return map to Σ_1 is the rotation (25).

Theorem 4.1. *Under the same conditions of Theorem 2.2, for all isoenergy level sets in $\mathcal{R}^1(h)\cup\mathcal{R}^2(h)$, the return map $F_{(e_1,h-e_1)}$ to the section Σ_1 is topologically conjugated to a Θ_2 rotation on the $[-\hat{\theta}_2^{\text{wall}}, \hat{\theta}_2^{\text{wall}})$ circle*:

$$\theta_2 \to \theta_2 + \Theta_2(e_1, h; q_{1,2}^{\text{wall}}) \mod 2\hat{\theta}_2^{\text{wall}}, \tag{25}$$

or, equivalently, to a 2*-IEM on the interval* $[-\hat{\theta}_2^{\text{wall}}, \hat{\theta}_2^{\text{wall}}]$ *with intervals lengths* $\lambda_A = 2\hat{\theta}_2^{\text{wall}} - \Theta_2^*$, $\lambda_B = \Theta_2^*$.

Proof. By Lemma 3.5 the flow on level sets belonging to $\mathcal{R}^1(h)$ is topologically conjugated to the $(\omega_1(e_1), \omega_2(h-e_1))$ directional flow on the torus $\mathbb{T}_1(e_1, h-e_1)$ of equation (21). Notice that if the level set is in the disallowed region of $\mathcal{R}^1(h)$, then $\hat{\theta}_2^{\text{wall}} = \varnothing$, hence $\mathbb{T}_1(e_1, h-e_1) = \varnothing$, so the Theorem trivially holds. For the nontrivial case, by (14), the transverse section Σ_1 to the flow is mapped, for a fixed level set, to the transverse section $\theta_1 = 0$ of the corresponding torus. Hence, to complete the proof we need to show that the return map to the section $\theta_1 = 0$ of the $(\omega_1(e_1), \omega_2(h-e_1))$ directional flow on $\mathbb{T}_1(e_1, e_2)$ is the rotation (25). Indeed, notice that for the level sets in $\mathcal{R}^1(h)$ the effective impact angle is $\hat{\theta}_1^{\text{wall}} = \pi$ (when motion is allowed), so $\Theta_2 = \Theta_2^{\text{smooth}}(e_1, h) = 2\pi\omega_2(h-e_1)/\omega_1(e_1)$ and thus (25) coincides with the return map on the $\mathbb{T}_1(e_1, h-e_1)$ torus. Similarly, by Lemma 3.5, the flow on level sets belonging to $\mathcal{R}^2(h)$ is topologically conjugated to the $(\omega_1(e_1), \omega_2(h-e_1))$ directional flow on the rotated torus $\mathbb{T}_2(e_1, e_2)$ of equation (21), namely on $\mathbb{T}_2(e_1, e_2) = \{(\theta_1, \theta_2) \mid \theta_1 \in [-\hat{\theta}_1^{\text{wall}}, \hat{\theta}_1^{\text{wall}}), \theta_2 \in [-\pi, \pi)\}$. The return map to the section $\theta_1 = 0$ on this torus is a rotation of the θ_2 angle on the 2π circle by $\omega_2(h-e_1)2\hat{\theta}_1^{\text{wall}}/(\omega_1(e_1))$, which is exactly Θ_2 (see (23)). Finally, since $\hat{\theta}_2^{\text{wall}} = \pi$ for the allowed level sets in $\mathcal{R}^2(h)$, (25) is verified. $\square$

Next, we establish that for level sets in $\mathcal{R}^c(h)$, the return map defines a three-interval map on the circle, namely a 5-IEM on the fundamental segment arises. Let

$$\begin{aligned}\chi_2(e_1, h; q_{1,2}^{\text{wall}}) &= \frac{\Theta_2^{\text{smooth}} - \Theta_2}{2\theta_2^{\text{wall}}} \\ &= \frac{T_1(e_1) - \tilde{T}_1(e_1; q_1^{\text{wall}})}{\tilde{T}_2(h-e_1; q_2^{\text{wall}})} \\ &= \frac{\omega_2(h-e_1)}{\omega_1(e_1)} \frac{\pi - \theta_1^{\text{wall}}(e_1; q_1^{\text{wall}})}{\theta_2^{\text{wall}}(h-e_1; q_2^{\text{wall}})}\end{aligned} \tag{26}$$

denote the ratio between the time spent above the step and the return time to the upper step boundary. The integer part of χ_2 corresponds to the minimal number of impacts with the upper boundary of the step during this passage:

$$K_2(e_1, h; q_{1,2}^{\text{wall}}) = \lfloor \chi_2 \rfloor. \tag{27}$$

Theorem 4.2. *Under the same conditions of Theorem 2.2, for all isoenergy level sets in* $\mathcal{R}^c(h)$*, the return map* $F_{(e_1, h-e_1)}$ *to the section* Σ_1 *is topologically conjugated to a* 3 *interval IEM on the* θ_2 *circle of the form*

$$(J_R, J_{K_2}, J_{K_2+1}) \to \Theta_2 + (J_R, J_{K_2+1}, J_{K_2}) \bmod 2\pi, \tag{28}$$

where the lengths of the intervals are

$$(\lambda_{J_R}, \lambda_{J_{K_2}}, \lambda_{J_{K_2+1}}) = (2\pi - 2\theta_2^{\text{wall}}, 2\theta_2^{\text{wall}}(1-\{\chi_2\}), 2\theta_2^{\text{wall}}\{\chi_2\}), \tag{29}$$

and the phase of the left boundary of J_R *is*

$$\theta_{J_R}^L = \theta_2^{\text{wall}} - \tfrac{1}{2}\Theta_2 \pmod{2\pi}. \tag{30}$$

In the above formulae $(\theta_2^{\text{wall}} = \theta_2^{\text{wall}}(h-e_1; q_2^{\text{wall}}), \Theta_2, \chi_2)$ *are defined by equations* (7), (23) *and* (26), *respectively, and the phase* θ_2 *is set by* (14). *The return time to* Σ_1 *for* $\theta_2 \in J_R$ *is* $\tilde{T}_1$ *whereas for* $\theta_2 \in J_{K_2} \cup J_{K_2+1}$ *it is* T_1. *Equivalently, the dynamics for each level set is conjugated to the induced* 5*-IEM on the* $[-\pi, \pi)$ *interval of* θ_2 *values. This* 5*-IEM is uniquely defined by equations* (28)–(30), *and apart of isolated points of* e_1 *values in* $\mathcal{R}^c(h)$, *all its* 5 *intervals are of positive lengths.*

Proof. By Lemma 3.6 the flow on level sets belonging to $\mathcal{R}^c(h)$ is topologically conjugated to the $(\omega_1(e_1), \omega_2(h-e_1))$ directional flow on SW — the swiss-cross surface defined by $\theta_1^{\text{wall}}(e_1; q_1^{\text{wall}})$ and $\theta_2^{\text{wall}}(h-e_1; q_2^{\text{wall}})$. In particular, the section Σ_1 of the return map is mapped by the action-angle conjugation to the vertical center of SW, the 2π circle of θ_2 phases (see Figure 8), so the return map on SW and the step dynamics return map to Σ_1 are smoothly conjugated. While the return map can be computed from the SW geometry alone, we find it convenient at times to consider the step dynamics.

We divide the θ_2 circle to two subintervals: J_R consisting of phases with trajectories which hit the right boundary of the step (equivalently, the right boundary of the vertical arm of SW) and return to Σ_1, and J_U consisting of phases with trajectories which do not hit the right boundary (equivalently, enter the horizontal arm of the SW), go above the step, possibly hitting the upper boundary of the step (equivalently, the horizontal boundaries of the SW horizontal arm), and then return to Σ_1 (see Figures 3 and 8 where the return map construction to Σ_1 in the configuration space and in the directional flow on the swiss-crossed shaped polygon are shown). Hence, the length of J_R is the length of the vertical right boundary of the SW, $\lambda_{J_R} = 2\pi - 2\theta_2^{\text{wall}} = 2\pi(1-\tilde{T}_2/T_2)$ and $\lambda_{J_U} = 2\theta_2^{\text{wall}}$.

The return time for trajectories belonging to J_R is $\tilde{T}_1$, the phase θ_2 for these trajectories increases at the constant speed $\omega_2(h-e_1)$, so, the interval J_R is rotated by $2(\omega_2(h-e_1)/\omega_1(e_1))\theta_1^{\text{wall}}$, namely by Θ_2 as defined in (23).

The return time for trajectories belonging to J_U is T_1. It is divided to the time $\tilde{T}_1$, where the trajectories are to the right of the step and to the time interval $T_1(e_1) - \tilde{T}_1(e_1; q_1^{\text{wall}})$ where the trajectories are above the step, possibly bouncing off its upper boundary. During the $\tilde{T}_1$ time segment the phase θ_2 increases, as before, by Θ_2. During the $T_1(e_1) - \tilde{T}_1(e_1; q_1^{\text{wall}})$ segment, the phase gain depends on the number of bounces. Denote the interval of θ_2 values for which trajectories hit the upper step k times by J_k. The function χ_2 (see (26)) provides the ratio between the time trajectories in J_U spend above the step and the return time of trajectories with energy $e_2 = h - e_1$ to the step upper boundary. Hence, the number of bounces of the trajectories belonging to J_U is either $K_2 = \lfloor \chi_2 \rfloor$ or $K_2 + 1$, namely, $J_U = J_{K_2} \cup J_{K_2+1}$. The phase gained during the $T_1(e_1) - \tilde{T}_1(e_1; q_1^{\text{wall}})$ segment by trajectories in J_k is $2(\pi - \theta_2^{\text{wall}})k + \omega_2 \tilde{T}_2 \chi_2 = 2(\pi - \theta_2^{\text{wall}})k + 2\theta_2^{\text{wall}}(\lfloor \chi_2 \rfloor + \{\chi_2\}) = 2\pi k + 2\theta_2^{\text{wall}}(K_2 - k) + 2\theta_2^{\text{wall}}\{\chi_2\}$, hence, applying this formula for $k = K_2$ and for $k = K_2 + 1$ we obtain

$$F(\theta_2) = \begin{cases} \theta_2 + \Theta_2 & \theta_2 \in J_R, \\ \theta_2 + \Theta_2 + 2\theta_2^{\text{wall}}\{\chi_2\} + 2\pi K_2 & \theta_2 \in J_{K_2}, \\ \theta_2 + \Theta_2 + 2\theta_2^{\text{wall}}(-1 + \{\chi_2\}) + 2\pi(K_2 + 1) & \theta_2 \in J_{K_2+1}, \end{cases} \tag{31}$$

where the intervals $(J_R, J_{K_2}, J_{K_2+1})$, correspond, respectively, to phases with trajectory segments which hit exactly once only the right side of the step (J_R), those which hit only the upper side of the step exactly K_2 times (J_{K_2}) and those hitting only the upper side exactly $K_2 + 1$ times (J_{K_2+1}), where $K = K_2(e_1, h)$; see (26)–(27). Notice that χ_2 is finite since $\tilde{T}_2 > 0$ for level sets in the step region (yet, χ_2 diverges at the step-region boundary when $q_2^{\text{wall}} > 0$; see Table 2).

The order of these intervals on the circle is $(J_R, J_{K_2}, J_{K_2+1})$; this follows from the geometry of the swiss-crossed surface or from realizing that the right (resp. left) most end point of J_R corresponds to a trajectory which hits the corner with positive (resp. negative) vertical velocity, hence, a small shift into the interval J_U will result in missing the step on the right side and hitting the upper part of the step on the left side, see Figure 11.

Under the return map to Σ_1 the two intervals J_{K_2}, J_{K_2+1} switch their position and J_U and J_R rotate by Θ_2; This follows from formulae (31). Indeed, the dividing trajectory between these two intervals is the trajectory that hits the corner from the direction above the step (i.e., with $p_1 > 0$, $p_2 < 0$), and this dividing trajectory is glued to the lower boundary of J'_R — since the return map is piecewise orientation preserving this implies that J_{K_2}, J_{K_2+1} must switch their positions — see Figure 11. In summary, we proved equation (28). The lengths of the intervals, λ_α of (29), follow either from the swiss-cross geometry, or, equivalently, from formulae (31), or by considering the phases of the trajectories which hit the step corner (see Figure 11):

$$\begin{aligned} \lambda_{J_{K_2+1}} &= 2\pi \frac{\tilde{T}_2}{T_2} \left\{ \frac{T_1 - \tilde{T}_1}{\tilde{T}_2} \right\} = 2\theta_2^{\text{wall}} \{\chi_2\} \\ \lambda_{J_{K_2}} &= 2\pi \frac{\tilde{T}_2}{T_2} \left(1 - \left\{ \frac{T_1 - \tilde{T}_1}{\tilde{T}_2} \right\} \right) = 2\theta_2^{\text{wall}}(1 - \{\chi_2\}) \end{aligned} \tag{32}$$

The form of the IEM on the circle is now fully determined by the rotation (23), the permutation (28), and the lengths of the intervals (29).

To determine the 5-IEM on the fundamental interval $[-\pi, \pi)$, we need to identify how the circle-intervals and their images J_α, J'_α, are cut by the chosen fundamental interval, here $[-\pi, \pi)$. Let $\theta^{L,R}_{J_\alpha}, \theta^{L,R}_{J'_\alpha} \in [-\pi, \pi)$ denote the left and right end points of the circle interval J_α, J'_α mod 2π. Namely, when $\theta^L_{J_\alpha} < \theta^R_{J_\alpha}$ the circle interval J_α is not cut by the fundamental interval, so $J^*_\alpha = [\theta^L_{J_\alpha}, \theta^R_{J_\alpha}) \subset [-\pi, \pi)$ whereas $\theta^L_{J_\alpha} > \theta^R_{J_\alpha}$ means that J_α is split to two intervals, so: $J^*_\alpha = J^1_\alpha \cup J^2_\alpha = [-\pi, \theta^R_{J_\alpha}) \cup [\theta^L_{J_\alpha}, \pi)$, and the same convention is applied to the intervals images. To obtain the 5-IEM, given an α such that $\theta^L_{J_\alpha} > \theta^R_{J_\alpha}$ we split that interval to two at the phase π. Similarly, given an α such that $\theta^L_{J'_\alpha} > \theta^R_{J'_\alpha}$ we split its preimage, J_α at θ^* — the preimage of π. In the nondegenerate case (i.e., when $\theta^{L,R}_{J_\alpha}, \theta^{L,R}_{J'_\alpha} \neq -\pi$, $J_\alpha \in \{J_R, J_{K_2}, J_{K_2+1}\}$), exactly one of the intervals and exactly one image of an interval is split, so, if additionally $\{\chi_2\} \neq 0$, we obtain a 5-IEM. We identify below the J_R interval end points and their images and demonstrate that this completely determines the 5-IEM on $[-\pi, \pi)$.

The left boundary of J_R, $\theta^L_{J_R}$, is the phase of the trajectory which reaches the corner from the right with negative vertical velocity, i.e., it is the phase on Σ_1 which arrives to the corner $(\theta^{\text{wall}}_1, \theta^{\text{wall}}_2)$ in the swiss-cross (see Figure 11). Since the time of passage from Σ_1 to Σ^-_1 is half of $\tilde{T}_1$, and since the phases in J_R are rotated by the phase Θ_2, we immediately obtain that

$$\begin{aligned} \theta^L_{J_R} &= \theta^R_{J_{K_2+1}} = \theta^{\text{wall}}_2 - \tfrac{1}{2}\Theta_2 \pmod{2\pi}, \\ \theta^L_{J'_R} &= \theta^R_{J'_{K_2}} = \theta^{\text{wall}}_2 + \tfrac{1}{2}\Theta_2 \pmod{2\pi}. \end{aligned} \tag{33}$$

This information, together with the order of the intervals (28) and their lengths (29) completely determines the 5 IEM. Indeed,

$$\theta^R_{J_R} = \theta^L_{J_{K_2}} = \theta^L_{J_R} + \lambda_{J_R} \pmod{2\pi}, \tag{34}$$

hence

$$\theta^L_{J'_{K_2+1}} = \theta^R_{J'_R} = \theta^R_{J_R} + \Theta_2 \pmod{2\pi}, \tag{35}$$

and

$$\theta^R_{J_{K_2}} = \theta^L_{J_{K_2+1}} = \theta^L_{J_{K_2}} + \lambda_{J_{K_2}} \pmod{2\pi}, \tag{36}$$

so

$$\theta^L_{J'_{K_2}} = \theta^R_{J'_{K_2+1}} = \theta^L_{J'_{K_2+1}} + \lambda_{J_{K_2+1}} \pmod{2\pi}, \tag{37}$$

and all the intervals' and their images' end points are thus determined by $\chi_2, \Theta_2, \theta^{\text{wall}}_2$ (all depending on (e_1, h) and on the parameters e.g., $q^{\text{wall}}_{1,2}$). In particular, the conditions under which one or more of the 5-intervals in $[-\pi, \pi)$

q_1^{wall}	q_2^{wall}	$\chi_2(h_1^{\text{step}}),\, \chi_2(h-h_2^{\text{step}})$	$\Theta_2(h_1^{\text{step}}),\, \Theta_2(h-h_2^{\text{step}})$
<0	<0	$0,\ \frac{A(h-h_2^{\text{step}})}{2\pi}$	$\Theta_2^{\text{smooth}}(h_1^{\text{step}},h),\ B(h-h_2^{\text{step}})$
<0	>0	$0,\ \infty$	$\Theta_2^{\text{smooth}}(h_1^{\text{step}},h),\ B(h-h_2^{\text{step}})$
>0	<0	$\frac{\Theta_2^{\text{smooth}}(h_1^{\text{step}},h)}{2\theta_2^{\text{wall}}(h-h_1^{\text{step}})},\ \frac{A(h-h_2^{\text{step}})}{2\pi}$	$0,\ B(h-h_2^{\text{step}})$
>0	>0	$\frac{\Theta_2^{\text{smooth}}(h_1^{\text{step}},h)}{2\theta_2^{\text{wall}}(h-h_1^{\text{step}})},\ \infty$	$0,\ B(h-h_2^{\text{step}})$

Table 2. The values of χ_2 and Θ_2 at the two edges of $\bar{\mathcal{R}}^c(h)$, where we use the shorthand notations

$$A(h-h_2^{\text{step}}) = \Theta_2^{\text{smooth}}(h-h_2^{\text{step}})\big(1-\theta_1^{\text{wall}}(h-h_2^{\text{step}})/\pi\big),$$
$$B(h-h_2^{\text{step}}) = \Theta_2^{\text{smooth}}(h-h_2^{\text{step}})(\theta_1^{\text{wall}}(h-h_2^{\text{step}})/\pi).$$

has zero length can be explicitly formulated:

$$\Theta_2(e_1,h,q_1^{\text{wall}}) \\ = \begin{cases} \Theta^{\text{smooth}}(e_1,h)-2K\theta_2^{\text{wall}}(h-e_1,q_2^{\text{wall}}) & \text{then } \lambda_{J_{K+1}}=0, \\ \pm 2\theta_2^{\text{wall}}(h-e_1,q_2^{\text{wall}})+2\pi(1+2M) & \text{then } -\pi\in\{\theta_{J_R}^{L,R},\theta_{J'_R}^{L,R}\}, \\ 2\theta_2^{\text{wall}}(h-e_1,q_2^{\text{wall}})(1-2\{\chi_2\})+2\pi(1+2M) & \text{then } -\pi\in\{\theta_{J_K}^{R},\theta_{J'_{K+1}}^{R}\}, \end{cases} \tag{38}$$

where $K, M\in\mathbb{Z}$. To complete the proof, we need to show that these conditions may be satisfied at most at isolated e_1 values. To this aim, we first notice

Lemma 4.3. *For level sets in the step region $\mathcal{R}^c$, the functions χ_2, Θ_2, θ_2^{wall} of e_1 are pairwise independent, and, when Θ_2^{smooth} is nonconstant, they are also pairwise independent of Θ_2^{smooth}.*

Proof. The independence follows from the observation that the functions are smooth nonconstant functions (see Tables 1 and 2) that depend nontrivially on e_1 through distinct parameters. For example, $\Theta_2=\Theta_2(e_1,h,q_1^{\text{wall}})$ whereas $\theta_2^{\text{wall}}=\theta_2^{\text{wall}}(h-e_1,q_2^{\text{wall}})$ and the dependence of these two functions on e_1 through $q_{1,2}^{\text{wall}}$ is nontrivial (i.e., it follows from equations (7) and (23) that

$$\frac{\partial^2\theta_2^{\text{wall}}}{\partial q_2^{\text{wall}}\partial e_1} = -\frac{d}{de_1}\frac{\omega_2(h-e_1)}{\sqrt{2(h-e_1-V_2(q_2^{\text{wall}}))}}$$

and

$$\frac{\partial^2\Theta_2}{\partial q_1^{\text{wall}}\partial e_1} = -\frac{d}{de_1}\frac{2\omega_2(h-e_1)}{\sqrt{2(e_1-V_1(q_1^{\text{wall}}))}}$$

hence, with, possibly, the exception of isolated e_1 values, these derivatives do not vanish for all level sets in $\mathcal{R}^c$). Hence, if they were functionally dependent, i.e., there was a $G(\theta_2^{\text{wall}}, \Theta_2; h, q_{1,2}^{\text{wall}}) \equiv 0$ then

$$\frac{d}{dq_2^{\text{wall}}} G(\theta_2^{\text{wall}}, \Theta_2; h, q_{1,2}^{\text{wall}}) = \frac{\partial G}{\partial \theta_2^{\text{wall}}} \frac{\partial \theta_2^{\text{wall}}}{\partial q_2^{\text{wall}}} + \frac{\partial G}{\partial q_2^{\text{wall}}} \equiv 0$$

and hence

$$\begin{aligned}\frac{d^2}{de_1 dq_2^{\text{wall}}} G(\theta_2^{\text{wall}}, \Theta_2; h, q_{1,2}^{\text{wall}}) &= \frac{\partial G}{\partial \theta_2^{\text{wall}}} \frac{\partial^2 \theta_2^{\text{wall}}}{\partial e_1 \partial q_2^{\text{wall}}} + \frac{\partial \frac{dG}{de_1}}{\partial \theta_2^{\text{wall}}} \frac{\partial \theta_2^{\text{wall}}}{\partial q_2^{\text{wall}}} + \frac{\partial \frac{dG}{de_1}}{\partial q_2^{\text{wall}}} \\ &= \frac{\partial G}{\partial \theta_2^{\text{wall}}} \frac{\partial^2 \theta_2^{\text{wall}}}{\partial e_1 \partial q_2^{\text{wall}}} \\ &= 0.\end{aligned}$$

Since $\partial^2 \theta_2^{\text{wall}}/(\partial e_1 \partial q_2^{\text{wall}}) \neq 0$ we conclude that $\partial G/\partial \theta_2^{\text{wall}} = 0$, namely, there is no such G with nontrivial dependence on both θ_2^{wall} and Θ_2). Similarly, since $\chi_2 = \chi_2(e_1, h, q_1^{\text{wall}}, q_2^{\text{wall}})$, and similarly to the above calculations, the dependence of χ_2 on both q_1^{wall} and q_2^{wall} is nontrivial in e_1, the pairs (χ_2, Θ_2) and $(\chi_2, \theta_2^{\text{wall}})$ are functionally independent. Finally, since $\Theta_2^{\text{smooth}} = \Theta_2^{\text{smooth}}(e_1, h)$, by the same argument as above, provided $\partial \Theta^{\text{smooth}}(e_1, h)/\partial_{e_1} \neq 0$ apart of isolated points, it is pairwise independent from each of the functions $\chi_2, \Theta_2, \theta_2^{\text{wall}}$. □

Now, we can show that (38) is satisfied at most at isolated e_1 values. For the first two possibilities, both sides of the equation are smooth functions of e_1 with the right hand side depending nontrivially on q_1^{wall} whereas the left hand side depending nontrivially on q_2^{wall}. Hence, by the same arguments as in Lemma 4.3, the right and left hand side are functionally independent and their difference vanish at most at isolated e_1 values.

For the last row, notice that

$$\chi_2(e_1, h, q_1^{\text{wall}}, q_2^{\text{wall}}) = \frac{T_2(h-e_1)}{\tilde{T}_2(h-e_1)} \frac{T_1(e_1) - \tilde{T}_1(e_1)}{T_2(h-e_1)} = \frac{\Theta_2^{\text{smooth}} - \Theta_2}{2\theta_2^{\text{wall}}}, \tag{39}$$

namely, $2\{\chi_u\}\theta_2^{\text{wall}} = \Theta_2^{\text{smooth}} - \Theta_2 - 2K_2\theta_2^{\text{wall}}$, hence the last equation becomes

$$\begin{aligned}&2\theta_2^{\text{wall}}(h-e_1; q_2^{\text{wall}})(1+2K_2) \\ &\qquad = 2\Theta_2^{\text{smooth}}(e_1, h) - \Theta_2(e_1, h, q_1^{\text{wall}}) - 2\pi(1+2M),\end{aligned} \tag{40}$$

which shows, as above, that it is also satisfied at most at isolated e_1 values.

Notice that $\theta_2^{\text{wall}} > 0$ for all level sets in $\mathcal{R}^c(h)$, so the circle map has always at least two nontrivial components (J_R and J_U), and in fact, with the exception

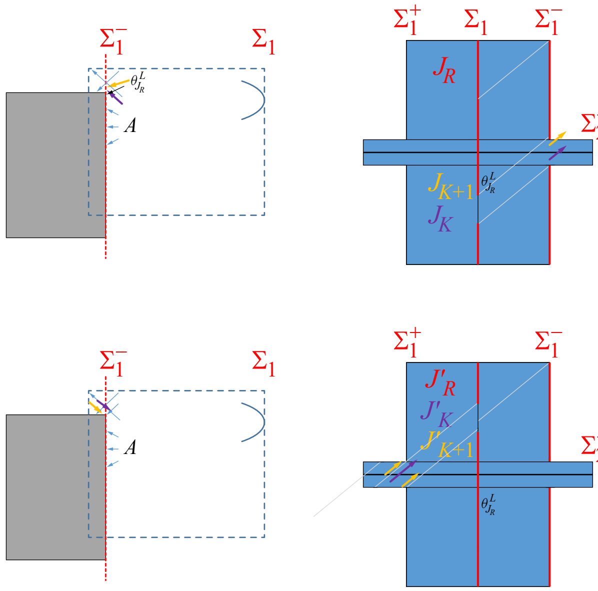

Figure 11. Order of intervals: the intervals J_{K_2}, J_{K_2+1} correspond to orbits that bounce, respectively, K_2, K_2+1 times above the step. On the SW surface these are the orbits that enter the horizontal arm and wrap, respectively, K_2, K_2+1 times around it before returning to the vertical arm. Thus, their order on Σ_1 is reversed by the flow. The phase $\theta^L_{J_R}$ denotes the left edge of J_R — the phase that separates the orbits that enter the horizontal arm from those that bounce off the vertical arm boundary, namely the vertical boundary of the step.

of isolated points within $\mathcal{R}^c(h)$, it has three nontrivial components since $\{\chi_2\}$ vanishes at most at isolated e_1 values. $\square$

5. Additional properties of the family of IEM

Theorem 4.2 implies that the dynamics for level sets in the step set are completely determined by the numerical properties of $\chi_2, \Theta_2, \theta_2^{\text{wall}}$. All these functions depend smoothly on e_1 for the level sets in $\mathcal{R}^c(h)$ and are nonconstant functions — indeed, their values at the boundaries of $\mathcal{R}^c(h)$ are always distinct — see Tables 1 and 2. Hence, these functions attain both rational and irrational values as e_1 is varied (in some cases, but not all, these functions are also monotone in e_1). While one may suspect that this implies that for almost all e_1 values the dynamics are uniquely ergodic, it is difficult to check directly when the corresponding IEM satisfies the Veech condition; see [13]. Indeed, while Lemma 4.3 states that the functions $\chi_2, \Theta_2, \theta_2^{\text{wall}}$ are pairwise independent, and, in Theorem 4.2

we established that the lengths of the intervals of the IEM are nonzero with the exception of isolated e_1 values, more delicate relations between the intervals lengths may arise. Indeed, rewriting equation (39) as

$$\Theta_2^{\text{smooth}}(e_1, h) \\ = 2\theta_2^{\text{wall}}(h - e_1, q_2^{\text{wall}})\chi_2(e_1, h, q_1^{\text{wall}}, q_2^{\text{wall}}) + \Theta_2(e_1, h, q_1^{\text{wall}}), \quad (41)$$

shows that in the linear case, where $\Theta_2^{smooth,\text{LO}} = 2\pi \frac{\omega_2}{\omega_1}$, the three functions are functionally related! The implications of this dependence on the dynamics and the properties of it for general nonlinear oscillators are yet to be explored. For now we show, by analyzing the properties of these functions, that, for some cases minimal dynamics arise and in others nonminimal dynamics arise.

In particular, we establish that there can be isolated strongly resonant level sets at which orbits of different periods coexist (e.g., if $\Theta_2/2\pi, 2\theta_2^{\text{wall}}/2\pi, \{\chi_2\} \in \mathbb{Q}$), level sets for which periodic and quasiperiodic motion coexist (e.g., when $\{\Theta/2\pi, 2\theta_2/2\pi\} \in \mathbb{Q}$, $\{\chi_2\} \notin \mathbb{Q}$ such a case may emerge) and isolated level sets in $\mathcal{R}^c(h)$ at which the IEM reduces to a rotation (when $\{\chi_2\} = 0$ so the directional flow on SW has a diagonal trajectory in the horizontal arm). Notice that the analogous computations for the return map to Σ_2 amounts to replacing $1 \leftrightarrow 2$ in all the above definitions.

In particular, we notice the special role the function χ_2 plays: its magnitude controls the number of bounces experienced by phases in J_{K_2} (recall that $K_2 = \lfloor \chi_2 \rfloor$) and its phase, $\{\chi_2\}$, controls the division of J_U to two intervals (recall that $\lambda_{J_{K_2+1}} = 2\theta_2^{\text{wall}}\{\chi_2\}$). Hence, we study the dependence of χ_2 on e_1 and on the parameters $q_{1,2}^{\text{wall}}$. We begin with two simple cases where we can completely characterize the dynamics.

Corllary 5.1. *For level sets in $\mathcal{R}^c(h)$ for which $\{\chi_2\} = 0$ the return map to Σ_1 is of only 2 intervals, namely it corresponds to a rotation by Θ_2, and is thus ergodic if and only if $\Theta_2/2\pi \notin \mathbb{Q}$.*

Proof. By (29), $\{\chi_2\} = 0$ implies that $\lambda_{J_{K_2}} = 2\theta_2^{\text{wall}} > 0$ and $\lambda_{J_{K_2+1}} = 0$, hence, (31) becomes a rotation by Θ_2. $\square$

In terms of the directed motion on the L-shaped billiard, the condition $\{\chi_2\} = 0$ corresponds to the case of a diagonal orbit connecting the corners of the horizontal arm. If, additionally, $\Theta_2/2\pi \in \mathbb{Q}$ then this orbit is also a diagonal of the vertical arm. Notably, if $q_2^{\text{wall}} > 0$, close to the boundary of $\mathcal{R}^c(h)$ the horizontal sleeve becomes narrow (see Figure 12) and thus there are many level sets at which $\{\chi_2\} = 0$.

Lemma 5.2. *If $q_2^{\text{wall}} > 0$, for all $h > h^{\text{step}}$, there are countable infinite level sets in $\mathcal{R}^c(h)$ for which $\{\chi_2\} = 0$.*

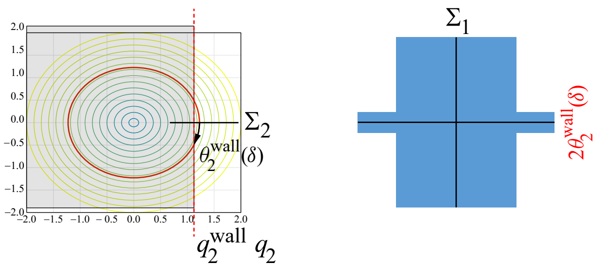

Figure 12. The dynamics for small θ_2^{wall}.

Proof. Since, for $q_2^{\mathrm{wall}} > 0$, $\tilde{T}_2(h - e_1; q_2^{\mathrm{wall}}) \to 0$ as $e_1 \to h - h_2^{\mathrm{step}}$ whereas $T_1(e_1) - \tilde{T}_1(e_1; q_1^{\mathrm{wall}})$ attains a finite positive limit (since $h > h^{\mathrm{step}}$), the smooth function $\chi_2(e_1, h) = (T_1(e_1) - \tilde{T}_1(e_1)/\tilde{T}_2(h - e_1))$ in the open interval $\mathcal{I}^c(h)$ becomes infinite on the interval right boundary, hence it passes through integer values at countable infinite values of e_1. □

Another case which allows a complete characterization of the motion is when Θ_2 is rational and θ_2^{wall} is small.

Lemma 5.3. *For level sets in $\mathcal{R}^c(h)$ for which $\Theta_2 = 2\pi m/n$ and $2\theta_2^{\mathrm{wall}} < 2\pi/n$, the IEM to Σ_1 is nonergodic. For such level sets, if $\{\chi_2\} \notin \mathbb{Q}$ the motion is dense on a union of open intervals and is periodic on its complement. If $\{\chi_2\} \in \mathbb{Q}$, all i.c., are periodic, yet, there are two distinct periods. All the above conditions are realizable for some level sets and wall positions.*

Proof. Let $I = [-\pi, \pi)\setminus \bigcup_{j=0}^{n-1} F^j(J_U) \subset J_R$ where $J_U = J_{K_2} \cup J_{K_2+1}$. Since here $\lambda_{J_U} = 2\theta_2^{\mathrm{wall}} < 2\pi/n$, this is a nonempty set. It is invariant since the end points of J_U belong to J_R, so the end points are n-periodic. Hence, all the i.c., in I are n periodic and thus F is nonergodic on the circle.

The dynamics in the complement to I, namely the invariant set $\bigcup_{j=0}^{n-1} F^j(J_U)$, depends on the numerical value of $\{\chi_2\}$. Notice that for all i.c., in J_{K_2}, $F^n(\theta_2) = \theta_2 + 2\theta_2^{\mathrm{wall}}\{\chi_2\} \in J_U$ whereas for all i.c., in J_{K_2+1}, $F^n(\theta_2) = \theta_2 - 2\theta_2^{\mathrm{wall}}(1 - \{\chi_2\}) \in J_U$, namely, $F^n(\theta_2)$ is a 2-IEM on J_U, hence it is periodic for $\{\chi_2\} = \frac{p}{q} \in \mathbb{Q}$ and is dense in J_U otherwise. In the periodic case, initial conditions in I are n-periodic whereas initial conditions in its complement are nq periodic. Finally, since the functions $\Theta_2, \chi_2, \theta_2^{\mathrm{wall}}$ are continuous (in fact, smooth) nonconstant functions of e_1 in $\mathcal{I}^c(h)$ and since $\Theta_2 = \Theta_2(e_1, h, q_1^{\mathrm{wall}})$ we obtain that for every h, q_1^{wall} there is a countable set of e_1 values in $\mathcal{I}^c(h)$, $e_1^* = e_1(m/n, h, q_1^{\mathrm{wall}})$ for which $\Theta_2 = 2\pi m/n$. Notice that Θ_2 does not depend explicitly on q_2^{wall}. Fixing $m/n, h, q_1^{\mathrm{wall}}$, there is a $q_2^{\mathrm{wall}}(\delta)$ value such that $2\theta_2^{\mathrm{wall}}(h - e_1^*, q_2^{\mathrm{wall}}) < 2\pi/n$ for all $q_2^{\mathrm{wall}} > q_2^{\mathrm{wall}}(\delta)$; indeed, choose $q_2^{\mathrm{wall}}(\delta) > 0$ such that $V_2(q_2^{\mathrm{wall}}(\delta)) = h - e_1^* - \delta$, so, by (7) and (18), for small δ, $\theta_2^{\mathrm{wall}}(\delta) = \theta_2^{\mathrm{wall}}(h - e_1^*, q_2^{\mathrm{wall}}(\delta))$ is monotone decreasing (in δ) to 0 (see Figure 12). In particular, there exists $\delta^*(n)$ such that for all $\delta \in (c\delta^*(n), \delta^*(n))$, for any $0 < c < 1$, the impact angle satisfies $2\theta_2^{\text{wall}}(c\delta^*(n)) < 2\theta_2^{\text{wall}}(\delta) < 2\pi/n$, so it is small yet bounded away from 0, as needed for the smooth dependence on e_1 near e_1^*. In particular, for this range of $q_2^{\text{wall}}(\delta)$ values, motion on the level set $(e_1^*, h - e_1^*)$ is n-periodic for the set I as described above. Moreover, on this level set, from (26), $\chi_2(\delta) = (\Theta^{\text{smooth}}(e_1^*, h) - 2\pi m/n)/\theta_2^{\text{wall}}(\delta) > 0$, hence, it is a continuous monotone increasing function of δ, and thus, $\{\chi_2\} \notin \mathbb{Q}$ for almost all δ values in the interval and there is a countable set of δ values for which $\{\chi_2\} \in \mathbb{Q}$. Namely, we established that these conditions are always realizable by varying the parameter q_2^{wall}. □

Notice that for sufficiently small c in the above proof the function $\chi_2(\delta)$ becomes large, as in Lemma 5.2, therefore, $\{\chi_2(\delta)\}$ vanishes at some isolated δ values. Finally, since χ_2 is continuous, its range for $e_1 \in \mathcal{I}^c(h)$ is at least as large as the interval $(\chi_2(h_1^{\text{step}}), \chi_2(h - h_2^{\text{step}}))$. When one of these values is an integer, the behavior below and above this energy changes. Thus, Table 2 provides conditions for energy values at which bifurcations occur. For linear oscillators, we can find the ranges explicitly, see Section 6.

All the above properties were stated for the return map to Σ_1, creating an artificial asymmetry between the horizontal and vertical directions. The same results apply to the return map to the Σ_2 section by reversing the roles of 1 and 2 and horizontal and vertical in all definitions.

6. The step dynamics for linear oscillators

For the quadratic potentials (2), the L-shaped billiard tables vertices are found explicitly and the direction of motion is fixed. We begin this section by proving Theorem 2.6 regarding the linear-oscillators-step dynamics and continue with additional observations regarding the singular level sets for this case.

Proof of Theorem 2.6. The transformation to action angle coordinates for linear oscillators, with the convention (14), becomes

$$(q_i(t), p_i(t)) = \left(\sqrt{\frac{2I_i}{\omega_i}}\cos\theta_i(t), -\sqrt{2I_i\omega_i}\sin\theta_i(t)\right), \qquad H_i = \omega_i I_i,$$

and $I_i = \frac{1}{2}\left(p_i^2/\omega_i + \omega_i q_i^2\right)$. Hence, for $e_i > h_i^{\text{step}} = \frac{1}{2}\omega_i^2(q_i^{\text{wall}})^2$:

$$\begin{aligned}\theta_i^{\text{wall,LO}}(e_i; q_i^{\text{wall}}) &= \arccos\sqrt{\frac{\omega_i}{2I_i}}q_i^{\text{wall}} \\ &= \arccos\frac{\omega_i q_i^{\text{wall}}}{\sqrt{2e_i}} \in \begin{cases}\left(\frac{\pi}{2}, \pi\right) & q_i^{\text{wall}} < 0, \\ \left(0, \frac{\pi}{2}\right) & q_i^{\text{wall}} > 0.\end{cases}\end{aligned} \tag{42}$$

Since the frequencies of linear oscillators are independent of the energy, the direction of motion in the isoenergetic billiard family, $\mathcal{B}(h)$, is fixed to (ω_1, ω_2) for all the level sets. Hence, for a given energy surface $h = e_1 + e_2 > h^{\text{step}}$, the linear oscillator step dynamics on each level set $(e_1, e_2 = h - e_1) \in \mathcal{R}^c(h)$ are conjugated to the directed billiard motion, in direction (ω_1, ω_2), in the L-shaped billiards $L(\pi, \pi, \arccos \omega_1 q_1^{\text{wall}}/\sqrt{2e_1}, \arccos \omega_2 q_2^{\text{wall}}/\sqrt{2(h-e_1)})$. Moreover, since

$$\frac{d\theta_1^{\text{wall,LO}}(e_1; q_1^{\text{wall}})}{de_1} = \frac{\omega_1 q_1^{\text{wall}}}{2e_1} \frac{1}{\sqrt{2e_1 - (\omega_1 q_1^{\text{wall}})^2}} \tag{43}$$

and

$$\frac{d\theta_2^{\text{wall,LO}}(h - e_1; q_1^{\text{wall}})}{de_1} = -\frac{\omega_2 q_2^{\text{wall}}}{2(h-e_1)} \frac{1}{\sqrt{2(h-e_1) - (\omega_2 q_2^{\text{wall}})^2}}, \tag{44}$$

the widths of the arms are monotone in e_1 and are of opposite monotonicity if and only if $q_1^{\text{wall}} q_2^{\text{wall}} > 0$. $\square$

As shown in Section 5, the monotonicity, bounds and limits of the functions $\Theta_2, \chi_2, \theta_2^{\text{wall}}$ determine the variety of behaviors of the dynamics on isoenergy surfaces. For linear oscillators, $\Theta_2^{\text{LO}}, \theta_2^{\text{wall,LO}}$ are monotone in the step region whereas:

Lemma 6.1. *For all $h > h^{\text{step}}$, the function $\chi_2^{\text{LO}}(e_1, h)$ is monotone if and only if $q_1^{\text{wall}} q_2^{\text{wall}} < 0$.*

Proof. Observe that for linear oscillators $q_i^{\text{wall}} \tilde{T}_i'^{\text{LO}}(e_i; q_i^{\text{wall}}) > 0$ (see equations (7) and (9) and recall that $T_i'^{\text{LO}} = 0$, hence the result follows from the definition (26) of $\chi_2(e_1, h)$, or, from direct differentiation of

$$\chi_2^{\text{LO}}(e_1, h) = \frac{\omega_2}{\omega_1} \frac{(\pi - \arccos(\omega_1 q_1^{\text{wall}}/\sqrt{2e_1}))}{\arccos(\omega_2 q_2^{\text{wall}}/\sqrt{2(h-e_1)})} = \frac{\omega_2}{\omega_1} \frac{\pi - \theta_1^{\text{wall,LO}}(e_1; q_1^{\text{wall}})}{\theta_2^{\text{wall,LO}}(h - e_1; q_2^{\text{wall}})}$$

(see (11)),

$$\chi_2^{\text{LO}'}(e_1) = \frac{\omega_2 \left(-\frac{\omega_1 q_1^{\text{wall}} \arccos \omega_2 q_2^{\text{wall}}/\sqrt{2(h-e_1)}}{2e_1 \sqrt{2e_1 - (\omega_1 q_1^{\text{wall}})^2}} + \frac{\omega_2 q_2^{\text{wall}} (\pi - \arccos \omega_1 q_1^{\text{wall}}/\sqrt{2e_1})}{2(h-e_1)\sqrt{2(h-e_1) - (\omega_2 q_2^{\text{wall}})^2}} \right)}{\omega_1 (\arccos \omega_2 q_2^{\text{wall}}/\sqrt{2(h-e_1)})^2}. \tag{45}$$

The denominator is always positive (it approaches 0 when $q_2^{\text{wall}} > 0$ and $e_1 \nearrow h - \frac{1}{2}(\omega_2 q_2^{\text{wall}})^2$) so the sign is determined by the numerator. If $q_1^{\text{wall}} q_2^{\text{wall}} < 0$ both terms in the numerator have the same sign so χ_2 is monotone. If $q_1^{\text{wall}} q_2^{\text{wall}} > 0$, the first term in the numerator diverges to $-\operatorname{sign}(q_1^{\text{wall}})\infty$ as $e_1 \searrow \frac{1}{2}(\omega_1 q_1^{\text{wall}})^2$, the second term diverges to $\operatorname{sign}(q_2^{\text{wall}})\infty$ as $e_1 \nearrow h - \frac{1}{2}(\omega_2 q_2^{\text{wall}})^2$, hence $\chi_2'(e_1)$ changes sign and χ_2 is nonmonotone. $\square$

q_1^{wall}	q_2^{wall}	$\chi_2^{\text{LO}}(h_1^{\text{step}}) \to \chi_2^{\text{LO}}(h - h_2^{\text{step}})$	$\Theta_2^{\text{LO}}(h_1^{\text{step}}) \to \Theta_2^{\text{LO}}(h - h_2^{\text{step}})$
< 0	< 0	$0 \nearrow\searrow \omega(1 - 1/\pi\theta_1^*(h))$	$2\pi\omega \searrow 2\omega\theta_1^*(h)$
< 0	> 0	$0 \nearrow \infty$	$2\pi\omega \searrow 2\omega\theta_1^*(h)$
> 0	< 0	$\omega\pi/\theta_2^*(h) \searrow \omega(1 - 1/\pi\theta_1^*(h))$	$0 \nearrow 2\omega\theta_1^*(h)$
> 0	> 0	$\omega\pi/\theta_2^*(h) \searrow\nearrow \infty$	$0 \nearrow 2\omega\theta_1^*(h)$

Table 3. The values of χ_2^{LO}, Θ_2^{LO} at the edges of $\mathcal{R}^c(h)$ and their monotonicity properties, where $\omega = \frac{\omega_2}{\omega_1}$.

Corllary 6.2. *If $q_2^{\text{wall}} > 0$, for all $h > h^{\text{step}}$, the step region has countable infinite level sets at which $\{\chi_2^{\text{LO}}\} = 0$, namely at which the return map to Σ_1 reduces to a two intervals rotation on the circle. For $q_2^{\text{wall}} < 0$, for sufficiently large h, the number, $N_{\text{osc}}^2(h)$, of such level sets when $q_1^{\text{wall}} < 0$ is at least $\left\lfloor \frac{1}{2}\frac{\omega_2}{\omega_1} \right\rfloor$ whereas if $q_1^{\text{wall}} > 0$ there are $\left\lfloor \frac{3}{2}\frac{\omega_2}{\omega_1} \right\rfloor$ such level sets. The same results hold for the return map to Σ_2 when replacing the roles of $1 \leftrightarrow 2$ in the above statements.*

Proof. First, it follows from (11) that in the step region $\chi_2^{\text{LO}}(e_1, h)$ is a smooth nonoscillatory function which diverges only at the step region upper boundary (and this occurs if and only if $q_2^{\text{wall}} > 0$). Hence, for any fixed h, there is at most countable infinite level sets $N_{\text{osc}}^2(h)$ at which $\{\chi_2^{\text{LO}}(e_1)\}$ may vanish. The edge values — the values of χ_2^{LO}, Θ_2^{LO} at the end points of the step-region (namely calculating (9), (11) at $e_1 = h_1^{\text{step}}$ and at $e_1 = h - h_2^{\text{step}}$) and their monotonicity property are listed in Table 3, where

$$\theta_1^*(h) = \theta_1^{\text{wall}}(h - h_2^{\text{step}}; q_1^{\text{wall}}) = \arccos \frac{\omega_1 q_1^{\text{wall}}}{\sqrt{2h - (\omega_2 q_2^{\text{wall}})^2}} \tag{46}$$

$$\theta_2^*(h) = \theta_2^{\text{wall}}(h - h_1^{\text{step}}; q_2^{\text{wall}}) = \arccos \frac{\omega_2 q_2^{\text{wall}}}{\sqrt{2h - (\omega_1 q_1^{\text{wall}})^2}}. \tag{47}$$

For any energy h, these values supply the range of χ_2^{LO} in the monotone cases (second and third rows in the tables) and a lower bound on its range in the nonmonotone cases (first and last rows). The number of isoenergy level sets at which $\{\chi_2^{\text{LO}} = 0\}$ (at which the directional motion in the horizontal arm of the SW surface is diagonal) is determined by the number of integer values contained in the range of χ_2^{LO}. The second and fourth rows of Table 3 show that the range is infinite when $q_2^{\text{wall}} > 0$, proving the first statement of the corollary. Table 4 shows the asymptotic edge values at large energies, using the observation that $\theta_{1,2}^*(h) \to \frac{\pi}{2}$. The rest of the corollary follows from this table — for $q_2^{\text{wall}} < 0$, the first row of Table 4 corresponds to the nonmonotone case whereas the third row

q_1^{wall}	q_2^{wall}	χ_2^{LO}	Θ_2^{LO}	N_{osc}^2	N_{osc}^1
<0	<0	$0 \nearrow\searrow \omega/2$	$2\pi\omega \searrow \pi\omega$	$\geqslant \lfloor\omega/2\rfloor$	$\geqslant \lfloor 1/2\omega\rfloor$
<0	>0	$0 \nearrow \infty$	$2\pi\omega \searrow \pi\omega$	∞	$\lfloor 3/2\omega\rfloor$
>0	<0	$2\omega \searrow \omega/2$	$0 \nearrow \pi\omega$	$\lfloor 3\omega/2\rfloor$	∞
>0	>0	$2\omega \searrow\nearrow \infty$	$0 \nearrow \pi\omega$	∞	∞

Table 4. The behavior of χ_2^{LO}, Θ_2^{LO} on $\mathcal{R}^c(h)$ at large h and the number of oscillations, N_{osc}^i(h), of $\{\chi_i^{\text{LO}}\}$ in the family of isoenergy return maps to Σ_i for sufficiently large h, where $\omega = \omega_2/\omega_1$.

q_1^{wall}	q_2^{wall}	χ_2^{LO}	Θ_2^{LO}	$N_{\text{osc}}^2(h^{\text{step}}+\eta)$
<0	<0	$0\nearrow\searrow a_1\omega$	$2\pi\omega\searrow 2\pi\omega(1-a_1)$	$\gtrsim \lfloor a_1\omega\rfloor$
<0	>0	$0\nearrow\infty$	$2\pi\omega\searrow 2\pi\omega(1-a_1)$	∞
>0	<0	$\omega(1+a_2)\searrow\omega(1-a_1)$	$0\nearrow\pi a_1$	$\lfloor\omega(a_1+a_2)\rfloor$
>0	>0	$\omega/a2\searrow\nearrow\infty$	$0\nearrow\pi a_1$	∞

Table 5. The values of χ_2^{LO}, Θ_2^{LO} at the edges of $\mathcal{R}^c(h=h^{\text{step}}+\eta)$ for small $\eta>0$, namely $\chi_2^{\text{LO}}(h_1^{\text{step}})$, $\chi_2^{\text{LO}}(\eta+h^{\text{step}}-h_2^{\text{step}})$ and $N_{\text{osc}}^2(h)$. The values of $N_{\text{osc}}^1(h)$ in the first and second rows are found by switching $1\leftrightarrow 2$ (as in Table 4). For shorthand notation we denote here $\omega=\omega_2/\omega_1$ and $a_i=\frac{1}{\pi}\sqrt{\eta/h_i^{\text{step}}}$, $i=1,2$.

corresponds to the monotone case. Since $N_{\text{osc}}^2(h)$ are integers, for sufficiently large h the limiting values and $N_{\text{osc}}^2(h)$ are identical. Finally, by symmetry, replacing the roles of $1 \leftrightarrow 2$, provides the estimates for $N_{\text{osc}}^1(h)$, the number of oscillations in the vertical arm before returning to the section Σ_2. $\square$

Table 5 displays the edge values at energies near h^{step} (i.e., for $h = h^{\text{step}} + \eta$, and small, positive, η). Notice that for such h values

$$\theta_i^*(h) = \sqrt{\eta/h_i^{\text{step}}} \quad \text{if } q_i^{\text{wall}} > 0$$

and

$$\theta_i^*(h) = \pi - \sqrt{\eta/h_i^{\text{step}}} \quad \text{if } q_i^{\text{wall}} < 0.$$

We see that when $q_2^{\text{wall}} > 0$, infinite number of oscillations occur for arbitrary small η, whereas in the other cases, the number of oscillations scales with $\sqrt{\eta}$.

7. Summary and discussion

An integrable mechanical Hamiltonian system with a step barrier in the configuration space which is aligned with the continuous symmetries of the integrable Hamiltonian produces dynamics that are not Liouville integrable, yet are unanalyzable. An experimental setup which realizes such a theoretical model has been suggested (Figure 1). In such models, the motion on energy surfaces is foliated by level sets, yet, the motion on a range of isoenergy level sets is nonintegrable and is conjugated to the motion on a family of genus 2 flat surfaces or, equivalently, to an L-shaped billiard (Theorem 2.2). The return map to a Poincaré section for this range of level sets is a 5 interval exchange map, and the lengths of the intervals change nontrivially along the isoenergy family of level sets (Theorem 4.2). For the case of Linear oscillators the L-shaped billiard dimensions and thus the intervals lengths are found explicitly (Theorem 2.6) whereas for general nonlinear oscillators they are given up to quadratures. While our main example included a single step, the same strategy may be applied to any barrier geometry which combines horizontal and vertical barriers. The flow of the HIS (1) with such barriers is conjugated, for any given level set, to a directional motion in the angles' space on nibbled a flat surface, and in some cases (see [12]) one obtains rectangles similar to those analyzed in [11]. An important conclusion is that above certain energy the energy surfaces of (1) are foliated by several families of level set surfaces; within any such family the geometry varies smoothly, and different families have distinct topology. Namely, on the same energy surface there are families of level-set surfaces with different number of connected components and different numbers of holes; see Corllary 2.3 and Figure 10.

The implications of our findings are intriguing; First, the statistics of a typical observable of such mechanical systems (i.e., an observable which does not depend only on the energy distribution among the degrees of freedom) are now related to the delicate theories derived for studying IEM and Teichmuler flows on moduli spaces. Second, by considering soft steep potentials instead of impacts, the topology of the energy surfaces remains as complex as the one constructed here (then the motion is not expected to be foliated to level sets). Higher dimensional extensions, other symmetries, potentials with local maxima (so that the smooth system has singular level sets of the Liouville foliation), and the influence of small perturbations and soft potentials are exciting directions to be further explored; see related results in [18; 22].

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becker@math.uni-bonn.de *The Weizmann Institute of Science, Rehovot, Israel*

stevenelliott517@protonmail.com *The Weizmann Institute of Science, Rehovot, Israel*

benjyjf@gmail.com *The Weizmann Institute of Science, Rehovot, Israel*

segev.gc@gmail.com *The Weizmann Institute of Science, Rehovot, Israel*

mipnueli@gmail.com *The Weizmann Institute of Science, Rehovot, Israel*

vered.rom-kedar@weizmann.ac.il *The Weizmann Institute of Science, Rehovot, Israel*

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Some remarks on the classical KAM theorem, following Pöschel

ABED BOUNEMOURA

We propose a slight correction and a slight improvement on the main result contained in "A lecture on Classical KAM Theorem" by J. Pöschel.

1. Introduction and results

The paper [5] contains a very nice exposition of the classical KAM theorem which has been very influential. It is our purpose in this short and non-self-contained note to add two remarks to this remarkable paper.

The first one concerns a technical mistake in the proof of the main abstract statement Theorem A,[1] which has been recently pointed out and corrected in the PhD thesis [3]. Yet a correction of this mistake, following Pöschel arguments, leads to a final statement which is both less elegant and quantitatively weaker. We would like to explain how, by modifying slightly the arguments using ideas due to Rüssmann (see for instance [7]), Theorem A of [5] can be proved without any changes. The aforementioned modifications consist of replacing the crude Fourier truncation by a more refined polynomial approximation, and then set an iterative scheme with a linear,[2] rather than super-linear, speed of convergence.

The second one concerns the application of Theorem A to an ε-perturbation of a nondegenerate integrable Hamiltonian system. This gives persistence of a set of positive measure of analytic invariant quasiperiodic tori with fixed diophantine frequencies, such that each torus in this set is at a distance of order $\sqrt{\varepsilon}$ to its associated unperturbed invariant torus. By using a more adapted version of Theorem A, we can actually show that the distance is of order ε/α, where α is the constant of the Diophantine vector. This is not a new result, as this was already

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[1]The choices of h_0 and K_0, page 23 in [5], violate the condition $h_0 \leq \alpha(2K_0^{\nu})^{-1}$.

[2]We would like to quote here the paper [6]: "It has often been said that the rapid convergence of the Newton iteration is necessary for compensating the influence of small divisors. But a deeper analysis shows that this is not true. The Newton method compensates not only the influence of small divisors but also many bad estimates veiling the true structure of the problems."

proved in [9] using a refinement of Kolmogorov approach (for an individual torus).

So let us recall the main result of [5], keeping the same notations. For a given domain $\Omega \subseteq \mathbb{R}^n$, consider a subset $\Omega_\alpha \subseteq \Omega$ of Diophantine vectors with constant $\alpha > 0$ and exponent $\tau \geq n-1$. Given $0 < r, s, h \leq 1$, define

$$D_{r,s} = \{I \mid |I| < r\} \times \{\theta \mid |\mathrm{Im}(\theta)| < s\} \subseteq \mathbb{C}^n \times \mathbb{C}^n, \quad O_h = \{\omega \mid |\omega - \Omega_\alpha| < h\} \subseteq \mathbb{C}^n$$

where $|\cdot|$ is the sup norm for vectors, and let $|\cdot|_{r,s,h}$ the sup norm for functions defined on $D_{r,s} \times O_h$ and $|\cdot|_L$ the Lipschitz seminorm with respect to ω. Let $N(I,\omega) = e(\omega) + \omega \cdot I$, which can be seen as a family N_ω of linear integrable Hamiltonian depending on parameters $\omega \in \Omega$; the family of embedding $\Phi_0 : \mathbb{T}^n \times \Omega \to \mathbb{R}^n \times \mathbb{T}^n$ defined by $\Phi_0(\theta,\omega) = (0,\theta)$ defines, for each $\omega \in \Omega$, a Lagrangian torus invariant by the Hamiltonian flow of N_ω and quasiperiodic of frequency ω.

Theorem A. *Let $H = N + P$. Suppose P is real-analytic on $D_{r,s} \times O_h$ with*

$$|P|_{r,s,h} \leq \gamma\alpha r s^\nu, \quad \alpha s^\nu \leq h \tag{1-1}$$

where $\nu = \tau + 1$ and γ is a small constant depending only on n and τ. Then there exist a Lipschitz map $\varphi : \Omega_\alpha \to \Omega$ and a Lipschitz family of real-analytic Lagrangian embedding $\Phi : \mathbb{T}^n \times \Omega_\alpha \to \mathbb{R}^n \times \mathbb{T}^n$ that defines, for each $\omega \in \Omega_\alpha$, a Lagrangian torus invariant by the Hamiltonian flow of $H_{\varphi(\omega)}$ and quasiperiodic of frequency ω. Moreover, Φ is real-analytic on $T_* = \{\theta \mid |\mathrm{Im}(\theta)| < s/2\}$ for each ω and

$$\begin{cases} |W(\Phi - \Phi_0)|, \quad \alpha s^\nu |W(\Phi-\Phi_0)|_L \leq c(\alpha r s^\nu)^{-1}|P|_{r,s,h}, \\ |\varphi - \mathrm{Id}|, \qquad\quad \alpha s^\nu |\varphi - \mathrm{Id}|_L \leq c r^{-1} |P|_{r,s,h}, \end{cases} \tag{1-2}$$

uniformly on $T_* \times \Omega_\alpha$ and Ω_α respectively, where c is a large constant depending only on n and τ, and $W = \mathrm{Diag}(r^{-1}\,\mathrm{Id}, s^{-1}\,\mathrm{Id})$.

As expressed in (1-2), the map (Φ,φ) is Lipschitz regular with respect to $\omega \in \Omega_\alpha$, and its Lipschitz norm (suitably weighted) is close to the one of (Φ_0, Id); this is all what is needed to transfer the positive measure in parameter space $\omega \in \Omega_\alpha$ to a positive measure of quasiperiodic solutions in phase space. One course one may ask whether (Φ,φ) is more regular with respect to $\omega \in \Omega_\alpha$ (since Ω_α is a closed set, smoothness has to be understood in the sense of Whitney). In fact, the sketch of proof we will give below implies the following: given any $l \in [1,+\infty[$, provided (1-1) is replaced by

$$|P|_{r,s,h} \leq \gamma(l)\alpha r s^\nu$$

for some $h > 0$ and some $\gamma(l) > 0$, (Φ,φ) is of class C^l with respect to ω: we simply chose $l = 1$ in Theorem A to obtain Lipschitz regularity. However, as

$l \to +\infty$, $\gamma(l) \to 0$ and thus we cannot conclude that (Φ, φ) is smooth. In order to reach such a statement, one can replace the linear scheme of convergence by the usual super-linear scheme (as described in [5] for instance) but then the exponent ν in (1-1) has to be deteriorate: given any $\mu > \nu$, we have that (Φ, φ) is smooth with respect to ω provided (1-1) is replaced by

$$|P|_{r,s,h} \leq \gamma(\mu, \nu)\alpha r s^{\mu}$$

for some $h > 0$ and some $\gamma(\mu, \nu) > 0$: again $\gamma(\mu, \nu) \to 0$ as $\mu \to \nu$. Popov (see [4]) showed that one can even go further and obtain some Gevrey smoothness of (Φ, φ) under a stronger smallness condition; without going into these rather technical issues, let us just say that (Φ, φ) can be shown to be Gevrey with exponent $1+\mu$ provided the polynomially small threshold s^{ν} in (1-2) is replace by a super-exponentially small threshold of order $\exp(-c(1/s)^{a})$ with $a = a(\mu, \nu) = \nu/(\mu - \nu)$. This is probably the best smoothness one can achieve in general.

Next we consider a small perturbation of a nondegenerate integrable Hamiltonian, that is a real-analytic Hamiltonian of the form

$$H(q, p) = h(p) + f(q, p), \quad |f| \leq \varepsilon$$

where $|f|$ is the sup norm on a proper complex domain. Introducing frequencies as independent parameters as in [5], one can write H as in Theorem A with

$$P = P_f + P_h, \quad |P_f| \leq \varepsilon, \quad |P_h| \leq Mr^2$$

where M is a bound on the Hessian of h. At that point, the best choice for r seems to be $r \simeq \sqrt{\varepsilon}$ so that the size of P is of order ε and Theorem A can be applied; yet with such a choice it is obvious that because of the estimates for φ in (1-2), the distance between the perturbed and unperturbed torus will be of order $\varepsilon/r \simeq \sqrt{\varepsilon}$. Such an argument, used in [5], do not take into account the fact that the term P_h is actually integrable and at least quadratic in I (that is, $P_h(0, \omega) = 0$ and $\nabla_I P_h(0, \omega) = 0$): this is an important point, as the size of P_h will effectively enter into the conditions (1-1) but not in the estimates (1-2), simply because P_h do not get involved in the approximation procedure nor contribute to the linearized equations one need to solve at each step of the iteration. Then, taking into account the estimate for P_h (which itself is a consequence of the fact that it is at least quadratic in I), the requirement

$$|P| \lesssim \alpha r s^{\nu}$$

is then obviously implied by the conditions

$$|P_f| \lesssim \alpha r s^{\nu}, \quad r \lesssim \alpha s^{\nu}$$

and thus we can state the following theorem (with a change of notations).

Theorem B. *Let $H = N + P + Q$. Suppose P, Q are real-analytic on $D_{r,s} \times O_h$, Q is integrable and at least quadratic in I with $|Q|_{r,h} \le Mr^2$ and*

$$|P|_{r,s,h} \le \gamma\alpha r s^{\nu}, \quad r \le \delta M^{-1}\alpha s^{\nu}, \quad \alpha s^{\nu} \le h \tag{1-3}$$

where $\nu = \tau + 1$, γ and δ are small constants depending only on n and τ. Then there exist a Lipschitz map $\varphi : \Omega_\alpha \to \Omega$ and a Lipschitz family of real-analytic Lagrangian embedding $\Phi : \mathbb{T}^n \times \Omega_\alpha \to \mathbb{R}^n \times \mathbb{T}^n$ that defines, for each $\omega \in \Omega_\alpha$, a Lagrangian torus invariant by the Hamiltonian flow of $H_{\varphi(\omega)}$ and quasiperiodic of frequency ω. Moreover, the estimates (1-2) *holds true.*

We may now choose r as large as possible, namely $r \simeq \alpha s^{\nu}$, and obtain as a consequence that the distance between perturbed and unperturbed torus is of order $\varepsilon(\alpha s^{\nu})^{-1}$. As we already said, this fact was proved in [9]; alternatively, a slight modification in the proof in [2] yields the same result.

2. Sketch of proof

In this section, we will sketch the proof of Theorems A and B; actually, we will simply indicate the modifications with respect to [5] and we will use the same convention for implicit constants depending only on n and τ.

Proposition 2.1. *Let $H = N + P$, and suppose that $|P|_{s,r,h} \le \varepsilon$ with*

$$\begin{cases} \varepsilon \cdot\!< \alpha\eta^2 r\sigma^{\nu}, \\ \varepsilon \cdot\!< hr, \\ h \le \alpha(2K^{\nu})^{-1}, \quad K =\cdot\, \sigma^{-1}\log(n\eta^{-2}) \end{cases} \tag{2-1}$$

where $0 < \eta < \frac{1}{8}$ and $0 < \sigma < \frac{s}{5}$. Then there exists a real-analytic transformation

$$\mathcal{F} = (\Phi, \varphi) : D_{\eta r, s-5\sigma} \times O_{h/4} \to D_{r,s} \times O_h$$

such that $H \circ \mathcal{F} = N_+ + P^+$ with

$$|P_+| \le 9\eta^2\varepsilon \tag{2-2}$$

and

$$\begin{cases} |W(\Phi - \mathrm{Id})|, \quad |W(D\Phi - \mathrm{Id})W^{-1}| \cdot\!< (\alpha r\sigma^{\nu})^{-1}\varepsilon, \\ |\phi - \mathrm{Id}|, \qquad h|D\varphi - \mathrm{Id}|_L \cdot\!< r^{-1}\varepsilon, \end{cases} \tag{2-3}$$

uniformly on $D_{\eta r, s-5\sigma} \times O_h$ and $O_{h/4}$, with $W = \mathrm{Diag}(r^{-1}\,\mathrm{Id}, \sigma^{-1}\,\mathrm{Id})$.

The above proposition is a variant of the KAM step of [5], which we already used in [1]. The only difference is that in [5], instead of (2-1) the following conditions are imposed

$$\begin{cases} \varepsilon \cdot\!< \alpha\eta r\sigma^{\nu}, \\ \varepsilon \cdot\!< hr, \\ h \le \alpha(2K^{\nu})^{-1}, \end{cases} \tag{2-4}$$

with a free parameter $K \in \mathbb{N}^*$, leading to the following estimate

$$|P_+| \lessdot (\varepsilon(r\sigma^\nu)^{-1} + \eta^2 + K^n e^{-K\sigma})\varepsilon. \tag{2-5}$$

instead of (2-2). The last two terms in the estimate (2-5) comes from the approximation of P by a Hamiltonian R which is affine in I and a trigonometric polynomial in θ of degree K; to obtain such an approximation, in [5] the author simply truncates the Taylor expansion in I and the Fourier expansion in θ to obtain the following approximation error

$$|P - R|_{s-\sigma,2\eta r,h} \lessdot (\eta^2 + K^n e^{-K\sigma}).$$

Yet we can use a more refined approximation result, which allows to get rid of the factor K^n in the above estimate. More precisely, we use Theorem 7.2 of [7] (choosing, in the latter reference, $\beta_1 = \cdots = \beta_n = \frac{1}{2}$ and $\delta^{1/2} = 2\eta$ for $\delta \leq \frac{1}{4}$); with the choice of K as in (2-1),[3] this gives another approximation $\tilde{R}$ (which is nothing but a weighted truncation, both in the Taylor and Fourier series, which is affine in I and of degree bounded by K in θ) and a simpler error

$$|P - \tilde{R}|_{s-\sigma,2\eta r,h} \leq 8\eta^2.$$

As for the first term in the estimate (2-5), it can be easily bounded by $\eta^2\varepsilon$ in view of the first part of (2-1) which is stronger than the first part of (2-4) required in [5].

Now, at variance with [5], we will use Proposition 2.1 in an iterative scheme with a linear speed of convergence as η will be chosen to be a small but fixed constant: for convenience, let us set

$$\eta = 10^{-1}4^{-\nu}, \quad \kappa = 9\eta^2.$$

Next, we define for $i \in \mathbb{N}$,

$$\sigma_0 = s/20, \quad \sigma_i = 2^{-i}\sigma_0, \quad s_0 = s, \quad s_{i+1} = s_i - 5\sigma_i$$

so that s_i converges to $s/2$. Then, for $K_i =\cdot\, \sigma_i^{-1}\log(n\eta^2) =\cdot\, \sigma_i^{-1}$, we set

$$h_i = \alpha(2K_i^\nu)^{-1} = 2^{-i\nu}h_0, \quad h_i \cdot\!= \alpha\sigma_i^\nu$$

and the condition $\alpha s^\nu \leq h$ implies in particular than $h_0 \leq h$. Finally, we put

$$\varepsilon_i = \kappa^i\varepsilon, \quad r_i = \eta^i r$$

and we verify that Proposition 2.1 can be applied infinitely many times: the third condition of (2-1) holds true by definition, whereas the first two conditions

[3] There is a constant depending only on n that we left implicit in the definition of K, which depends on the precise choice of norms for real and integer vectors, see [8] for instance.

of (2-1) amount to $\varepsilon_i \cdot\!< \alpha r_i \sigma_i^\nu$ which, in view of our choice of η, holds true for all $i \in \mathbb{N}$ provided it holds true for $i = 0$; for $i = 0$ the condition is satisfied in view of the threshold $\varepsilon \le \gamma \alpha r s^\nu$. Once we can iterate Proposition 2.1 infinitely many times, the convergence proof and the final estimates follow exactly as in [5], since the sequences $\varepsilon_i (h_i r_i)^{-1}$and $\varepsilon_i (h_i^2 r_i)^{-1}$ decrease geometrically, again by our choice of η. This concludes the sketch of proof.

To prove Theorem B, one needs the following variant of Proposition 2.1.

Proposition 2.2. *Let $H = N + P + Q$, suppose that $|P|_{s,r,h} \le \varepsilon$, $|Q|_{r,h} \le Mr^2$ with Q integrable and at least quadratic in I and*

$$\begin{cases} \varepsilon \cdot\!< \alpha \eta^2 r \sigma^\nu, \\ r \cdot\!< M^{-1} \alpha \eta^2 \sigma^\nu, \\ \varepsilon \cdot\!< hr, \\ h \le \alpha (2K^\nu)^{-1}, \qquad K = n\sigma^{-1} \log(\eta^{-2}), \end{cases} \tag{2-6}$$

where $0 < \eta < \frac{1}{4}$ and $0 < \sigma < \frac{s}{5}$. Then there exists a real-analytic transformation

$$\mathcal{F} = (\Phi, \varphi) : D_{\eta r, s-5\sigma} \times O_{h/4} \to D_{r,s} \times O_h$$

such that $H \circ \mathcal{F} = N_+ + P_+ + Q$ with the estimates (2-2) *and* (2-3).

Let $\tilde{R}$ be the approximation of P; if $\{\cdot\,,\cdot\}$ denotes the Poisson bracket and $[\,\cdot\,]$ averaging over the angles, we solve the equation

$$\{F, N\} = \tilde{R} + Q - [\tilde{R} + Q]$$

which, since Q is integrable, is exactly the equation

$$\{F, N\} = \tilde{R} - [\tilde{R}]$$

that is solved in [5] (with, of course, R instead of $\tilde{R}$ as we explained above). This justifies that the transformation in Proposition 2.2 is the same as in Proposition 2.1, and in particular it satisfy the estimates (2-2). The only difference is that the new Hamiltonian writes

$$H \circ \mathcal{F} = N_+ + P_+ + Q, \qquad N_+ = N + [\tilde{R}]$$

with

$$P_+ = \int_0^1 \{(1-t)[\tilde{R}] + t\tilde{R} + Q, F\} \circ X_F^t dt + (P - \tilde{R}) \circ X_F^1.$$

As compared to [5], there is an extra term in P_+ coming from Q, whose contribution is easily bounded by the simple Poisson bracket

$$|\{Q, F\}| \lessdot Mr(\alpha\sigma^\nu)^{-1}\varepsilon$$

and, in view of the extra condition we imposed in (2-6), one can easily arrange the estimate (2-3). This justifies Proposition 2.2, and the iteration leading to Theorem B is exactly the same as the one leading to Theorem A.

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bounemoura@ceremade.dauphine.fr

Université Paris Dauphine, CEREMADE, Paris, France

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Some recent developments in Arnold diffusion

CHONG-QING CHENG AND JINXIN XUE

This survey paper grows out of the lecture notes of the nine-hour lectures that the authors delivered in the special semester on Hamiltonian dynamics at MSRI in the fall of 2018. It can be considered as an introduction to our work on Arnold diffusion.

1. Introduction

In the Hamiltonian formalism of the classical mechanics, a smooth Hamiltonian function H on a symplectic manifold (M, ω) is given, and defines a vector field X through $\omega(\cdot, X) = dH$. The main problem is to study the dynamics, which is the long time behavior, of the solution of the differential equation $x' = X(x)$, $x \in M$, determined by the vector field X. The dynamics of a Hamiltonian system in general can be very complicated and deny analytical approaches. From dynamical perspectives, the most well-understood class of Hamiltonian systems is integrable systems. The classical Liouville–Arnold theorem states as follows.

Theorem 1.1 (Liouville–Arnold). *Let $H_1 = H : M^{2n} \to \mathbb{R}$ be a Hamiltonian and suppose there are $H_2, \dots, H_n : M \to \mathbb{R}$ satisfying*:

(a) $\{H_i, H_j\} \equiv 0$, *for all $i, j = 1, \dots, n$.*

(b) *The level set $M_{\mathbf{a}} := \{(q, p) \in M \mid H_i(q, p) = a_i, i = 1, \dots, n\}$ is compact.*

(c) *At each point of $M_{\mathbf{a}}$, the n vectors DH_i, $i = 1, \dots, n$ are linearly independent.*

Then:

(1) *$M_{\mathbf{a}}$ is diffeomorphic to $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$ and is invariant under the Hamiltonian flow of each H_i.*

(2) *$M_{\mathbf{a}}$ is a Lagrangian submanifold, i.e., for any $u, v \in T_x M_{\mathbf{a}}$, $\forall x \in M_{\mathbf{a}}$, we have $\omega(u, v) = 0$.*

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(3) *In a neighborhood U of $M_{\mathbf{a}}$, there is a symplectic transform $\Phi(q, p) = (\theta, I)$ such that*

$$\Phi(U) = \mathbb{T}^n \times (-\delta, \delta)^n$$

for some $\delta > 0$.

(4) *In the new coordinates, each $K_i := H_i \circ \Phi^{-1}$ is a function of I only so the Hamiltonian equation is*

$$\dot{\theta} = \omega_i(I) := \frac{\partial K_i}{\partial I}, \quad \dot{I} = 0.$$

Integrable systems are also important in algebraic geometry, representation theory, etc; see Hitchin [27]. For the purpose of studying dynamics of Hamiltonian systems, the Liouville–Arnold theorem gives a good description of the dynamics of integrable systems. Each regular level set $M_{\mathbf{a}}$ is an invariant torus under the Hamiltonian flow and the dynamics on it is linear flow. However, integrable systems are very rare. In nature, a system always undergoes some internal or external perturbations. Therefore the next interesting and natural class of Hamiltonian systems is nearly integrable systems which are small perturbations of integrable systems. This class of systems models many interesting natural phenomena including in particular the Newtonian N-body problem. It turns out that this class of systems has rich dynamics and also approachable to a large extent by analytic tools. From the Liouville–Arnold theorem, we see that the natural phase space for studying nearly integrable systems is the symplectic manifold $T^*\mathbb{T}^n$ or its subsets endowed with the standard symplectic structure. We will call a system of the following form a nearly integrable system

$$H(x, y) = h(y) + \varepsilon P(x, y), \quad (x, y) \in \mathbb{T}^n \times \mathbb{R}^n = T^*\mathbb{T}^n \tag{1-1}$$

which gives rise to the Hamiltonian equation

$$\begin{cases} \dot{x} = \partial_y h(y) + \varepsilon \partial_y P(x, y), \\ \dot{y} = -\varepsilon \partial_x P(x, y). \end{cases} \tag{1-2}$$

The natural regularity assumption on H is C^r, $r \geq 2$ including ∞ and ω (meaning analytic).

The celebrated Kolmogorov–Arnold–Moser theorem says that under certain isoenergetic nondegeneracy condition, when ε is sufficiently small, most volume of the phase space is occupied by invariant Lagrangian tori, each of which carries irrational flow with Diophantine frequency. Systems with $n = 1$ are integrable, so are well understood by Liouville–Arnold theorem. For systems with $n = 2$, the KAM theorem gives lots of disjoint two-dimensional tori separating the three dimensional level set, so each orbit is either on a invariant torus or trapped between two nearby tori. We may use the oscillation of the action variable y

along an orbit as a measurement of the instability of the system. In both the cases $n = 1$ and $n = 2$, we see that the oscillation of y along each orbit is small ($o(1)$ as $\varepsilon \to 0$) so we think the systems as being stable. However, the cases of $n \geq 3$ is drastically different. The KAM tori are n-dimensional invariant sets of codimension $n - 1 > 1$ on each energy level set, so the complement of the union of the KAM tori is connected (there may be other Lagrangian tori which are not given by the KAM theorem). This leaves room for the possibility of having orbits wandering in the complements of these tori. Moreover, Arnold constructed an example in which one action variable can indeed oscillate as far as possible. Thus Arnold proposed the following conjecture.

Conjecture [2; 4]. *For any two points y' and y'' on the connected level hypersurface of h in the action space there exist orbits of* (1-2) *connecting an arbitrary small neighborhood of the torus $y = y'$ with an arbitrary small neighborhood of the torus $y = y''$, provided that $\varepsilon \neq 0$ is sufficiently small and P is generic.*

The statement can be found in [2; 4], as well as in the book [5] in Problems 1963-1, 1966-3, 1994-33 etc. We make the following remarks concerning the statement of the conjecture.

Remark 1.2. (1) In some circumstances the statement of Arnold talks about only "general" or "typical" systems without specifying the regularity of the Hamiltonian; see [2]. In [4], Arnold considered generic analytic Hamiltonians. The KAM theory applies to both analytic Hamiltonians and smooth (C^r, r large or ∞) Hamiltonians. However, when talking about genericity in differential topology and Riemannian geometry, the C^∞ category is the one used since it allows to construct bump functions and partition of unity. So for this conjecture, the analytic category and the smooth category are essentially different.

(2) The genericity as in this conjecture is not the usual Baire second category, since the smallness parameter ε may depend on the perturbation P. We will introduce a cusp-residual genericity similar to Mather [35].

(3) In [4] Arnold also talked about generic unperturbed part h. In particular, he mentioned Lorentzian type mechanical systems as the first step to study the conjecture for nonconvex h. Our variational method applies only to the convex case i.e., D^2h is positive definite, which includes already lots of physical models, since mechanical systems (kinetic energy plus potential energy) have positive definite kinetic energy part.

The conjecture is in essence asking for an understanding of the global dynamics in the complement of the KAM tori, where the dynamics is expected to be very chaotic but is very resistant to analysis. A related problem called standard map conjecture states that the system

$$(x, y) \mapsto (x + y + k \sin x,\, y + k \sin x)$$

has positive Lyapunov exponent for a positive Lebesgue measure set for all or some parameter $k \in \mathbb{R}$. The conjecture expect that the complement of the KAM curves are nonuniformly hyperbolic in the sense of Pesin theory. Having an orbit with wandering action variable is a way to measure the instability. It was foreseen by Arnold [4] that the major difficulty is caused by the double resonance, where the system can be reduced to a nonperturbative mechanical system.

We next state our main result as follows, which is an answer to the above conjecture in the smooth category for convex systems and in the sense of cusp-residual genericity. In the main body of the survey, we will sketch the main ingredients of our proof in a series of papers [16; 9; 8; 10; 11]. Readers are also referred to [14; 15; 6; 18; 19; 37; 7; 35; 28; 24; 32; 37] for other relevant work. Denote by $\mathfrak{S}_1$ the unit sphere in $C^r(T^*\mathbb{T}^n)$ (or $C^r(\mathbb{T}^n)$) with $r \in [7, \infty]$, we have:

Theorem 1.3. *Given any small $\delta > 0$, and finitely many small balls $B_\delta(y_i) \subset \mathbb{R}^n$, where $y_i \in h^{-1}(E)$ with $E > \min h(y)$, there exists a residual set $\mathfrak{C} \subset \mathfrak{S}_1$ such that the following holds for the system* (1-1). *For each $P \in \mathfrak{C}$ there exists an $\varepsilon_P > 0$, such that there is a residual set of ε in $(0, \varepsilon_P)$, the Hamiltonian flow admits orbits visiting the balls $B_\delta(y_i)$ in any prescribed order.*

The paper is organized as follows. In the main body of the paper, we explain Arnold diffusion in *a priori* unstable systems and the proof of Theorem 1.3 in the case of $n = 3$. We postpone the general $n > 3$ case to Appendix C due to its technicality. Though a bit technical, Appendix C may still serve as a road-map of our paper [11] for readers who want to understand the detailed proof. In Section 2, we explain Arnold's example. In Section 3, we explain the variational method using the pendulum and Arnold's example. We also provide our mechanism of changing cohomology classes. In Section 4, we explain the main difficulties in the proof of Arnold diffusion for *a priori* unstable systems and how to overcome them. In Section 5, we derive the resonant normal form. Section 6 is the important section, which is about mechanical systems with two degrees of freedom. In Section 7, we explain how to construct diffusing orbit in systems with three degrees of freedom, in particular how to overcome the main difficulty of the strong double resonance. In Section 8, we briefly discuss the issue of genericity. Finally, we have three appendices. In Appendix A, we provide the basic concepts in Mather theory and in Appendix B, we provide the theorem of normally hyperbolic invariant manifolds. In Appendix C, we explain how to construct diffusing orbit in systems of arbitrary degrees of freedom.

2. Arnold's example

2A. ***The pendulum.*** The mathematical pendulum is prominent in the study of Arnold diffusion. The Hamiltonian is

$$H_0(x, y) = \tfrac{1}{2}y^2 + (\cos 2\pi x - 1), \quad (x, y) \in T^*\mathbb{T}.$$

First, as a system of one degree of freedom, the Liouville–Arnold theorem can be applied to the regular values of H. Thus the phase space dynamics is further determined by the critical values of H.

Near the fixed points $O = (0, 0)$, the Hamiltonian can be linearized as $y^2/2 - (2\pi x)^2/2$. The linearized Hamiltonian equation is

$$\begin{cases} \dot{x} = y, \\ \dot{y} = 4\pi^2 x, \end{cases}$$

so the fixed point is hyperbolic. Let O be the hyperbolic fixed point and ϕ^t, $t \in \mathbb{R}$, be the flow generated by the Hamiltonian vector field, we define the stable (W^s) and unstable (W^u) manifolds of the fixed point O as

$$W^s(O) = \{z \in T^*\mathbb{T} \mid \phi^t(z) \to O, \ \text{as } t \to +\infty\},$$
$$W^u(O) = \{z \in T^*\mathbb{T} \mid \phi^t(z) \to O, \ \text{as } t \to -\infty\}.$$

For the pendulum, we see that $W^s(O)$ coincides with $W^u(O)$ consisting of two entire homoclinic orbits denoted by $\{(x_0(t), \pm y_0(t)), t \in \mathbb{R}\}$ with $(x_0(t), \pm y_0(t)) \to (0, 0)$ as $t \to \pm\infty$.

It was discovered by Poincaré that the stable and unstable manifold will split (i.e., will not coincide) if a generic time-periodic perturbation is added. Let us consider the perturbed Hamiltonian

$$H_\varepsilon(x, y, t) = \tfrac{1}{2}y^2 + (\cos 2\pi x - 1) + \varepsilon H_1(x, y, t), \quad (x, y) \in T^*\mathbb{T},$$

where $H_1(x, y, t) = H_1(x, y, t + 1)$ and $\partial_x H_1(0, 0, t) = \partial_y H_1(0, 0, t) = 0$ for all $(x, y, t) \in T^*\mathbb{T} \times \mathbb{T}$. The latter assumption on H_1 implies that O remains a fixed point for the perturbed system H_ε. In this case, the Hamiltonian equation is time-dependent, so its solution is not an $\mathbb{R}$-action on $T^*\mathbb{T}$. Instead, we consider the time-1 map denoted by ϕ_ε^1, whose iterations give rise to a $\mathbb{Z}$-action on $T^*\mathbb{T}$, due to the 1-periodic dependence on t of H_1. We redefine the stable and unstable manifolds as

$$W_\varepsilon^s(O) = \{z \in T^*\mathbb{T} \mid \phi_\varepsilon^n(z) \to O, \ \text{as } n \to +\infty\},$$
$$W_\varepsilon^u(O) = \{z \in T^*\mathbb{T} \mid \phi_\varepsilon^n(z) \to O, \ \text{as } n \to -\infty\}.$$

The splitting of $W_\varepsilon^s(O)$ and $W_\varepsilon^u(O)$ is one of the main mechanisms responsible for the nonintegrability of the perturbed system. The general method of measuring the separatrix splitting to the first order is the Melnikov function

$$\begin{aligned}\mathcal{M}(\alpha) &= \int_{\mathbb{R}} \{H_0, H_1\}(x_0(t), y_0(t), t+\alpha)\, dt,\\ \{H_0, H_1\} &= \partial_x H_0 \cdot \partial_y H_1 - \partial_y H_0 \cdot \partial_x H_1.\end{aligned} \tag{2-1}$$

2B. ***Arnold's example.*** Arnold in [1] constructed the following example for which he first discovered the phenomena called now Arnold diffusion

$$\begin{aligned}&H(\theta, I, x, y, t)\\ &\quad = \frac{I^2}{2} + \frac{y^2}{2} + \varepsilon(\cos(2\pi x) - 1)(1 + \mu(\cos(2\pi\theta) + \sin(2\pi t))),\end{aligned} \tag{2-2}$$

where $(\theta, I; x, y; t) \in T^*\mathbb{T}^1 \times T^*\mathbb{T}^1 \times \mathbb{T}$. It is proved in [1] that

Theorem 2.1 (Arnold). *In the system* (2-2), *for any given* $A < B$, $\varepsilon > 0$, *there is an orbit* $\{(\theta(t), I(t), x(t), y(t))\}$ *of the system and time* $t_1 < t_2$ *with* $I(t_1) \le A$ *and* $I(t_2) \ge B$, *provided* $\mu > 0$ *is small enough.*

We first consider the case of $\mu = 0$. The resulting system has two degrees of freedom. Away from the set $\{y^2/2 + \varepsilon(\cos(2\pi x) - 1) = 0\}$, the system is integrable in the Liouville–Arnold sense.

The product of the hyperbolic fixed point $O = (0, 0)$ of the system H_0 and the phase space of the subsystem $\tilde{H} = I^2/2$ gives rise to the following cylinder in the product space $T^*\mathbb{T}^2$

$$\mathcal{C} = \{(\theta, I, x, y) = (\theta, I, 0, 0), I \in \mathbb{R}, \theta \in \mathbb{T}^1\}.$$

Each circle $\mathcal{C}(I) := \{I = \text{const}, \theta \in \mathbb{T}, x = 0, y = 0\}$ in the cylinder is invariant under the Hamiltonian flow of H_0. When restricted to $\mathcal{C}$, the resulting Hamiltonian system is given by the integrable Hamiltonian $\tilde{H} = I^2/2$. The frequency ω along $\mathcal{C}$ has the form $(I, 0)$ (item (4) of Theorem 1.1), so the cylinder on which the Liouville–Arnold theorem does not apply has resonant frequency, i.e., for all integer vector $k \in \mathbb{Z}^2$ of the form $(0, *)$, we have $\omega \cdot k = 0$. Each circle $\mathcal{C}(I)$ also has stable and unstable manifolds denoted by $W_I^{u,s}$.

When the time-dependent perturbation is turned on, using the Melnikov function (2-1) in the previous subsection, it can be verified that the stable W_I^s and unstable manifolds W_I^u of $\mathcal{C}(I)$ intersect transversely for all I. Therefore the transversality implies that W_I^u intersects $W_{I'}^s$ transversely if I and I' is sufficiently close. Then orbits can be found to shadow a sequence of $W^{u/s}$ chain to have large oscillation of I. We refer readers to [25] for a shadowing lemma developed recently. It is important to point out that the particularly chosen perturbation in Arnold's example gives a vanishing perturbation to the Hamiltonian vector field on the cylinder $\mathcal{C}$, so that the dynamics on $\mathcal{C}$ remains unperturbed. It is not the case for a generic perturbation, which constitutes the main difficulty for *a priori* unstable systems.

3. The variational method

In this section, we briefly introduce the variational method after Mather [33; 34] and Mañé [31]. Formal definitions of the objects in this theory are summarized in the appendix. Here we only illustrate some of the key points using mainly the pendulum.

3A. ***Variational methods in terms of rotator and pendulum.*** Let $L : T\mathbb{T}^n \to \mathbb{R}$ be a Tonelli Lagrangian system. Let η be a closed 1-form with cohomology class $[\eta] = c \in H^1(\mathbb{T}^n, \mathbb{R})$. We take infimum among all the invariant probability measures μ supported on $T\mathbb{T}^n$

$$-\alpha(c) := \inf_{\mu} \int L(x, \dot{x}) - \eta \, d\mu.$$

We define Mather set as $\widetilde{\mathcal{M}}(c) := \cup \operatorname{supp} \mu$ where the union is taken over all the measures attaining the above infimum.

Let us first give an illuminating example. In the pendulum the hyperbolic fixed point $O = (0, 0)$ the Hamiltonian is linearized as $H_0 = \frac{1}{2}y^2 - (2\pi)^2 x^2$, so after Legendre transform, the corresponding Lagrangian is $L_0 = \frac{1}{2}\dot{x}^2 + (1/(2\pi)^2)x^2$. The probability measure minimizing the action $\inf_\mu \int L_0 \, d\mu$ is easily seen to be the Dirac-δ supported at O. So we see the link

Minimal measure (Dirac-δ)

$\leftrightarrow$ *Nondegenerate global maximum of the Hamiltonian*

$\to$ *Hyperbolic fixed point.*

This is a guiding principle for us to locate the Mather set with hyperbolicity for nearly integrable systems.

In the example of the mathematical pendulum, the Mather set $\tilde{\mathcal{M}}(c)$ is supported on the hyperbolic fixed point when $c = 0$ and there are orbits homoclinic to the hyperbolic fixed point. In variational methods, we introduce the Aubry set and Mañé set to capture the homoclinic orbits and heteroclinic orbits. The Aubry set $\tilde{\mathcal{A}}(c)$ is the lift to $T^*\mathbb{T}^n$ of the following projected Aubry set

$$\mathcal{A}(c) = \{x \in \mathbb{T}^n \mid h_c(x, x) = 0\},$$

where

$$h_c(x, y) := \liminf_{t \to \infty} \inf_{\gamma} \int_0^t L(\gamma(s), \dot{\gamma}(s)) - \eta + \alpha(c) \, ds$$

and $\gamma : [0, t] \to \mathbb{T}^n$ is a C^1 curve with $\gamma(0) = x$ and $\gamma(t) = y$, $x, y \in \mathbb{T}^n$. On $\mathcal{A}(c)$, we can introduce an equivalence relation: $x \sim y$ if $h_c(x, y) = 0$. Then we get the quotient $\bar{\mathcal{A}}(c)$ called the Aubry class.

Denoting by $\phi^t : T\mathbb{T}^n \to T\mathbb{T}^n$, $t \in \mathbb{R}$, the Lagrangian flow, we can again define the stable and unstable sets analogous to that in hyperbolic dynamics so we can introduce

$$W_c^u = \{z \in T\mathbb{T}^n \mid \phi^t z \to \tilde{\mathcal{A}}(c), t \to -\infty\},$$
$$W_c^s = \{z \in T\mathbb{T}^n \mid \phi^t z \to \tilde{\mathcal{A}}(c),\ t \to +\infty\}.$$

Here we use the notations $W_c^{u,s}$, though the Aubry set $\tilde{\mathcal{A}}(c)$ may not be hyperbolic.

In case when the Aubry class consists of a single point, these sets are defined as graphs of the gradients of the backward/forward weak KAM solutions u_c^- and $u_c^+ : \mathbb{T}^n \to \mathbb{R}$ respectively, which are known to be unique up to an additive constant. We call the difference $B_c(x) = u_c^-(x) - u_c^+(x)$ the barrier function, whose critical points correspond to the intersection of W_c^u and W_c^s. If $z = (x, y) \in W_c^u \cap W_c^s$ and x is a global minimal point of B_c, then by definition $\phi^t(z)$ approaches $\widetilde{\mathcal{M}}(c)$ in both the future and the past, such an orbit is a prototypical orbit in the Mañé set $\tilde{\mathcal{N}}(c)$. The barrier function is in general only known to be Lipschitz, however, it has the remarkable property of being differentiable at its global minimal points. We refer readers to the appendix for formal definitions of the Mather set $\widetilde{\mathcal{M}}(c)$, Aubry set $\tilde{\mathcal{A}}(c)$, Mañé set $\tilde{\mathcal{N}}(c)$ and weak KAM solutions $u_c^{\pm}$ and their basic properties. We also refer readers to [13] for how to realize these objects in the pendulum.

We next explain the effect of changing cohomology class. In Liouville–Arnold theorem, the action variable I is constructed by integrating the Liouville 1-form pdq along a basis of the first homology group $H_1(M_{\mathbf{a}}, \mathbb{Z})$. In variational methods, the changing of the cohomological class has the effect of selecting the corresponding action variable for integrable systems hence selecting the Lagrangian torus. Let $H(I) : T^*\mathbb{T}^n \to \mathbb{R}$ be a convex integrable Hamiltonian independent of the angular variable $\theta \in \mathbb{T}^n$. The corresponding Lagrangian is denoted by $L(\dot{\theta})$. We next show how to find the minimizer of the variational problem $\inf_\mu \int L(\dot{\theta}) - \eta\, d\mu$ with $[\eta] = c \in H^1(\mathbb{T}^n, \mathbb{Z}) \in \mathbb{R}^n$. For simplicity, we take $\eta = cd\theta$, so the minimization problem is solved by Legendre transform as

$$-\alpha(c) := \inf_{\dot{\theta} \in \mathbb{R}^n} L(\dot{\theta}) - c \cdot \dot{\theta} = -H(c).$$

The infimum is attained as the point $\dot{\theta} = \partial_c H(c)$ and $c = \partial_{\dot{\theta}} L(\dot{\theta}) = I$. So we see that for integrable systems the cohomology class c agrees with the action variable I, the Mather set is the corresponding invariant torus $\{\dot{\theta} = \partial_c H(c)\} \times \mathbb{T}^n \subset T\mathbb{T}^n$.

3B. ***Arnold's example in the variational language.*** Recall that in Arnold's example, orbits are found to shadow different circles $\mathcal{C}(I)$s. Each circle can be realized as the Aubry set with cohomology class $c = (I, 0) \in H^1(\mathbb{T}^2, \mathbb{R})$. Thus in variational terms, Arnold diffusing orbit corresponds to orbits shadowing different Aubry sets $\tilde{\mathcal{A}}(c)$s. To find orbit shadowing Aubry sets with different cohomology classes, we have the following variational version of Arnold's mechanism of constructing diffusing orbit using the intersection of the stable and unstable manifolds.

Theorem 3.1 (Type-h orbit). *Let $\Gamma : [0, 1] \to H^1(M, \mathbb{R})$ be a continuous curve. Suppose there exist a certain finite covering $\check{\pi} : \check{M} \to M$, two open domains $N_1, N_2 \subset \check{M}$ with $d(N_1, N_2) > 0$, and for each $s \in [0, 1]$, there exist a codimenion one disk D_s and small numbers $\delta_s, \delta'_s > 0$ such that*:

1. *The projected Aubry sets satisfy $\mathcal{A}(\Gamma(s)) \cap N_1 \neq \varnothing$, $\mathcal{A}(\Gamma(s)) \cap N_2 \neq \varnothing$ and $\mathcal{A}(\Gamma(s')) \cap (N_1 \cup N_2) \neq \varnothing$ for each $|s' - s| < \delta_s$.*
2. *$\check{\pi}\mathcal{N}(\Gamma(s), \check{M})|_{D_s} \backslash (\mathcal{A}(\Gamma(s)) + \delta'_s)$ is nonempty and totally disconnected, where the $+\delta'_s$ notation means a δ'_s neighborhood.*

Then there exists an orbit $d\gamma \subset T^*M$ such that $\boldsymbol{\alpha}(\gamma) \subset \tilde{\mathcal{A}}(\Gamma(0))$ and $\boldsymbol{\omega}(\gamma) \subset \tilde{\mathcal{A}}(\Gamma(1))$.

We call orbits in the theorem type-h, standing for *heteroclinic*. Bernard [6] introduced a similar variational mechanism called forcing relations. The way the theorem applies to Arnold's example is as follows. We treat the x-variable in (2-2) as being defined on $\mathbb{R}/(2(2\pi\mathbb{Z}))$, in other words, we lift the pendulum component to the double covering space of $T^*\mathbb{T}$. Thus, the Aubry set for each cohomology class $c = (I, 0)$ has two copies and the second assumption is satisfied due to the transversal intersection of the stable manifold of one component of the Aubry set and the unstable manifold of the other component, for each cohomology class $(I, 0)$, hence the theorem applies to Arnold's example. This advantage of the lifting procedure here is that it produces orbits in the Mañé set but not in the Aubry set. The last point is subtle, and we refer readers to [13] for the description of Mañé set and Aubry set in the pendulum example.

Summarizing the above, we have the following dictionary:

hyperbolic objects	variational objects
hyperbolic set	Aubry set
stable/unstable manifold	graph of differential of weak KAM
intersection of stable/unstable manifolds	critical point of the barrier function
homo- or hetero-clinic orbits	Mañé set\Mather set
Arnold's orbit shadowing different $\mathcal{C}(I)$s	type-h orbit

The main advantage of the variational methods is that the existence of the variational objects such as Mather sets, Aubry sets and Mañé sets are always assured. Without requiring good regularities of the variational objects, diffusing orbits can still be constructed.

This dictionary goes far beyond Arnold's example and *a priori* unstable systems. In the next subsection, we will introduce a new way of changing cohomology classes, which will be used crucially in the proof of Arnold diffusion in *a priori* stable systems, in addition to Arnold's mechanism.

3C. *Type-c orbit.* In this section, we introduce the second way of finding orbits shadowing Aubry sets with different cohomology classes, which we call type-c, standing for *cohomology equivalence*. The basic idea is that the cohomology class can be changed in the orthogonal complement of the homology of a section of the Mañé set. This mechanism first appeared in [34] proved in [14] for nonautonomous systems. The version for autonomous systems that we are going to give here was first established in [29; 30]; see Section 3.1 of [8].

We suppose that there exists Σ_c nondegenerately embedded $(n-1)$-dimensional torus on $\mathbb{T}^n$ given by an embedding $\varphi\colon \mathbb{T}^{n-1} \to \mathbb{T}^n$ with $\Sigma_c = \varphi(\mathbb{T}^{n-1})$ the image of φ, and the induced map $\varphi_*\colon H_1(\mathbb{T}^{n-1}, \mathbb{Z}) \hookrightarrow H_1(\mathbb{T}^n, \mathbb{Z})$ is an injection. We can simply choose Σ_c in the nonautonomous setting to be the configuration space with $\{t = 0\}$.

Let $\mathfrak{C} \subset H^1(\mathbb{T}^n, \mathbb{R})$ be a connected set. For each class $c \in \mathfrak{C}$, we assume that there exists a nondegenerate embedded $(n-1)$-dimensional torus $\Sigma_c \subset \mathbb{T}^n$ such that each c-semistatic curve γ transversally intersects Σ_c. Let

$$\mathbb{V}_c = \bigcap_U \{i_{U*} H_1(U, \mathbb{R}) : U \text{ is a neighborhood of } \mathcal{N}(c) \cap \Sigma_c \text{ in } \mathbb{T}^n\},$$

here $i_U\colon U \to M$ denotes inclusion map. Denote by $\mathbb{V}_c^\perp$ the annihilator of $\mathbb{V}_c$, i.e., if $c' \in H^1(\mathbb{T}^n, \mathbb{R})$, then $c' \in \mathbb{V}_c^\perp$ if and only if $\langle c', h\rangle = 0$ for all $h \in \mathbb{V}_c$. Clearly,

$$\mathbb{V}_c^\perp = \bigcup_U \{\ker i_U^* : U \text{ is a neighborhood of } \mathcal{N}(c) \cap \Sigma_c \text{ in } \mathbb{T}^n\}.$$

Note that there exists a neighborhood U of $\mathcal{N}(c) \cap \Sigma_c$ such that $\mathbb{V}_c = i_{U*} H_1(U, \mathbb{R})$ and $\mathbb{V}_c^\perp = \ker i_U^*$.

Definition 3.2 (c-equivalence). We say that $c, c' \in H^1(M, \mathbb{R})$ are *c-equivalent* if there exists a continuous curve $\Gamma\colon [0, 1] \to \mathfrak{C}$ such that $\Gamma(0) = c$, $\Gamma(1) = c'$, $\alpha(\Gamma(s))$ keeps constant for all $s \in [0, 1]$, and for each $s_0 \in [0, 1]$ there exists $\epsilon > 0$ such that $\Gamma(s) - \Gamma(s_0) \in \mathbb{V}_{\Gamma(s_0)}^\perp$ whenever $s \in [0, 1]$ and $|s - s_0| < \epsilon$.

Theorem 3.3 (Type-c orbit). *Suppose that two cohomology classes c and c' are c-equivalent, then there exists an orbit whose $\boldsymbol{\alpha}$-limit set is in $\tilde{\mathcal{A}}(c)$ and $\boldsymbol{\omega}$-limit set is $\tilde{\mathcal{A}}(c')$, and vice versa.*

Proof. We only prove the case when $|c-c'|$ is sufficiently small. The details of changing c in the large scale (global connecting orbits) can be found in Section 5 of [14]. We first denote by U^c a small neighborhood of $\mathcal{N}(c) \cap \Sigma_c$. We next modify the Lagrangian $L_c := L(\gamma, \dot\gamma) - \langle c, \dot\gamma\rangle$ to $L_{c+\eta\rho} := L(\gamma, \dot\gamma) - \langle c + \eta\rho(t), \dot\gamma\rangle$ where η is a de Rham closed one-form with cohomology class $[\eta] = c' - c$ whose support lies in U^c and $\rho(t) \in C^\infty$ satisfies $\rho(t) = 0$ for $t \le 0$ and $\rho(t) = 1$ for $t \ge \varepsilon$ for ε small. Such a closed one-form exists following from the definition of the c-equivalence, $c - c' \perp H_1(\mathcal{N}(c)|_\Sigma, \mathbb{R})$. The free time global minimizer (defined as the semistatic curves, see appendix) of the action $\int L_{c+\eta\rho}\, dt$ is taken over all the curves with endpoints in $\widetilde{\mathcal{M}}(c)$ and $\widetilde{\mathcal{M}}(c')$. First it is known that the minimizer stays close to the Mañé set $\tilde{\mathcal{N}}(c)$ if $|c-c'|$ is small enough so it also passes through U. The proof of this fact is the same as that of the upper-semicontinuity of the Mañé set; see Section 2 of [14]. We claims that the minimizer satisfies the Euler–Lagrange equation. As we know, adding a closed 1-form to the Lagrangian does not change the E-L equation. If we keep track of the orbit, before entering U, the Lagrangian is L_c. In U, since $\operatorname{supp}\eta \cap U = \varnothing$, the Lagrangian is still L_c. When the orbit gets outside of U, for ε small enough, the Lagrangian is now actually $L_{c'}$. In all the cases, the E-L equation is the same as that of L so we have constructed an orbit $d\gamma$. Since orbits in $\tilde{\mathcal{N}}(c) \setminus \tilde{\mathcal{M}}(c)$ does not recur, as $t \to \infty$, the orbit $d\gamma$ stays in a region where the cohomology class is $\eta(c')$ hence the $\boldsymbol{\omega}$-limit set is $\tilde{\mathcal{A}}(c')$ and similarly, the $\boldsymbol{\alpha}$-limit set is $\tilde{\mathcal{A}}(c)$. □

4. a priori unstable systems

We now explain the main difficulty of constructing diffusing orbit in the so-called *a priori* unstable system, which are generalizations of Arnold's example but maintaining the structure of normally hyperbolic invariant cylinder (NHIC). We refer readers to the appendix for the definition of normally hyperbolic invariant manifold (NHIM) and a theorem on its persistence under perturbations. A prototypical form of the *a priori* unstable system is

$$H = \frac{I^2}{2} + \frac{y^2}{2} + (\cos(2\pi x) - 1) + \varepsilon P(\theta, I, x, y, t), \tag{4-1}$$

where $(\theta, I, x, y, t) \in T^*\mathbb{T}^2 \times \mathbb{T}^1$. This kind of system appears as the single resonance normal form (see Section 5 below), thus the following problem is the first step towards the conjecture of Arnold diffusion.

For C^r-generic P with $2 \le r \le \infty$ and for any $A < B$, the system (4-1) *admits an orbit $\{(\theta(t), I(t), x(t), y(t)), t \in \mathbb{R}\}$ and t_1, t_2 such that $I(t_1) \le A$ and $I(t_2) \ge B$ provided ε is sufficiently small.*

The problem is solved by different authors using different methods. In this section, we briefly explain the main difficulties and the solution of Cheng and Yan [14; 15].

First, note that when $\varepsilon = 0$, the system admits a NHIC given by

$$\mathcal{C} = \{x = y = 0, (\theta, I) \in \mathbb{T} \times \mathbb{R}\}.$$

In order to apply the theorem of NHIM, we first replace the perturbation εP by $\varepsilon \chi P$ where $\chi : T^*\mathbb{T}^2 \to \mathbb{R}$ such that $\chi = 1$ for $|I| < R$ and $|y| < 10$, and $\chi = 0$ for $|I| > R + 1$ and $|y| > 11$ for some large R with $R > \max\{|A|, |B|\}$. Our orbit will stay within the region where $\chi = 1$ so it is also an orbit of the original system. For the perturbed system, we shall consider the time-1 map denoted by $\phi_\varepsilon^1 : T^*\mathbb{T}^2 \to T^*\mathbb{T}^2$. By the theorem of NHIM so we get a NHIC $\mathcal{C}_\varepsilon$ close to $\mathcal{C}$ and is invariant under ϕ_ε^1. Restricted to $\mathcal{C}_\varepsilon$, the map ϕ_ε^1 is a twist map, so we can then apply KAM theorem to get that for ε small enough, there are uncountably many invariant circles on $\mathcal{C}_\varepsilon$ that are homologically nontrivial. In general there are also other homologically nontrivial invariant circles that are not given by the KAM theorem.

Here comes the first main difficulty. The distances between two neighboring circles may be of order $\sqrt{\varepsilon}$. However, the size of separatrix splitting is only of order ε. This means that Arnold's mechanism of utilizing the intersection of stable and unstable manifolds fails to find orbit crossing the $\sqrt{\varepsilon}$-gaps. This is called the "big gap" problem.

The way to overcome this problem is to invoke the cohomology equivalence mechanism in Section 3C. The reason is that for each $c \in H^1(\mathbb{T}^2, \mathbb{R})$ such that $\tilde{\mathcal{N}}(c)$ lies in the gap, the Mañé set is contractible so Definition 3.2 is verified. Now the general strategy is to apply the c-equivalence mechanism whenever there is a big gap and to apply Arnold's mechanism (variationally type-h orbit) whenever nearby invariant circles are close enough to have transversely intersecting stable and unstable manifolds.

Here comes the second main difficulty. There are uncountably many invariant circles for which we want their stable and unstable manifolds to intersect transversely in order to implement Arnold's mechanism. It is easy to add a perturbation to create the intersection for one such circle. However, it is not allowed to add uncountably many perturbations for the consideration of genericity.

The key to this problem is the following regularity result, which holds for nearly integrable twist maps on $T^*\mathbb{T}^1$ or equivalently nearly integrable Hamiltonian systems of one and a half degrees of freedom.

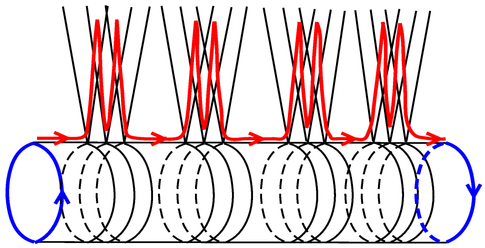

Figure 1. Phase space dynamics of the mechanism in [14; 15].

Theorem 4.1. *Let $H : T^*\mathbb{T} \times \mathbb{T} \to \mathbb{R}$ be a time-dependent nearly integrable Tonelli Hamiltonian system and $u_c^\pm : \mathbb{T} \to \mathbb{R}$, $c \in H^1(\mathbb{T}, \mathbb{R})$ be its weak KAM solutions. Then for all c, c' in a bounded subset of $H^1(\mathbb{T}, \mathbb{R})$ and such that $\widetilde{\mathcal{M}}(c)$ and $\widetilde{\mathcal{M}}(c')$ are invariant circles, there is a uniform constant C such that*

$$\|u_c^\pm(\cdot) - u_{c'}^\pm(\cdot)\|_{C^0} \leq C\|c - c'\|^{1/2}.$$

A similar regularity result holds for the barrier function of the full system. We thus see that the set $\mathcal{S}$ of all weak KAM solutions corresponding to invariant circles on $\mathcal{C}_\varepsilon$ is a set of finite box dimension in $C^0(\mathbb{T}^2, \mathbb{R})$. We have seen in Section 3A that the intersection of the stable and unstable manifolds can be interpreted as the minimal point of the barrier function. Thus we need the barrier function to be nonconstant outside $\mathcal{C}_\varepsilon$. Note that a C^0 function $f : \mathbb{T} \to \mathbb{R}$ being constant on an interval $J \subset \mathbb{T}$ is of infinite codimension. Since $\mathcal{S}$ has finite box dimension, it is easy to find an arbitrarily small $\tilde{u}$ such that the entire set $\tilde{u} + \mathcal{S}$ avoids the infinite codimensional space of functions that are constants over some sets of the form $\mathbb{T} \times J$, where $J \subset \mathbb{T}$ is an interval. In this way, we thus have verified assumption (2) of Theorem 3.1 and can facilitate Arnold's mechanism. We refer readers to [14; 15] for details of this argument. We finally emphasize that the regularity of the weak KAM solutions of the form 4.1 is the essential ingredient in the proof of the genericity.

We finally remark on the literature. The use of box dimension to the genericity problem goes back to Moeckel [36] in which the author studied the iteration of a pair of twist maps where the regularity problem is straightforward. The regularity result Theorem 4.1, its generalization to the full system and the genericity argument for *a priori* unstable systems first appeared in [14; 15]. Bernard [6] gave a different mechanism for constructing diffusing orbit using only Arnold's mechanism designed for the variational objects, without a genericity argument. The regularity result adapted to the mechanism of [6] was given in [38].

5. The normal form

When applied to nearly integrable systems, the variational method is greatly enhanced by the normal form theory. The basic objects such as Mather sets, Aubry sets and Mañé sets are invariant under symplectomorphisms. In the normal form theory, we will apply a symplectic transformation to reduce the Hamiltonian to a normal form to reveal the rotator-pendulum structure. We have seen from Arnold's example that the rotator-pendulum structure is intimately related to the appearance of resonances. The normal form theory reveals this link in this section.

5A. ***Homogenization.*** For nearly integrable systems of the form (1-1), the natural scale to work with is $\sqrt{\varepsilon}$ in the space of action variables. In this section, we introduce a procedure called homogenization used to blow up a $O(\sqrt{\varepsilon})$ ball in the space of action variables to the unit size. The main outcome of the homogenization procedure is a mechanical system with a fast drift and a small perturbation.

Consider an autonomous Hamiltonian H defined on $T^*\mathbb{T}^n$. Picking a point $y^\star \in \mathbb{R}^n$, we introduce the homogenization operator

$$\mathfrak{H}: \quad y - y^\star := \sqrt{\varepsilon}Y, \quad H(x, y) = \varepsilon \mathsf{H}(x, Y), \tag{5-1}$$

where Y, τ, H are the homogenized action variable and Hamiltonian respectively. We will simultaneously rescale the time t to the new time $\tau = t\sqrt{\varepsilon}$, The Hamiltonian (1-1) becomes

$$\mathsf{H}(x, Y) = \frac{h(y^\star)}{\varepsilon} + \frac{1}{\sqrt{\varepsilon}}\langle \omega^\star, Y\rangle + \frac{1}{2}\langle \mathsf{A}Y, Y\rangle + \mathsf{V}(x) + \mathsf{P}(x, \sqrt{\varepsilon}Y), \tag{5-2}$$

where:

(1) $\frac{h(y^\star)}{\varepsilon} + \frac{1}{\sqrt{\varepsilon}}\langle \omega^\star, Y\rangle + \frac{1}{2}\langle \mathsf{A}Y, Y\rangle$ is the first three terms of the Taylor expansion of $h(y)$ around $y^\star$.

(2) $\omega^\star = \frac{\partial h}{\partial y}(y^\star)$.

(3) $\mathsf{A} = \frac{\partial^2 h}{\partial y^2}(y^\star)$ is a positive definite constant matrix.

(4) $\mathsf{V}(x) = P(x, y^\star)$ is the constant term in the Taylor expansion of $P(x, y)$ with respect to the variable y.

(5) $\mathsf{P}(x, \sqrt{\varepsilon}Y)$ consists of all the remaining terms and we have the estimate $\|\mathsf{P}\|_{C^r} = O(\sqrt{\varepsilon})$ if $\|Y\| < C$.

5B. ***Normal form.*** We next state a normal form proposition for the homogenized system. Simply put, the normal form deduces the rotator+pendulum structure from a resonance.

Definition 5.1. A frequency vector $\omega \in \mathbb{R}^n \setminus \{0\}$ is said to be *resonant* if we have $\langle \omega, \mathbf{k}_i \rangle = 0$ for some linearly independent $\mathbf{k}_1, \dots, \mathbf{k}_m \in \mathbb{Z}^n \setminus \{0\}$, $1 \le m \le n-1$. The number m is called the *multiplicity of the resonance*. We call ω a *complete resonance* if $m = n-1$, in which case ω is a nonzero multiple of a rational vector.

Proposition 5.2 [11, Proposition 3.10]. *For any $\delta > 0$, there exists ε_0 such that for all $\varepsilon < \varepsilon_0$ the following holds. Suppose $\omega^\star \in \mathbb{R}^n$ admits m independent resonance relations $\langle \mathbf{k}_i, \omega^\star \rangle = 0$ with $|\mathbf{k}_i| \le \delta^{-1/2}$, $i = 1, \dots, m$, and $|\langle \mathbf{k}, \omega^\star \rangle| > \varepsilon^{1/3}$ for any $|\mathbf{k}| \le \delta^{-1/2}$ and $\mathbf{k} \notin \mathrm{span}_{\mathbb{Z}}\{\mathbf{k}_1, \dots, \mathbf{k}_m\}$. Then there exists a symplectic transformation ϕ, which is $o_\varepsilon(1)$ close to identity in the C^{r-2} norm in the domain $\{|Y| \le 1\}$, such that the Hamiltonian system* (5-2) *is transformed to the following*

$$\begin{aligned} &\mathsf{H}\circ\phi(x, Y) \\ &\quad = \tfrac{1}{\varepsilon} h(y^\star) + \tfrac{1}{\sqrt{\varepsilon}} \langle \omega^\star, Y \rangle + \tfrac{1}{2} \langle \mathsf{A} Y, Y \rangle + V(\langle \mathbf{k}_1, x \rangle, \dots, \langle \mathbf{k}_m, x \rangle) + \delta \mathsf{R}(x, Y), \end{aligned} \tag{5-3}$$

where:

(1) *V consists of all the Fourier modes of* V *in* $\mathrm{span}_{\mathbb{Z}}\{\mathbf{k}_1, \dots, \mathbf{k}_m\}$.

(2) *The remainder $\delta \mathsf{R}(x, Y) = \mathsf{R}_I(x) + \sqrt{\varepsilon} \mathsf{R}_{II}(x, Y)$, where $\delta \mathsf{R}_I$ consists of all the Fourier modes in V with $|\mathbf{k}| > \delta^{-1/2}$.*

(3) *If the perturbation P in* (1-1) *satisfies $\|P(x, y)\|_{C^r} \le 1$, then the norms of V, R_I, R_{II} satisfy $\|V\|_{C^r}$, $\|\mathsf{R}_I\|_{C^{r-2}}$, $\|\mathsf{R}_{II}(x, Y)\|_{C^{r-2}} \le 1$.*

Sketch of proof. We sketch an argument to give the main idea of the proof and refer readers to [11]. We consider the pullback of H by the time-1 map $\phi^1_{\sqrt{\varepsilon} F}$ of another Hamiltonian $\sqrt{\varepsilon} F$ to be determined. Then we get by the definition of the Poisson bracket $\big(\frac{d}{dt}|_{t=0} \mathsf{H}(\phi^t_{\sqrt{\varepsilon} F})\big) := \{\mathsf{H}, \sqrt{\varepsilon} F\} = \frac{\partial \mathsf{H}}{\partial x} \frac{\partial \sqrt{\varepsilon} F}{\partial y} - \frac{\partial \mathsf{H}}{\partial y} \frac{\partial \sqrt{\varepsilon} F}{\partial x}$ and Taylor expansion that

$$\begin{aligned} \mathsf{H}\circ\phi^1_{\sqrt{\varepsilon} F} &= \mathsf{H} + \{\mathsf{H}, \sqrt{\varepsilon} F\} + \varepsilon \int_0^1 (1-t) \{\{\mathsf{H}, F\}, F\} \circ \phi^t_F \, dt \\ &= \tfrac{1}{\varepsilon} h(y^\star) + \tfrac{1}{\sqrt{\varepsilon}} \langle \omega^\star, Y \rangle + \tfrac{1}{2} \langle \mathsf{A} Y, Y \rangle + \mathsf{V}(x) + \langle \omega^\star, \partial_x F \rangle + O(\varepsilon^{1/3}). \end{aligned} \tag{5-4}$$

We next decompose $\mathsf{V}(x) = V + \tilde{V}$ where V consists of all the Fourier modes of V in $\mathrm{span}_{\mathbb{Z}}\{\mathbf{k}_1, \dots, \mathbf{k}_m\}$, and $\tilde{V}$ consists of the rest. We further decompose $\tilde{V} = \tilde{V}_1 + \tilde{V}_2$ where $\tilde{V}_1$ consists of those Fourier modes with $|\mathbf{k}| \le \delta^{-1/2}$ and $\tilde{V}_2$ consists of the rest. Note that $\tilde{V}_2$ has C^{r-2} norm less than δ by the decay of Fourier coefficients. Then we can solve the equation $\tilde{V}_1 + \langle \omega^\star, \partial_x F \rangle = 0$ by taking Fourier expansion and using the assumption $|\langle \mathbf{k}, \omega^\star \rangle| > \varepsilon^{1/3}$ for any $\mathbf{k} \in \mathbb{Z}^n$ with $|\mathbf{k}| \le \delta^{-1/2}$ and $\mathbf{k} \notin \mathrm{span}_{\mathbb{Z}}\{\mathbf{k}_1, \dots, \mathbf{k}_m\}$. We thus obtain the normal form. $\square$

Once we have the normal form, we can then find a matrix $M \in \mathrm{SL}(n, \mathbb{Z})$ whose first m rows are $\mathbf{k}_1, \dots, \mathbf{k}_m$ such that $M\omega^\star$ has 0 first m entries. Thus, after a linear symplectic transformations $(x, Y) \mapsto (M^{-1}x, M^t Y)$, the potential V is a function of $x_1, \dots, x_m$. This allows us to reduce the normal form to a "pendulum+rotator" structure as in Arnold's example.

5C. ***The pendulum+rotator structure near resonance.*** For example, we consider the following Hamiltonian

$$H(x, y) = \tfrac{1}{2}\|y\|^2 + \varepsilon P(x), \quad (x, y) \in T^*\mathbb{T}^n.$$

We remark that we have chosen the kinetic energy part of the form $\frac{1}{2}\|y\|^2$ to simplify the discussion. A general kinetic energy of the form $\frac{1}{2}\langle \mathsf{A}Y, Y\rangle$ will create some new difficulty in separating the rotator and the pendulum. We have developed systematic tools (shear transformation and undo-shear etc) in [11] to deal with this issue. We avoid this complication by restricting ourselves to the simple example and refer interested readers to [11] for more details in the general case.

Suppose $y^\star = (0, \hat{\omega}^\star)$ where $\hat{\omega}^\star \in \mathbb{R}^{n-m}$ is Diophantine. Then the Hamiltonian has the following normal form up to an additive constant

$$\mathsf{H}(x, Y) = \tfrac{1}{\sqrt{\varepsilon}}\langle \hat{\omega}^\star, \hat{Y}\rangle + \tfrac{1}{2}\|\hat{Y}\|^2 + \tfrac{1}{2}\|\tilde{Y}\|^2 + V(\tilde{x}) + \delta \mathsf{R}(x, Y), \tag{5-5}$$

where we use notation $x = (\tilde{x}, \hat{x})$ and $Y = (\tilde{Y}, \hat{Y})$, where $\tilde{}$ means the first m variables and $\hat{}$ means the last $n - m$ variables. This Hamiltonian system is split naturally into a product system if we discard the $\delta\mathsf{R}$ term. The subsystem $\hat{\mathsf{H}}(\hat{x}, \hat{Y}) = \frac{1}{\sqrt{\varepsilon}}\langle \hat{\omega}^\star, \hat{Y}\rangle + \frac{1}{2}\|\hat{Y}\|^2$ is integrable and can be considered as a rotator. Suppose V has a nondegenerate global maximum at 0 so the subsystem

$$\tilde{\mathsf{H}}(\tilde{x}, \tilde{Y}) = \tfrac{1}{2}\|\tilde{Y}\|^2 + V(\tilde{x}) \tag{5-6}$$

has a hyperbolic fixed point $(0, 0)$. The Hamiltonian H now has the form of "pendulum+rotator" structure as in Arnold's example. In particular, single resonance normal form gives rise to an *a priori* unstable system of the form (4-1) (the pendulum subsystem has one degree of freedom).

We warn the readers that the normal form becomes singular as $\varepsilon \to 0$, which is reflected in the term $\frac{1}{\sqrt{\varepsilon}}\langle \omega^\star, Y\rangle$ in (5-3) implying that the dynamics on the NHIC is fast rotating ($\dot{\hat{x}} = O(\varepsilon^{-1/2})$ in example (5-5)). This presents a technical difficulty in the proof. The way we solve the problem is to notice that its contribution to the variational equation disappears since $\omega^\star$ is a constant, hence it has no contribution to the differential of the time-1 map of the Hamiltonian system! This fact enables us to perform the graph transform as in [21; 26] to obtain a version of the theorem of NHIM in this setting, with which we turn on the coupling $\delta\mathsf{R}$ in (5-5) (recall that in Theorem B.2, the assumptions are made on the differential of the map $f : M \to M$ but not on the vector field generating the flow). Details of the statement and the proof can be found in Appendix E of [11].

6. Mechanical systems with two degrees of freedom

In this section, we study the dynamics of a mechanical system of two degrees of freedom of the following form where A is positive definite

$$\mathsf{G}(x, Y) = \tfrac{1}{2}\langle \mathsf{A}Y, Y\rangle + V(x), \quad (x, Y) \in T^*\mathbb{T}^2. \tag{6-1}$$

This system appears naturally in the double resonance normal form. We will see in the next section that such a system is inevitable in constructing diffusing orbits for system (1-1) with $n = 3$.

This system is hard to analyze in general due to its nonperturbative nature. However, the two-dimensionality enables us to obtain enough information on the structure of Mather sets and Mañé sets so that diffusing orbit can be constructed passing through the double resonance.

6A. ***Two degrees of freedom: positive energy levels.*** We have the following theorem describing Mather sets of rational rotation vectors.

Theorem 6.1 [16, Theorem 2.1]. *Given a Tonelli Hamiltonian $H : T^*\mathbb{T}^2 \to \mathbb{R}$ and a class $g \in H_1(\mathbb{T}^2, \mathbb{Z})$ and a closed interval $[\nu^-, \nu^+]$ with $\nu^+ > \nu^- > 0$, there exists an open-dense set $\mathfrak{V} \subset C^r(\mathbb{T}^2, \mathbb{R})/\mathbb{R}$ with $r \geq 5$ such that for each $V \in \mathfrak{V}$ normalized by* $\max V = 0$, *it holds simultaneously for all $\nu \in [\nu^-, \nu^+]$ that the Mather set $\mathcal{M}_{\nu g}$ for $H + V$ consists of hyperbolic periodic orbits. Indeed, except for finitely many ν_j, the Mather set consists of two hyperbolic periodic orbits, for all other $\nu \in [\nu^-, \nu^+]$ it consists of exactly one hyperbolic periodic orbit.*

For each fixed positive energy level, the existence of periodic orbits as the Mather set and its generic uniqueness were known in the Aubry–Mather theory for twist maps. However, it is highly nontrivial to show that these periodic orbits form smooth families and the finiteness of the bifurcations when varying energy levels. This theorem completely describes the structure of the Mather set with rotation vectors along a rational ray in the frequency space. These Mather sets constitute a NHIC. At the bifurcation values ν_j, the two components of the Mather sets are connected by heteroclinic orbits in the Mañé set. When the system is perturbed by a time-periodic perturbation, again we have a system of *a priori* unstable type.

6B. ***Two degrees of freedom: the zeroth energy level.*** We next study the zero frequency case. This was done in [8]. Instead of studying the dynamics in the

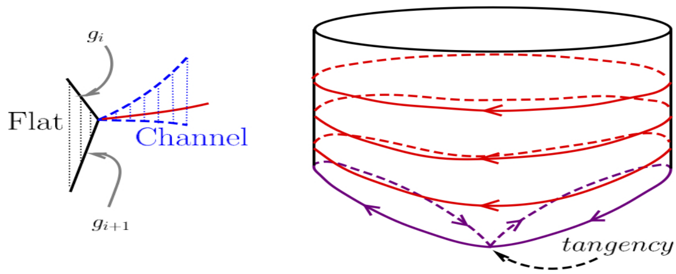

Figure 2. Channel connected to a vertex of $\partial\mathbb{F}_0$.

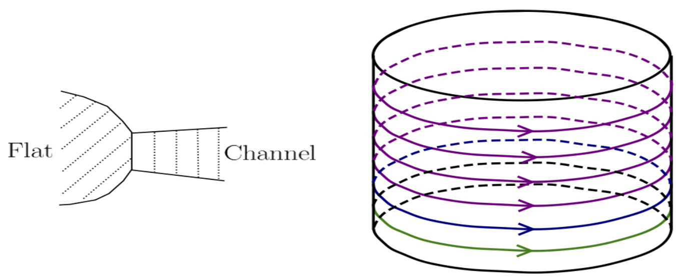

Figure 3. Channel connected to an edge of $\partial\mathbb{F}_0$.

frequency space, we switch to the space of cohomology classes. This passage has the effect of blowing up singularities.

We denote $\mathbb{F}_0 = \alpha_{\mathsf{G}}^{-1}(0)$ and call it the flat, which is a convex set and by $\partial\mathbb{F}_0$ the boundary of $\mathbb{F}_0$. A simple example is the product of two identical pendulums whose $\mathbb{F}_0$ is a square. We next introduce

$$\partial^*\mathbb{F}_0 = \{c \in \partial\mathbb{F}_0 : \mathcal{M}(c)\backslash\{x=0\} \neq \varnothing\}.$$

The set $\partial^*\mathbb{F}_0$ can be nonempty. An example of a system with $\partial^*\mathbb{F}_0 \neq \varnothing$ was given in Section 2 of [9]. When $\partial^*\mathbb{F}_0 \neq \varnothing$ happens, then $\partial\mathbb{F}_0$ has infinitely many edges; see [39].

We next introduce a subset $G_{m,c} \subset H_1(\mathbb{T}^2, \mathbb{Z})$ be a subset that $g \in G_{m,c}$ if there is a minimal homoclinic orbit $(\gamma, \dot{\gamma})$ in $\tilde{\mathcal{A}}(c)$ with $[\gamma] = g$. Given an edge $\mathbb{E}_i$, we define $G_{m,\mathbb{E}_i} = G_{m,c}$ for each $c \in \operatorname{int}\mathbb{E}_i$ since all classes in $\operatorname{int}\mathbb{E}_i$ share the same Aubry set.

The following theorem was proved in [8].

Theorem 6.2. *Let* $\mathbb{F}_0 = \alpha_{\mathsf{G}}^{-1}(\min\alpha_{\mathsf{G}})$ *be a two dimensional flat, and* $\mathcal{M}(c_0)$ *be a singleton for* $c_0 \in \operatorname{int}\mathbb{F}_0$. *Let* $\mathbb{E}_i$ *denote an edge of* $\mathbb{F}_0$ *(not a point), then:*

(1) *Either* $\mathbb{E}_i \cap \partial^*\mathbb{F}_0 = \varnothing$ *or* $\mathbb{E}_i \subset \partial^*\mathbb{F}_0$.

(2) *If* $\mathbb{E}_i \cap \partial^*\mathbb{F}_0 = \varnothing$, *then* $G_{m,\mathbb{E}_i}$ *contains exactly one element, if* $\mathbb{E}_i \subset \partial^*\mathbb{F}_0$, *all curves in* $\mathcal{M}(\mathbb{E}_i)\backslash\{0\}$ *have the same rotation vector.*

(3) *If* $c \in \partial\mathbb{E}_i$ *and* $c \notin \partial^*\mathbb{F}_0$ *then* $G_{m,c}$ *contains exactly two elements.*

(4) *If* $\mathbb{E}_i, \mathbb{E}_j \subset \partial^*\mathbb{F}_0$, *then either* $\mathbb{E}_i = \mathbb{E}_j$, *or* $\mathbb{E}_i$ *and* $\mathbb{E}_j$ *are disjoint.*

(5) *If* $\mathbb{E}_i \subset \partial^*\mathbb{F}_0$, $\mathcal{M}(c) = \mathcal{M}(c')$ *holds for* $c \in \partial\mathbb{E}_i$ *and* $c' \in int\mathbb{E}_i$.

(6) *If* μ_c *is an ergodic c-minimal measure for* $c \in \partial^*\mathbb{F}_0$ *and* $\omega(\mu_c)$ *is irrational, then the class c is an extremal point of* $\mathbb{F}_0$.

(7) *If* $c \in \partial\mathbb{F}_0\backslash\partial^*\mathbb{F}_0$ *and* $\tilde{\mathcal{A}}(c)$ *consists of the fixed point and one homoclinic orbit* $(\gamma, \dot{\gamma})$ *only, then c is located in the interior of certain edge* $\mathbb{E}_i$.

(8) *Each edge in* $\partial\mathbb{F}_0\backslash\partial^*\mathbb{F}_0$ *is joined by two edges in* $\partial\mathbb{F}_0\backslash\partial^*\mathbb{F}_0$.

The result is summarized in the following dictionary. For each cohomology class c in the right column, the corresponding Aubry set $\tilde{\mathcal{A}}(c)$ is in the left column:

phase space	$H^1(\mathbb{T}^2, \mathbb{R})$
hyperbolic fixed point	convex disk int $\mathbb{F}_0$
homoclinic or periodic orbit	edge of $\mathbb{F}_0$
two homoclinic orbits	vertex of $\mathbb{F}_0$
homology class of homoclinic orbits	$\perp$ edge
NHIC foliated by periodic orbits	channel connected to $\mathbb{F}_0$

To relate this dictionary to Theorem 6.1, we see that the NHIC foliated by periodic orbits given in Theorem 6.1 gives the channel in the last row of the dictionary. We may let the energy level to approach zero. The fact that there is no infinite bifurcation in this limiting procedure is proved in the following Theorem 6.4. In the limit, the Mather set may remain a periodic orbit or degenerate to a homoclinic orbit as in the second line of the dictionary (see Figure 2) or degenerate to two homoclinic orbits as in the third line of the dictionary (see Figure 3). The purpose of a careful study of the structure of $\partial\mathbb{F}_0$ and its dynamical correspondence is to understand the dynamics on small positive energy levels, as we shall talk about in the next subsection.

6C. *Dynamics around the strong double resonance.* It is shown in [8] that for all $c \in \partial\mathbb{F}_0$, the projected Mañé set $\mathcal{N}(c)$ (the projection of $\tilde{\mathcal{N}}(c)$ from $T^*\mathbb{T}^2$ to $\mathbb{T}^2$) does not cover the two torus.

Theorem 6.3 [8, Theorem 3.1]. *Consider the Hamiltonian* G *of the type* (6-1). *There exists a residual set in* $C^r(\mathbb{T}^2)/\mathbb{R}$, $r \geq 2$ *such that for each* V *in the set normalized by* $\max V = 0$, *and for each* $c \in \partial\mathbb{F}_0$, *the Mañé set* $\mathcal{N}(c)$ *does not cover the whole configuration space, i.e.,* $\mathcal{N}(c) \subsetneq \mathbb{T}^2$ *for all* $c \in \partial\mathbb{F}_0$. *Moreover, the upper-semicontinuity of* $\mathcal{N}(c)$ *with respect to c implies that there is a* $\Delta = \Delta(V) > 0$ *such that the same conclusion holds for all* $c \in \alpha_{\mathsf{G}}^{-1}([0, \Delta])$.

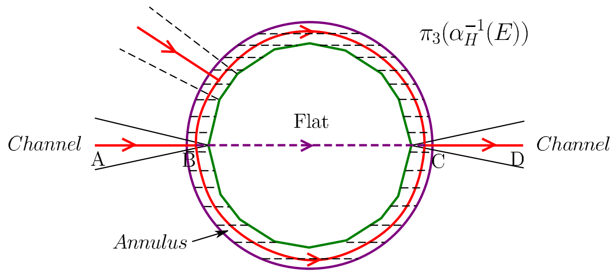

Figure 4. Turning around strong double resonance.

This theorem can be understood as that along the circle $\partial\mathbb{F}_0$, the dynamics is similar to that of the Birkhoff instability region of the twist map where there is no invariant circles. However, the facts that the dynamics on the zero energy level of G cannot be written as a twist map, the destruction of $\mathcal{N}(c)$ for all $c \in \partial\mathbb{F}_0$ and the nonperturbative nature of the system G make the result highly nontrivial. We refer readers to [8] for details.

The theorem implies that any two cohomology classes $c, c' \in \partial(\alpha_0^{-1}(E))$, $E \in [0, \Delta]$, are equivalent which gives rise to an orbit shadowing Mather sets $\widetilde{\mathcal{M}}(c)$ and $\widetilde{\mathcal{M}}(c')$; see Theorem 3.3. When viewed in the frequency space, this implies in particular that for any two rational rays starting from 0, there is an orbit shadowing Mather sets with rotation vectors lying on the two rays.

In general, it seems not easy to see the dynamical picture of orbits constructed here in the phase space. On very small energy levels when two channels are close, it seems natural that orbit shadows heteroclinics between periodic orbits on two channels, but the dynamics seems much richer when $\partial^*\mathbb{F}_0 \neq \varnothing$. We also remark that the number Δ here is obtained by the upper-semicontinuity of the Mañé set, hence does not admit an estimate, but it is certainly independent of ε. The numerical experiment of [23] seems to indicate that for dynamics around double resonance should mostly follow the mechanism here.

6D. ***Cylinders with a hole.*** The phase space picture of the dynamics near double resonance was studied by many authors. The idea is that the NHICs in Theorem 6.1 can reach the zero energy level and even extend slightly to the negative energy levels. On the zero energy level, the Poincaré return map takes infinitely long time to return. This makes it hard to verify the smoothness of the cylinder near the zero energy level. The classical theorem of normally hyperbolic invariant manifold does not apply since the cylinder here is constructed from periodic orbits but not perturbed from a known cylinder, while the theorem of normally hyperbolic invariant manifold is a theorem about the persistence of center manifolds under perturbations. The problem of the C^1 regularity of the cylinders was addressed in [17]. We state the main result of [17] in the general setting.

$$H(x, y) = \frac{1}{2}\langle Ay, y\rangle + V(x), \quad z = (x, y) \in \mathbb{T}^n \times \mathbb{R}^n, \tag{6-2}$$

where the matrix A is positive definite and the smooth potential V attains its maximum at a unique point $x_0 \in \mathbb{T}^n$. In this case, $z_0 = (x_0, 0)$ is a fixed point of the Hamiltonian flow Φ^t_H and there exist some orbits homoclinic to the fixed point known after the work of Bolotin. Be aware that the system admits a symmetry $\mathbf{s}: (x, y) \to (x, -y)$, we see that if $z^+(t) = (x^+(t), y^+(t))$ is an orbit, $z^-(t) = \mathbf{s}z^+(t) = (x^+(-t), -y^+(-t))$ is also an orbit. Hence, nonshrinkable homoclinic orbits emerge paired.

To formulate our result, by a translation of variables $x \to x - x_0$ and $V \to V - V(x_0)$ we assume $x_0 = 0$, $V(0) = 0$. We study k pairs of homoclinic orbits $\{z_1^{\pm}(t), \dots, z_k^{\pm}(t)\}$ and denote by $\Gamma_i^{\pm}$ the closure of $\{z_i^{\pm}(t) \mid t \in \mathbb{R}\}$. A periodic orbit $z^+(t)$ is said to *shadow the orbits* $\{z_1^+(t), \dots, z_k^+(t)\}$ if the period admits a partition $[0, T] = [0, t_1] \cup [t_1, t_2] \cup \cdots \cup [t_{k-1}, T]$ such that $z^+(t)|_{[t_{i-1}, t_i]}$ falls into a small neighborhood of $z_i^+(t)$. In this case, its $\mathbf{s}$-symmetric counterpart $z^-(t) = \mathbf{s}z^+(t)$ shadows the orbits $\{z_k^-(t), \dots, z_1^-(t)\}$.

The case of $k = 1$ will be studied in the original phase space $\mathbb{T}^n \times \mathbb{R}^n$. To study the case $k \geq 2$, we work in the covering spaces $\bar{\pi}_h\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{T}^n_h \times \mathbb{R}^n$ and $\pi_h : \mathbb{T}^n_h \times \mathbb{R}^n \to \mathbb{T}^n \times \mathbb{R}^n$, where $\mathbb{T}^n_h = \{(x_1, x_2, \dots, x_n) \in \mathbb{R}^n : x_i \mod h_i \in \mathbb{N}\backslash 0\}$. To decide the class $h = (h_1, \dots, h_n)$, we let $\bar{z}_1(t)$ be the lift of $z_1^+(t)$ to $\mathbb{R}^{2n}$ such that $\lim_{t\to-\infty} \bar{z}_1(t) = 0$, then choose a lift $\bar{z}_2(t)$ of $z_2^+(t)$ with $\lim_{t\to-\infty} \bar{z}_2(t) = \lim_{t\to\infty} \bar{z}_1(t)$. In the way, we get successively a lift $\bar{z}_i(t)$ of $z_i^+(t)$ for each i and define h to be the integer vector $\lim_{t\to\infty} \bar{z}_k(t)$. Let $\overline{\Gamma}$ be the closure of $\big\{\cup_{i\leq k}\bar{z}_i(t)) \mid t \in \mathbb{R}\big\}$, then we construct a shift $\sigma\overline{\Gamma}$ as follows. We define $\bar{z}'_1(t) \subset \sigma\overline{\Gamma}$ to be the lift of $z_1^+(t)$ such that $\lim_{t\to-\infty} \bar{z}'_1(t) = \lim_{t\to\infty} \bar{z}_k(t)$. Other $\bar{z}'_i(t)$, $i = 2, \dots, k$, is successively constructed. Let $\sigma\overline{\Gamma}$ be the closure of $\big\{\cup_i \bar{z}'_i(t)) \mid t \in \mathbb{R}\big\}$. We make the following assumption:

> *For k pairs of homoclinic orbits $\{z_1^{\pm}(t), \dots, z_k^{\pm}(t)\}$, there exists a nonnegative integer ℓ and a covering space $\bar{\pi}_h\colon \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{T}^n_h \times \mathbb{R}^n$ such that $\bar{\pi}_h(\overline{\Gamma} \cup \sigma\overline{\Gamma} \cup \cdots \cup \sigma^{\ell}\overline{\Gamma})$ is a closed curve without self-intersection.* **(H)**

Theorem 6.4. *Under certain genericity assumptions including* (**H**) (*see* [17, Theorem 1.1]) *there exists a continuation of periodic orbits from the homoclinic orbits* $\{z_1^{\pm}(t), \dots, z_k^{\pm}(t)\}$. *More precisely, some* $E_0 > 0$ *exists such that*:

(1) *For any* $E \in (0, E_0]$, *on the energy level* E *there exist unique periodic orbit* $z_E^+(t)$ *and its* $\mathbf{s}$*-symmetric orbit* $z_E^-(t) = \mathbf{s}z_E^+(t)$ *shadowing the orbits* $\{z_1^+(t), \dots, z_k^+(t)\}$ *and* $\{z_k^-(t), \dots, z_1^-(t)\}$ *respectively. The set* $\{z_E^{\pm}(t) \mid t \in \mathbb{R}\}$ *depending on* E *approaches* $\cup_i \Gamma_i^{\pm}$ *in Hausdorff metric as* $E \downarrow 0$.

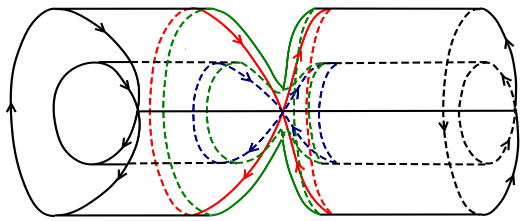

Figure 5. Cylinder with a hole.

(2) *For any* $E \in [-E_0, 0)$ *there exists a unique periodic orbit* $z_{E,i}$ *shadowing the orbits* $\{z_i^+(t), z_i^-(t)\}$ *for* $i = 1, \dots, k$. *As a set depending on* E, $\{z_{E,i}(t) \mid t \in \mathbb{R}\}$ *approaches* $\Gamma_i^+ \cup \Gamma_i^-$ *in Hausdorff metric as* $E \uparrow 0$.

Let $\Pi = \Pi^+ \cup_{1 \le i \le k} (\Pi_i^- \cup \Gamma_i^+ \cup \Gamma_i^-)$ *where* $\Pi^+ = \cup_{E>0}(\cup_t z_E^+(t) \cup z_E^-(t))$ *and* $\Pi_i^- = \cup_{E<0} \cup_t z_{E,i}(t)$. *For* $k = 1$, *it makes up a* C^1*-NHIC with one hole. For* $k \ge 2$, *each connected component in the pull-back* $\pi_h^{-1}\Pi$ *of* Π *to* $\mathbb{T}_h^n \times \mathbb{R}^n$ *is a* C^1*-NHIC with* $(\ell + 1)k$ *holes. The homoclinic orbits are contained inside of the manifold.*

In [17], to which readers are referred to, the authors give two more mechanisms of crossing the double resonance utilizing the geometric structure of cylinders with a hole. Compared to the first mechanism of turning around double resonance using c-equivalence, in this mechanism using cylinders with holes, orbits has to cross zero energy level hence we expect that the orbit should be much slower than that in the first mechanism hence is less likely. This is an interesting subject for future study.

7. Systems with three degrees of freedom

In this section, we give an overview of the proof of Theorem 1.3 in the case of $n = 3$.

7A. ***Design resonance paths and separate single and double resonances.*** We first show how to apply the homogenization and normal form to design resonance paths along which we construct diffusing orbit. We consider the case of three degrees of freedom for simplicity. Let $\varepsilon = 0$ in (1-1), now the frequency vector $\omega(y) := Dh(y) : \mathbb{R}^3 \to \mathbb{R}^3$ has range defined on a sphere when h is restricted to an energy level $E > \min h$. For any integer vector $\mathbf{k} \in \mathbb{Z}^3 \setminus \{0\}$, the resonance condition $\langle \mathbf{k}, \omega(y) \rangle = 0$ defines a circle on the sphere. Given two balls on the sphere, one can connect them by some of the resonant circles (in general at least 2). Along each resonance circle $S_{\mathbf{k}} := \{\langle \mathbf{k}, \omega(y) \rangle = 0, h(y) = E\}$, we show that the perturbation $P(\,\cdot\,, y) : \mathbb{T}^3 \to \mathbb{R}$, $y \in S_{\mathbf{k}}$ generically has a unique nondegenerate global max, up to finitely many bifurcation points where there are two nondegenerate global max (see Proposition 8.1 below for a version of this type of parametric transversality result). As we have explained in Section 5, we will cover such resonant circles by balls of radius $\Lambda\sqrt{\varepsilon}$ centered at $y^\star \in S_{\mathbf{k}}$, and perform the homogenization in each ball. The global max of $P(\cdot, y^\star)$ gives rise to a hyperbolic fixed point in a pendulum-like subsystem as we have seen in Section 5C. In particular, the normal hyperbolicity is uniform for all the homogenized systems around $S_{\mathbf{k}}$ due to the uniform nondegeneracy of the global max of $P(\cdot, y)$, $y \in S_{\mathbf{k}}$. The uniform normal hyperbolicity gives a bound d_0 of the maximal allowable C^1-norm of the perturbation so that the theorem of NHIM is valid. Note that this d_0 is independent of ε but depends only on P.

Let δ be a small number but independent of ε and apply the normal form Proposition 5.2 and we consider only finitely many integer vectors of lengths less than $\delta^{-1/2}$. Along $S_{\mathbf{k}}$, there might be a second resonance, i.e., there is $\mathbf{k}'$ with $|\mathbf{k}'| < \delta^{-1/2}$ linearly independent of $\mathbf{k}$ such that $\langle\omega(y_*), \mathbf{k}'\rangle = \langle\omega(y_*), \mathbf{k}\rangle = 0$, $y_* \in S_{\mathbf{k}}$. For each such point y_*, outside of its $O(\varepsilon^{1/3})$-neighborhood, we can apply Proposition 5.2 with single resonance ($m = 1$), and within such an $O(\varepsilon^{1/3})$-neighborhood, we apply Proposition 5.2 with double resonance ($m = 2$). In the former case, the problem is essentially reduced to the *a priori* unstable case after some highly nontrivial work (recall example (5-5) with $m = 1$). In the latter case, the potential $V(\langle\mathbf{k}, x\rangle, \langle\mathbf{k}', x\rangle)$ in (5-3) can be decomposed into $\overline{V}(\langle\mathbf{k}, x\rangle) + \tilde{V}(\langle\mathbf{k}, x\rangle, \langle\mathbf{k}', x\rangle)$, where $\tilde{V}$ depends on $\langle\mathbf{k}', x\rangle$ nontrivially and its C^2 norm is estimated as $C|\mathbf{k}'|^{-(r-2)}$ for fixed $\mathbf{k}$ and $P \in C^r$. When $\|\tilde{V}\|_{C^2} < d_0$, we can still apply the theorem of NHIM by treating $\tilde{V}$ as a perturbation so we call this case *weak double resonance* and treat it in a similar manner as a single resonance. Then the remaining case $\|\tilde{V}\|_{C^2} \ge d_0$ is called *strong double resonance*. Note that there are only finitely many of them, whose number is independent of ε, δ. The $O(\varepsilon^{1/3})$-neighborhood of a strong double resonance can be further divided into the $O(\varepsilon^{1/2})$-neighborhood and the region outside the $O(\varepsilon^{1/2})$-neighborhood. The former case is reduced to the setting of Section 6 as we will see in the next subsection. The latter case is the regime of transiting from single to double resonance regimes. It can be treated as the high energy level sets in the system (6-1) and in the normal form Proposition 5.2, the frequency $\omega^\star/\sqrt{\varepsilon}$ goes from $O(\varepsilon^{-1/6})$ to $O(1)$. It is shown in [8] that the cylinder in Theorem 6.1 in the high energy level regime consists of a single piece, without bifurcation and the normal hyperbolicity is uniform, so this transiting regime can also be treated as a system of *a priori* unstable type. In the following, we focus on the strong double resonances.

7B. ***The double resonance.*** In a $\Lambda\sqrt{\varepsilon}$ ball centered at a double resonance, we apply the homogenization and the normal form followed by a linear symplectic transform to get the following Hamiltonian at double resonance

$$\mathsf{H}(x,Y)=\tfrac{\omega_3}{\sqrt{\varepsilon}}Y_3+\tfrac{1}{2}\langle \mathsf{A}Y,Y\rangle+V(x_1,x_2)+\delta\mathsf{R}(x,Y),$$
$$(x;Y)=(x_1,x_2,x_3;Y_1,Y_2,Y_3).$$

We perform a standard energetic reduction (fixing an energy level and solve for $\mathsf{Y}_{\text{double}}:=(\omega_3/\sqrt{\varepsilon})Y_3$ as the new Hamiltonian and its conjugate $\tau=(\sqrt{\varepsilon}/\omega_3)x_3$ as the new time) to get

$$\mathsf{Y}_{\text{double}}=\tfrac{1}{2}\langle\tilde{\mathsf{A}}\tilde{Y},\tilde{Y}\rangle+V(\tilde{x})+\delta\tilde{\mathsf{R}}\left(\tilde{x},\frac{\omega_3\tau}{\sqrt{\varepsilon}},\tilde{Y}\right),\quad (\tilde{x};\tilde{Y})=(x_1,x_2;Y_1,Y_2) \tag{7-1}$$

where $\tilde{\mathsf{A}}$ is obtained from A by removing the third row and column, which are absorbed in $\delta\tilde{\mathsf{R}}$ during the reduction. We thus arrive at a system that is a small time-dependent perturbation of the nonperturbative mechanical system G of two degrees of freedom. Note that the τ-dependence in $\delta\tilde{\mathsf{R}}$ is fast oscillating as $\varepsilon\to 0$. This singular behavior does not invalidate the theorem of NHIM since it does not enter the estimate of the differential of the time-1 map for the similar reason to the discussion near the end of Section 5. We again refer readers to Appendix E of [11] for this point. We remark that Arnold [4] already identified this as the main difficulty for Arnold diffusion.

Let us now see how the action variable changes if a diffusion orbit is to be constructed. Suppose we want to move y along the resonant circles determined by

$$S_1:=\{\langle\omega(y),\mathbf{k}_1\rangle=0\}\quad\text{and}\quad S_2:=\{\langle\omega(y),\mathbf{k}_2\rangle=0\}.$$

For simplicity we assume $\mathbf{k}_1=(0,1,0)$ and $\mathbf{k}_2=(1,0,0)$ hence along S_1 the frequency has the form $\omega(y)=(\omega_1(y),0,\omega_3(y))$ and along S_2 we have $\omega(y)=(0,\omega_2(y),\omega_3(y))$. When two resonances occur simultaneously we have $\omega(y)=(0,0,\omega_3(y))$. Along the resonant circle S_1, we apply the normal form Proposition 5.2 with $m=1$, then by the argument following Proposition 5.2, we reduce the problem to an *a priori* unstable system in Section 4 so that we can move y freely on the resonant circle S_1 provided there is no second resonance. When the second resonance appears, in a neighborhood of $S_1\cap S_2$ we apply Proposition 5.2 with $m=2$ to yield the normal form (7-1) after the energetic reduction. The energetic reduction treats the third angular variable x_3 as the new time, hence for the system (7-1), the frequency vector is obtained by removing the third entry from $\omega(y)$. So along S_1 the reduced frequency vector has the form $\omega_a:=(a,0)$, $a\in\mathbb{R}$ and along S_2 it has the form $\omega_b:=(0,b)$, $b\in\mathbb{R}$, and the double resonance corresponds to the frequency vector $(0,0)$. To cross the strong double resonance $S_1\cap S_2$, we have to construct orbit moving along ω_a close to $(0,0)$ then along ω_b.

Equipped with the knowledge in Section 6 on the mechanical system G of two degrees of freedom, we are ready to construct diffusing orbits moving around the double resonance. We interpret the frequency ω_a or ω_b as the rotation vector of a Mather set, which is the velocity averaged against the minimizing measure. Theorem 6.1 enables us to move the frequencies along ω_a and ω_b using the mechanism of *a priori* unstable systems up to a small neighborhood of 0. Next, we apply Theorem 6.3 and the c-equivalence mechanism to find orbit shadowing Mather sets with rotation vectors on the frequency segments ω_a and ω_b. Therefore we overcome the difficulty of strong double resonance and global diffusing orbits are constructed in the case of $n = 3$.

8. The genericty

The genericity of the perturbations is a central issue and is closely related to the dynamics. For *a priori* unstable systems, we have outlined the genericity argument in Section 4, which is also applicable to *a priori* stable systems in the regime of single resonances and transition from single to double resonances, where the problem is essentially reduced to *a priori* unstable systems after some work, though highly nontrivial. Near double resonance, the genericity of the perturbations are given in Theorem 6.1 and 6.3. In Theorem 6.1, the genericity originates from the following parametric transversality result; see [16].

Proposition 8.1. *Let $F_s : \mathbb{T}^1 \to \mathbb{R}$, $s \in [0, 1]$ be a family of C^r, $r > 4$ functions that is Lipschitz in s. Then there is an open and dense subset $\mathcal{R}$ of $C^r(\mathbb{T})$ such that for each $V \in \mathcal{R}$, the function $F_s + V$ admits a unique nondegenerate global minimum for all but finitely many parameters $s_1, \ldots, s_n$ for which $F_{s_i} + V$, $i = 1, \ldots, n$ admits two nondegenerate global minimums.*

The genericity in Theorem 6.3 is achieved by only finitely many perturbations in the proof. Since the proof is a bit involved, we refer readers to [9] for details.

Note that in the main terms of the normal form (5-3) as well as the system (6-1), the system is of the form of mechanical systems (kinetic energy+potential energy). In particular, the potential part depends only on the angular variables. That is why we consider only Mañé perturbations (perturbations depending only on angular variables) in the statements of Theorem 6.1 and 6.3, which are the only allowed perturbations.

In the statement of Theorem 1.3, the perturbation P can either depend on all variables or simply Mañé. To achieve the genericity of Mañé perturbation, one of the main difficulties is to do it for *a priori* unstable systems, considering that Theorem 6.1 and 6.3 are stated for Mañé perturbations. Indeed, this is exactly the content of Section 4.2 of [9], where we refer interested readers.

Appendix A: Preliminary Hamiltonian dynamics

In this section, we give some preliminaries on Hamiltonian dynamics.

Definition A.1 (Tonelli Lagrangian). Let M be a closed manifold. A C^2-function $L\colon TM \times \mathbb{T} \to \mathbb{R}$ is called a *Tonelli Lagrangian* if it satisfies the following conditions:

(1) Positive definiteness: for each $(x, t) \in M \times \mathbb{T}$, the Lagrangian function is C^2 strictly convex in velocity, i.e., the Hessian $\partial_{\dot{x}\dot{x}} L$ is positive definite.

(2) Super-linear growth: we assume that L has fiber-wise superlinear growth: for each $(x, t) \in M \times \mathbb{T}$, we have $L/\|\dot{x}\| \to \infty$ as $\|\dot{x}\| \to \infty$.

(3) Completeness: all solutions of the Euler–Lagrange equation are well defined for the whole $t \in \mathbb{R}$.

We have the following remarks:

- (Euler–Lagrange equation) Given a Lagrangian L, its Lagrangian flow is solved from the *Euler–Lagrange equation* $\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$; see [3, Chapter 3].
- (autonomous, nonautonomous, twist maps) We say that L is *autonomous* if it does not depend on t, otherwise it is called *nonautonomous*. A nonautonomous system $L : T\mathbb{T}^n \times \mathbb{T} \to \mathbb{R}$ will be said to have $n + \frac{1}{2}$ degrees of freedom. When $n = 1$, a Tonelli Lagrangian of 1.5 degrees of freedom has time-1 map defined on $T\mathbb{T}$.
- (Tonelli Hamiltonian) A Hamiltonian $H : T^*M \times \mathbb{T} \to \mathbb{R}$ is called Tonelli, if it is the Legendre transform of a Tonelli Lagrangian, i.e.,

$$H(x, y, t) = \max_{\dot{x}} \langle y, \dot{x} \rangle - L(x, \dot{x}, t).$$

  For instance, any *mechanical Hamiltonian* of the form $H(x, y) = \frac{1}{2}\|y\|^2 + V(x)$, $(x, y) \in T^*\mathbb{T}^n$ is *Tonelli*, since it is the Legendre transform of $L(x, \dot{x}) = \frac{1}{2}\|\dot{x}\|^2 - V(x)$, $(x, \dot{x}) \in T\mathbb{T}^n$.
- (energetic reduction) Given an autonomous Hamiltonian $H : T^*\mathbb{T}^n \to \mathbb{R}$, denoting $x = (\hat{x}, x_n) \in \mathbb{T}^{n-1} \times \mathbb{T}$, $y = (\hat{y}, y_n) \in U (\subset \mathbb{R}^{n-1} \times \mathbb{R})$ where U is a bounded domain, if we know $\frac{\partial H}{\partial y_n} \neq 0$, then we can apply the implicit function theorem to the Hamiltonian $H(\hat{x}, x_n, \hat{y}, y_n) = E$ restricted to the constant energy level E, to solve for $y_n = y_n(\hat{x}, x_n, \hat{y})$. Now y_n can be considered as a nonautonomous Hamiltonian of $n - \frac{1}{2}$ degrees of freedom with angular variables $\hat{x}$, action variables $\hat{y}$ and x_n as the time variable; see [3, Section 45, Chapter 9].

Appendix B: The theorem of normally hyperbolic invariant manifolds

In this section we give the version of normally hyperbolic invariant manifold theorem that we used in the proof of our main theorem. The standard references are [26; 22]. Readers are also referred to [20]. There are some subtleties of applying the theorem in the proof concerning the fast oscillatory nature in the nonresonant degrees of freedom. Readers can find more details in the appendix of [11].

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

$$T_x M = E^s(x) \oplus E^u(x) \oplus T_x N$$

in such a way that

$$\begin{aligned} v \in E^s(x) &\Leftrightarrow |Df^n(x)v| \le C\lambda^n |v|, \quad && n \ge 0, \\ v \in E^u(x) &\Leftrightarrow |Df^n(x)v| \le C\lambda^{|n|} |v|, \quad && n \le 0, \\ v \in T_x N &\Leftrightarrow |Df^n(x)v| \le C\mu^n |v|, \quad && n \in \mathbb{Z}. \end{aligned}$$

Here the Riemannian metric $|\cdot|$ can be any prescribed one, which may change the constant C but not λ, μ.

Theorem B.2. *Suppose N is a NHIM under the C^r, $r > 1$, diffeomorphism $f : M \to M$. Denote $\ell = \min\{r, |\ln\lambda|/|\ln\mu|\}$. Then for any C^r f_ϵ that is sufficiently close to f in the C^1 norm*:

(1) *There exists a NHIM N_ϵ that is a C^ℓ graph over N.*

(2) (*Invariant splitting*) *There exists a splitting for $x \in N_\epsilon$*

$$T_x M = E^u_\epsilon(x) \oplus E^s_\epsilon(x) \oplus T_x N_\epsilon \tag{B-1}$$

invariant under the map f_ϵ. The bundle $E^{u,s}_\epsilon(x)$ is $C^{\ell-1}$ in x.

(3) *There exist C^ℓ stable and unstable manifolds $W^s(N_\epsilon)$ and $W^u(N_\epsilon)$ that are invariant under f and are tangent to $E^s_\epsilon \oplus TN_\epsilon$ and $E^u_\epsilon \oplus TN_\epsilon$ respectively.*

(4) *The stable and unstable manifolds $W^{u,s}(N_\epsilon)$ are fibered by the corresponding stable and unstable leaves $W^{u,s}_{x,\epsilon}$:*

$$W^u(N_\epsilon) = \cup_{x \in N_\epsilon} W^u_{x,\epsilon}, \quad W^s(N_\epsilon) = \cup_{x \in N_\epsilon} W^s_{x,\epsilon}.$$

(5) *The maps $x \mapsto W^{u,s}_{x,\epsilon}$ are $C^{\ell-j}$ when $W^{u,s}_{x,\epsilon}$ is given C^j topology.*

(6) *If f and f_ϵ are Hamiltonian and* $\dim E^s = \dim E^u$, *then N_ϵ is symplectic and the map f_ϵ restricted to N_ϵ is also Hamiltonian* [20].

Appendix C: Systems of arbitrary degrees of freedom

In this appendix, we illustrate how to construct diffusing orbit in the general $n > 3$ case. The main difficulty is that it is not avoidable to study the dynamics around the complete resonance where the system is reduced to a mechanical system of $(n-1)$ degrees of freedom, which is in general nonperturbative. The high dimensional and nonperturbative nature of the problem creates serious difficulties in general. For example, for a nonperturbative mechanical system of $(n-1)$ degrees of freedom, Mather sets with rational rotation vectors may not be periodic orbits and when they are periodic they are not necessarily hyperbolic. So the theory in Section 6 cannot be recovered in this case. However, it turns out that close to codimension 1 and 2 KAM tori, we can find a connected set where perturbative techniques can be applied to reduce the problem to a multiscale system such that in each scale we have only single or double resonances. In this way, the methods in the previous sections can be applied to construct diffusing orbits. The general strategy is as follows:

(1) Try to find NHIC homeomorphic to $T^*\mathbb{T}\times\mathbb{T}$ to apply the method of *a priori* unstable system (4-1).

(2) Apply the mechanism of c-equivalence when there is a strong double resonance.

(3) Introduce new ideas to cross resonances of higher multiplicity.

In case (1), we require the NHIC to be homeomorphic to $T^*\mathbb{T}$ instead of $T^*\mathbb{T}^k$, $k > 1$, mainly because the regularity Theorem 4.1 is only established in the case of $T^*\mathbb{T}$.

C1. ***Choosing the frequency path.*** We describe an algorithm to choose the frequency lines along which the diffusion orbits are constructed.

The diffusing orbit will be constructed along some resonant path in order to utilize the resonant normal form. We design a procedure to construct a frequency path with special hierarchy structure. In the first step we start with a frequency segment of the form

$$\omega_a = \rho_a\left(a,\, \frac{p_2}{q_2}\omega_2^*,\, \frac{p_3}{q_3}\omega_2^*,\, \hat{\omega}_{n-3}^*\right) \in \mathbb{R}^n, \tag{C-1}$$

where $(\omega_2^*, \hat{\omega}_{n-3}^*) = (\omega_2^*, \omega_4^*, \omega_5^*, \dots, \omega_n^*) \in \mathbb{R}^{n-2}$ is a Diophantine vector in $\mathbb{R}^{n-2}$, and a lies in an interval, $p_2/q_2,\, p_3/q_3 \in \mathbb{Q}$ irreducible. For all a, the vector ω_a admits a resonant integer vector $\mathbf{k}_1 = (0, q_2p_3, -q_3p_2, 0, \dots, 0)$. After a linear transform by a matrix in $\mathrm{SL}(n,\mathbb{Z})$, we get $\check{\omega}_a = \rho_a(a, 0, \frac{p}{q}\omega_2^*, \hat{\omega}_{n-3}^*) \in \mathbb{R}^n$. We want to show that a can be moved arbitrarily. More precisely, for any a', $a'' \in \mathbb{R}$ and δ sufficiently small, there is an orbit $(x(t), y(t))$, $t \in [t', t'']$, such that $\omega(y(t))|_{[t',t'']}$ lies in a δ neighborhood of ω_a, $a \in [a', a'']$. The frequency $\check{\omega}_a$ has at most two resonance relations, one of which is always $(0, 1, 0, \ldots, 0)$, so the normal form Proposition 5.2 with either $m = 1$ or $m = 2$ applies.

We first consider region where Proposition 5.2 with $m = 1$ applies. In this case the function V in (5-3) is defined on $\mathbb{T}^1$. Similar to Section 3A and the example after the statement of Proposition 5.2, we see that the system admits a NHIC homeomorphic to $T^*\mathbb{T}^{n-1}$ corresponding to the global max of V. In the case of $m = 2$, the function V is defined on $\mathbb{T}^2$. We can then separate a subsystem of the form (6-1), similar to the example after Proposition 5.2, and apply Theorem 6.1 to it to find a NHIC, which gives rise to a NHIC homeomorphic to $T^*\mathbb{T}^{n-1}$ for the full system slightly away from the strong double resonance.

To proceed, we need the following observations:

(1) The Hamiltonian system restricted to the NHIC is still Hamiltonian with one less degree of freedom.

(2) The hyperbolicity of the NHIC is determined by the nondegeneracy of the global max of the potential V.

(3) The remainder $\delta \mathsf{R}$ can be made as small as we wish.

(4) The normal form Proposition 5.2 with $m = 1$ or 2 holds in a neighborhood U of the frequency segment ω_a. The size of the neighborhood depends on δ.

Using (2) and (3), we choose δ so small that the perturbation $\delta \mathsf{R}$ does not destroy the NHIC constructed above. We then fix δ to proceed to the next step. Using (1), we obtain a Hamiltonian system restricted to the NHIC which is still nearly integrable has $n - 1$ degrees of freedom. Item (4) implies that the restricted Hamiltonian has frequencies (or rotation vectors of Mather sets, more precisely) in a neighborhood of $\rho_a\big(a, \frac{p}{q}\omega_2^*, \hat{\omega}_{n-3}^*\big) \in \mathbb{R}^{n-1}$ which is obtained from $\check{\omega}_a$ by removing the zero entry corresponding to the normal to the NHIC. So we can modify in the neighborhood U the first component ω_4^* of the vector $\hat{\omega}_{n-3}^*$ to a rational multiple of ω_2^*, so that the new frequency segment denoted by $\bar{\omega}_a = \big(a, \frac{p}{q}\omega_2^*, \frac{p_4}{q_4}\omega_2^*, \hat{\omega}_{n-4}^*\big)$ has a similar structure as ω_a so we can repeat the above procedure. Note that the rational $\frac{p_4}{q_4}$ necessarily has large denominator depending on δ. In the original system the means that we modify the frequency segment ω_a to $\omega_a' = \rho_a\big(a, \frac{p_2}{q_2}\omega_2^*, \frac{p_3}{q_3}\omega_2^*, \frac{p_4}{q_4}\omega_2^*, \hat{\omega}_{n-4}^*\big)$ hence introduces a second resonant integer vector $\mathbf{k}_2$ such that $\langle \mathbf{k}_2, \omega_a' \rangle = 0$ for all a. We have $|\mathbf{k}_2| \gg |\mathbf{k}_1|$ (more precisely, as $\delta \to 0$, we have $|\mathbf{k}_1|$ fixed but $|\mathbf{k}_2| \to \infty$) and moreover, the two vectors are not determined at once, instead, after $\mathbf{k}_1$ is determined and δ is fixed, we can then determine $\mathbf{k}_2$ by choosing p_4/q_4.

After $n-3$ steps, the above algorithm gives a final frequency segment of the form

$$\boldsymbol{\omega}_a^\sharp = \rho_a^\sharp\left(a, \frac{p_2}{q_2}, \frac{p_3}{q_3}, \dots, \frac{p_n}{q_n}\right) \in \mathbb{R}^n$$

with a special *hierarchy structure*: for fixed p_i/q_i, we then choose p_{i+1}/q_{i+1} sufficiently close to a Diophantine number $\omega_{i+1}^*/\omega_2^*$. We choose p_{i+1}/q_{i+1} so close to $\omega_{i+1}^*/\omega_2^*$ that the resonance integer vector $\mathbf{k}_i$ has a large norm and the Fourier modes $\Pi_{\mathbf{k}_i} P$ are so small that it does not destroy the NHIC obtained in the previous step applying the theorem of NHIM. Now the frequency vector $\boldsymbol{\omega}_a^\sharp$ has at least $n-2$ resonant integer vectors $\mathbf{k}_i$, $i = 1, 2, \dots, n-2$ with $|\mathbf{k}_i| \ll |\mathbf{k}_{i+1}|$ for all a in an interval. For some a, there might be another resonant vector $\mathbf{k}''$ whose length is comparable to one of $\mathbf{k}_i$. We note that the vectors $\mathbf{k}_i$, $i = 1, \dots, n-2$ are not determined at once, instead, we determine $\mathbf{k}_{i+1}$ after $\mathbf{k}_i$ is fixed.

Suppose we finish moving a and want to move the second component of the frequency vector. The idea is to send a close to a Diophantine number that is much closer than $|p_n/q_n - \omega_n^*/\omega_2^*|$ and start moving p_2/q_2 applying the above algorithm.

Carrying out the above procedure, we get the existence of NHICs outside a small neighborhood of the complete resonance. With the presence of the NHICs, we can consider the system as an *a priori* unstable system and construct diffusing orbit. We thus have the following statement (except part (3)(c) to be explained in the next subsection).

Theorem C.1 [11, Theorem 2.9]. *Let the Hamiltonian system $H = h + \varepsilon P \in C^r(T^*\mathbb{T}^n, \mathbb{R})$, $7 \le r \le \infty$, be as in* (1-1) *restricted to the energy level $E > \min h$. For any $\varrho > 0$, and any M open balls $B_1, \dots, B_M$ of radius ϱ centered on $h^{-1}(E)$, there exist some $\varepsilon_0 > 0$ and an open-dense set $\mathfrak{R} \subset \mathfrak{S}_1$, such that for each $P \in \mathfrak{R}$ there exist ε_P and a residual set $R_P \subset (0, \min\{\varepsilon_P, \varepsilon_0\})$ such that for all $\varepsilon \in R_P$ the following hold*:

(1) *There exists a continuous frequency path $\omega(t)$ with $\partial\beta(\omega(t)) \in \alpha^{-1}(E)$, $t \in [1, M]$ satisfying*:
   (a) $(\partial h)^{-1}(\omega(i)) \cap B_i \neq \varnothing$, $i = 1, 2, \dots, M$.
   (b) *Each point $\omega(t)$ is resonant with multiplicity at least $n-2$. There are finitely many marked points on $\omega(t)$ denoted by $\omega_1, \dots, \omega_m$, where m is independent of ε, that are resonant with multiplicity $n-1$.*

(2) *On the energy level E there are finitely many disjoint C^r normally hyperbolic invariant cylinders homeomorphic to $T^*\mathbb{T} \times \mathbb{T}$.*

(3) *For each ω_i, $i = 1, \dots, m$, there exists $\lambda_i > 0$ such that*:
   (a) *The Mather sets of rotation vectors $\omega(t)$ with $|\omega(t) - \omega_i| \ge \lambda_i\sqrt{\varepsilon}$ for all $i = 1, 2, \dots, m$, lie in the NHICs.*

(b) *Any continuous curve lying in the interior of* $\{\partial\beta(\omega(t)) \mid |\omega(t)-\omega_i| \geq \lambda_i\sqrt{\varepsilon}\} \subset \alpha^{-1}(E)$ *satisfies Theorem 3.1.*

(c) *The two neighboring connected components* $\{\partial\beta(\omega(t)) \mid |\omega(t)-\omega_i| \geq \lambda_i\sqrt{\varepsilon}\} \subset \alpha^{-1}(E)$ *near* $\partial\beta(\omega_i)$ *are c-equivalent.*

Remark C.2. Each marked point corresponds to a strong double resonance point appearing at some step of the reduction of order where there is a resonant integer vector $\mathbf{k}''$ whose length is comparable to some $\mathbf{k}_i$. We avoid getting too close to the double resonance. The reason is that the NHIC, if it exists, has only $C^{1+\alpha}$ smoothness where $\alpha > 0$ can be close to 0 since $|\ln\lambda/\ln\mu|$ can be close to one in Theorem B.2 near the strong double resonant point. The regularity is too low to perform further reduction of order.

C2. ***Crossing the complete resonance.*** In the previous subsection, we have shown how to construct NHICs away from complete resonances. In this section, we show how to cross the complete resonance hence prove part (3)(c) in Theorem C.1. Similar to the case of $n = 3$, the complete resonance causes essential difficulty to construct diffusing orbit in the higher dimensional case.

The normal form near the complete resonance. Applying Proposition 5.2 repeatedly, we derive the following Hamiltonian normal form at the complete resonant frequency $\boldsymbol{\omega}_a^\sharp$; see Section 7.5 of [11]. After a linear transform in $\mathrm{SL}(n,\mathbb{Z})$, we transform $\boldsymbol{\omega}_a^\sharp$ to $(0,\dots,0,\omega_n)$

$$H_{n-1} = \tfrac{1}{\sqrt{\varepsilon}}\omega_n Y_n + \tfrac{1}{2}\langle A_{n-1}Y, Y\rangle + \sum_{i=2}^{n-1}\delta_i V_i(x_1,\dots,x_i) + \delta_n R(x,Y),$$

where $(x,Y)\in T^*\mathbb{T}^n$, $V_i \in C^r$, and $R\in C^{r-2}$. The Hamiltonian has the following properties which originate from the hierarchy structure in the choice of the frequency line in the previous section:

(1) $\delta_{i+1} \ll \delta_i$, $\delta_2 = 1$, *and we have the freedom to choose* δ_{i+1} *as small as we wish once* $\delta_i V_i$ *is fixed, and* V_{i+1} *depends on* δ_{i+1} *but* $\|V_{i+1}\|_{C^r}$ *is uniformly bounded as* $\delta_{i+1}\to 0$*. The number* δ_{i+1} *is chosen so that the* δ_{i+1}*-perturbation does not destroy the NHIC constructed in the previous step whose normal hyperbolicity depends on* δ_i*.*

(2) *The positive definite matrix* A_{n-1} *depends on* δ_i *in the following way: the first* $i\times i$ *block depends only on* $\delta_2,\dots,\delta_i$ *but does not depend on* $\delta_{i+1},\dots,\delta_{n-1}$ *for* $i=2,\dots,n-1$*. Such dependence on* δ_i *appears due to our introduction of the linear symplectic map after applying the normal form.*

We next perform a standard energetic reduction to solve for $Y_n(x, x_n, y)$ as the solution of the equation

$$H_{n-1}(x, x_n, y, Y_n(x, x_n, y)) = E^* > \min \alpha_{H_{n-1}}$$

to arrive at the normal form which is a nonautonomous system with $n + 1/2$ degrees of freedom

$$Y_\delta := -Y_n \tfrac{\omega_n}{\sqrt{\varepsilon}} = \tfrac{1}{2}\langle Ay, y\rangle + \sum_{j=2}^{n-1} \delta_i V_i(x_1, \ldots, x_i) + \delta_n \tilde{R}\big(x, \tfrac{\tau}{\sqrt{\varepsilon}}, y\big), \tag{C-2}$$

where we update the notation $x = (x_1, \ldots, x_{n-1})$, $y = (Y_1, \ldots, Y_{n-1})$, and A denotes an $(n-1) \times (n-1)$ matrix obtained by removing the last row and column in A_{n-1}.

In these coordinates, one case of crossing the complete resonance is to move the frequency $a(1, 0, \ldots, 0) \in \mathbb{R}^{n-1}$ from some positive a to some negative a along an orbit with the obstruction being the zero frequency.

The algorithm of constructing diffusing orbit crossing the complete resonance. For simplicity, we consider the case $n = 4$ and assume $A = \mathrm{Id}_3$. The general case is more complicated and we refer readers to Section 6 of [11] for details. We also discard the term $\delta_4 \tilde{R}$ in Y_δ since it is useless in our argument of passing complete resonance.

Step 1 *The cohomology space picture.* We get the Hamiltonian

$$Y_\delta = \tfrac{1}{2}\|y\|^2 + V(x_1, x_2) + \delta V_3(x_1, x_2, x_3), \quad (x, y) \in T^*\mathbb{T}^3. \tag{C-3}$$

We first study the picture of $\mathbb{F}_0 = \alpha_{Y_\delta}^{-1}(0)$ in $H^1(\mathbb{T}^3, \mathbb{R})$. This has the shape of a big pizza (see Figure 6): $O(1)$ in the c_1, c_2 direction and very tiny $O(\sqrt{\delta})$ in the c_3 direction where $c = (c_1, c_2, c_3) \in H^1(\mathbb{T}^3, \mathbb{R})$, since the hyperbolicity of the hyperbolic fixed point is weak in the x_3, y_3 component. Each NHIC (homeomorphic to $T^*\mathbb{T}^1$) provided by Theorem C.1 corresponds in $H^1(\mathbb{T}^3, \mathbb{R})$ to an open set that we call a channel connected to $\mathbb{F}_0$. The correspondence is in the following sense. Each NHIC consists of hyperbolic periodic orbits in the Mather sets with rotation vectors lying in the frequency line $(a, 0, 0)$, $a \in \mathbb{R} \setminus \{0\}$ and the channels are the images of the frequency line under the map $\partial\beta : H_1(\mathbb{T}^3, \mathbb{R}) \to H^1(\mathbb{T}^3, \mathbb{R})$. One case of crossing the complete resonance is to find an orbit shadowing Mather sets with rotation vectors $(a, 0, 0)$ and $(-a, 0, 0)$, $a \neq 0$. Note that the picture of the pizza and channels is centrally symmetric since the system Y_δ is reversible (invariant under the change $y \to -y$). Our goal is to move the cohomology class c from one channel to another, hence by symmetry $c \to -c$. We have the following algorithm.

Step 2 ***a priori** unstable dynamics and center-straightening.* The NHIC provided by Theorem C.1 is obtained in the following way. First, since the subsystem $\mathsf{G} = \frac{1}{2}(y_1^2 + y_2^2) + V(x_1, x_2)$ has two degrees of freedom, we apply Theorem 6.1 to get a NHIC foliated by action minimizing periodic orbits in the homology class $g = (1, 0) \in H_1(\mathbb{T}^2, \mathbb{Z})$. Moreover, action-angle coordinates (θ, I) on the cylinder can be introduced to reduce the subsystem to a system $\tilde{h}(I)$ of one degree of freedom restricted to the NHIC. This reduces the Hamiltonian Y_δ to the form

$$\overline{Y}_\delta = \tilde{h}(I) + \tfrac{1}{2}y_3^2 + \delta Z(\theta, I, x_3), \quad (\theta, I, x_3, y_3) \in T^*\mathbb{T}^1 \times \mathbb{R}^2,$$

to which we can apply Theorem 6.1 again to get a NHIC foliated by action minimizing periodic orbits in the homology class $g = (1, 0) \in H_1(\mathbb{T}^2, \mathbb{Z})$. This gives the NHIC in Theorem C.1. Recovering the $\delta_4 \tilde{R}$ perturbation, diffusing orbits can be constructed moving along the NHIC (channel in $H^1(\mathbb{T}^3, \mathbb{R})$) up to a $o_{\delta_4 \to 0}(1)$-neighborhood of the pizza using the method of *a priori* unstable systems.

Step 3 *The cohomology equivalence.* As a result of the previous step, we have arrived at a neighborhood of the pizza where the cohomology class $c = (c_1, c_2, c_3)$ satisfies $\alpha_{\mathsf{G}}(c_1, c_2) \in (0, \Delta)$ and c_3 close to zero; see Theorem 6.3 for the definition of Δ. We now view the system Y_δ as a small perturbation of the subsystem G. By Theorem 6.3 and the upper-semicontinuity of the Mañé set, for small enough δ, the Mañé set $\tilde{\mathcal{N}}(c)$ when projected to $\mathbb{T}^2 (\ni (x_1, x_2))$ does not cover $\mathbb{T}^2$. We apply the c-equivalence mechanism (Theorem 3.3) to get that the cohomology class (c_1, c_2, c_3) is c-equivalent to $(-c_1, -c_2, c_3)$.

Step 4 *The ladder climbing.* Here comes an intrinsic problem due to the high dimensionality. The two channels are *centrally symmetric* due to the reversibility of the mechanical system. Namely, the projection of the two channels to the c_3 coordinate axis, may not overlap. So for $c = (c_1, c_2, c_3)$ in one channel, the point $(-c_1, -c_2, c_3)$ does not lie in the opposite channel. We have to find a way to change c_3 to $-c_3$. The idea is to notice that restricting the system Y_δ to the NHIC (homeomorphic to $T^*\mathbb{T}^2$) obtained by applying Theorem 6.1 to G, we get $\overline{Y}_\delta$. The center manifold which is the phase space of $\overline{Y}_\delta$, has stable and unstable manifolds hence we are in a situation similar to Arnold's example. Restricted to an energy level of the system Y_δ, the energy of the subsystem $\overline{Y}_\delta$ is also fixed, so we get a curve $\alpha_{\overline{Y}_\delta}(c)$ =const in $H^1(\mathbb{T}^2, \mathbb{R})$. Along this curve, we can move c_3 significantly by Arnold's mechanism, so we send

$$(-c_1, -c_2, c_3) \to (-c_1, -c_2, -c_3).$$

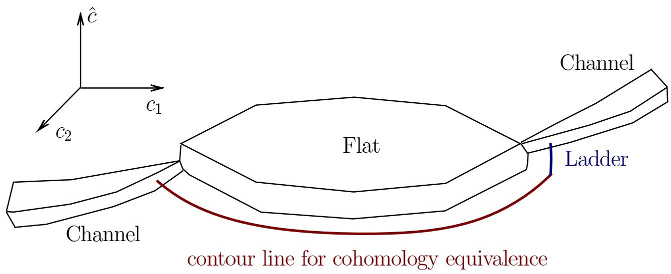

Figure 6. Turning around complete resonance Channel:NHIC; Red:c-equivalence; Blue:ladder.

To see the last mechanism clearly, we modify Arnold's Hamiltonian slightly to yield

$$H = \frac{y_1^2}{2} + \frac{y_2^2}{2} + \frac{y_3^2}{2} + (\cos x_3 - 1)(1 + \varepsilon(\cos x_1 + \sin x_2)).$$

In this system, for each $E > 0$ there exists diffusing orbit along which (y_1, y_2) moves arbitrarily on the circle $\{y_1^2 + y_2^2 = 2E\}$. In our case, the system Y_δ plays the role of H here and the subsystem $\overline{Y}_\delta$ plays the role of $\frac{1}{2}(y_1^2 + y_2^2)$ which lies on the NHIM $\{x_3 = y_3 = 0\}$.

As in the case of *a priori* unstable systems, we need a regularity result similar to Theorem 4.1 to show that the barrier functions $\overline{B}_c(x)$ of the system $\overline{Y}_\delta$ for $\alpha_{\overline{Y}_\delta}(c)$ =constant can be parametrized into a Hölder family. This is proved in [12].

We complete the sketch of the proof here and refer interested readers to [11] for more details.

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chengcq@nju.edu.cn — *School of Mathematical Sciences, Nanjing Normal University, Nanjing, China*

jxue@tsinghua.edu.cn — *Department of Mathematical Sciences, Tsinghua University, Beijing, China*

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Viscosity solutions of the Hamilton–Jacobi equation on a noncompact manifold

ALBERT FATHI

We study the continuous viscosity solutions of the evolutionary Hamilton–Jacobi equation

$$\partial_t U(t,x) + H(x, \partial_x U(t,x)) = 0,$$

on $[0,+\infty[\, \times M$, where H is a Tonelli Hamiltonian on the noncompact manifold M. We establish that all such solutions are given by the Lax–Oleinik formula. Moreover, we show that a finite everywhere Lax–Oleinik evolution is necessarily continuous and a viscosity solution on $]0,+\infty[\, \times M$.

The goal is also to provide a convenient reference for the evolutionary Hamilton–Jacobi equation for Tonelli Hamiltonians on noncompact manifolds.

1. Introduction

This work was started in February 2017 in Rome, following a conversation with Piermarco Cannarsa, Andrea Davini, Antonio Siconolfi and Afonso Sorrentino. We discussed the problem of the Lax–Oleinik evolution $\hat{u}$ (see Definition 8.2) of a continuous function u on a noncompact manifold. Although on a compact manifold, it was known that the Lax–Oleinik evolution of a continuous function is always locally concave and a solution of the Hamilton–Jacobi equation in evolution form, at that moment, the situation on a noncompact manifold was not clear, even assuming the continuity of the Lax–Oleinik evolution. The main problem was that it was not clear that the inf in Definition 8.2 of $\hat{u}$ was attained. After about a month, to my astonishment, I realized that no condition beyond finiteness was necessary; see Theorem 1.1.

This brought back the problem of uniqueness of a solution of the Hamilton–Jacobi equation in evolution form given an initial condition. In May 2016 in

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Shanghai, Kaizhi Wang, Lin Wang and Jun Yan, while discussing [11], brought to my attention that, contrary to my belief, the uniqueness of a continuous solution of the Hamilton–Jacobi equation in evolution form given an initial condition on a noncompact manifold was not known at that time (and therefore the Lax–Oleinik formula could not be established) unless the solution was uniformly continuous. The best results on this problem were those contained, for example, in Hitoshi Ishii's lecture notes [10], on whose methods this present work heavily relies. The difficulty here is that the maximum principle could not be applied directly, since it requires some compactness. In 2018 and 2019, I was able to show directly the Lax–Oleinik formula for arbitrary continuous solutions (see Theorem 1.2) and therefore I obtained the uniqueness as a consequence.

Beyond the new results mentioned above, the goal of this work is to provide a convenient reference for the *evolutionary* Hamilton–Jacobi equation

$$\partial_t U + H(x, \partial_x U) = 0$$

for a Tonelli Hamiltonian H on a *possibly noncompact* manifold, thus extending the results of the survey [7].

We will assume that the reader is familiar with [7], which is well adapted to our manifold setting. Other classic treatments of viscosity solutions of the Hamilton–Jacobi equation are [2; 1].

We consider a ***connected*** manifold M endowed with a ***complete*** Riemannian metric. We will denote by $\|\cdot\|_x$ the induced norm on either T_xM or T_x^*M, the fibers above x of the tangent TM or cotangent T^*M bundle of M. We will denote by d the Riemannian distance on M obtained from the Riemannian metric. It might be useful to recall that, due to the completeness of the Riemannian metric, bounded sets for d are relatively compact. Therefore the distance d is also complete.

We endow $\mathbb{R} \times M$, $\mathbb{R} \times M \times M$, and $M \times M$ with the product Riemannian metrics, and Riemannian distances, where the Riemannian metric on $\mathbb{R}$ is the usual one.

Throughout the paper $H : T^*M \to \mathbb{R}$ will denote a continuous function which we will call the Hamiltonian.

We will study (continuous) viscosity subsolutions, supersolutions and solutions of the evolutionary Hamilton–Jacobi equation

$$\partial_t U(t, x) + H(x, \partial_x U(t, x)) = 0, \tag{1-1}$$

on a subset of $\mathbb{R} \times M$.

In fact, the main results of this work will be proved for Tonelli Hamiltonians (Definition 3.1). The statements use the (negative) Lax–Oleinik semigroup T_t^-, $t \geq 0$ (see Definition 8.1).

The main results are given in the next two theorems.

Theorem 1.1. *Assume* $u : M \to [-\infty, \infty]$ *is a function such that its Lax–Oleinik evolution* $\hat{u} : [0, +\infty[\times M \to [-\infty, +\infty]$, $(t, x) \mapsto T_t^- u(x)$ *is finite at some point* (T, X), *with* $T > 0$ *and* $X \in M$. *Then the function* $\hat{u}$ *is continuous and even locally semiconcave on* $]0, T[\times M$. *Moreover*, *the function* $\hat{u}$ *is a viscosity solution of the evolutionary Hamilton–Jacobi equation* (1-1) *on* $]0, T[\times M$.

Note that we do not assume any continuity property on u. As we already said the result above is surprising, even when u is continuous.

Theorem 1.2. *Suppose* $H : T^*M \to \mathbb{R}$ *is a Tonelli Hamiltonian. Assume that*, *for some* $T > 0$ *the function* $U :]0, T[\times M \to \mathbb{R}$ *is a continuous viscosity solution of the evolutionary Hamilton–Jacobi equation* (1-1). *Define* $u : M \to [-\infty, \infty]$ *by*

$$u(x) = \liminf_{t \to 0} U(t, x).$$

Then $U = \hat{u}$ *on* $]0, T[\times M \to \mathbb{R}$, *where* $\hat{u} : [0, +\infty[\times M \to [-\infty, +\infty]$, $(t, x) \mapsto T_t^- u(x)$ *is the Lax–Oleinik evolution of* u.

Obviously, Theorem 1.2 implies that continuous viscosity solutions of the evolutionary Hamilton–Jacobi equation (1-1) satisfy the Lax–Oleinik formula and also the uniqueness given a continuous boundary condition on $\{0\} \times M$.

Remark 1.3. (1) Discussions in June 2019 in Rome, with A. Davini, Hitoshi Ishii and Antonio Siconolfi pointed to the fact that the results above hold true even if H is not C^2, but still satisfies the other Tonelli conditions see 3.1.

(2) The method of this work does not allow to extend the results to the case when H is time-dependent. For example, the proof of Proposition 2.2 is not adaptable to the time-dependent case.

2. Approximation by Lipschitz subsolutions

We will assume in this section that $H : T^*M \to \mathbb{R}$ is a continuous function, which we will call the Hamiltonian. Our goal is to show that we can approximate locally continuous viscosity subsolutions of the evolutionary Hamilton–Jacobi equation (1-1) with U defined on an open subset of $\mathbb{R} \times M$ by Lipschitz viscosity subsolutions, under a coercivity condition on H.

These results are well-known when M is the Euclidean space (see Hitoshi Ishii's lectures [10] for example), but the arguments in [10] can easily be adapted to the manifold setting as we now proceed to do.

2.1. ***Sup-convolution in one variable.*** The usefulness of sup-convolution to improve regularity of viscosity subsolutions is already well established. As said above, our treatment in this section follows closely [10] which dealt with the Euclidean space case.

Let $u : V \to \mathbb{R}$, be a continuous function, where V is an open subset of $\mathbb{R} \times M$. Assume $K \subset V$ is compact subset. By continuity of u and compactness of K, we can find an open subset $O_1 \subset V$, with $K \subset O_1$, such that

$$m = \sup_{O_1} |u| < +\infty. \tag{2-1}$$

Again by compactness of K, we can find $\delta > 0$ and an open neighborhood $O_2 \subset O_1$ of K, with compact closure $\bar{O}_2 \subset O_1$, and such that $[t-\delta, t+\delta] \times \{x\} \subset O_1$, for every $(t, x) \in \bar{O}_2$.

For $\epsilon > 0$, we define $u_\epsilon : \bar{O}_2 \to \mathbb{R}$ by

$$u_\epsilon(t, x) = \max_{s \in [-\delta, +\delta]} u(t+s, x) - \frac{s^2}{\epsilon}. \tag{2-2}$$

Note that u_ϵ is continuous by continuity of u and compactness of $[-\delta, +\delta]$.

We summarize the properties of u_ϵ in the following proposition.

Proposition 2.1. (1) *For every $\epsilon > 0$, we have $u_\epsilon \geq u$.*

(2) *For every $0 < \epsilon < \epsilon'$, we have $u_\epsilon < u_{\epsilon'}$.*

(3) *If $(t, x) \in \bar{O}_2$, and $s_\epsilon \in [-\delta, +\delta]$ is such that $u_\epsilon(t, x) = u(t+s_\epsilon, x) - (s_\epsilon)^2/\epsilon$, then $|s_\epsilon| \leq \sqrt{2\epsilon m}$, where m is given by* (2-1).

(4) *For every $(t, x) \in \bar{O}_2$, we have $u_\epsilon(t, x) \to u(t, x)$, when $\epsilon \to 0$. The convergence is uniform on $\bar{O}_2$.*

(5) *If $\sqrt{2\epsilon m} < \delta$, for each $(t, x), (t', x) \in \bar{O}_2$, with $|t - t'| < \delta - \sqrt{2\epsilon m}$, we have*

$$|u_\epsilon(t', x) - u_\epsilon(t, x)| \leq \frac{2\sqrt{2\epsilon m} + |t - t'|}{\epsilon} |t - t'| \leq \frac{\sqrt{2\epsilon m} + \delta}{\epsilon} |t - t'|.$$

Moreover, if $\sqrt{2\epsilon m} < \delta$, for every $x \in M$, the map $t \mapsto u_\epsilon(t, x)$ is Lipschitz on every connected component of $O_2 \cap \{x\} \times \mathbb{R}$ with Lipschitz constant $\leq 2\sqrt{2m/\epsilon}$.

Proof. Parts (1) and (2) are obvious. For part (3), we notice that

$$u_\epsilon(t, x) = u(t+s_\epsilon, x) - (s_\epsilon)^2/\epsilon \geq u(t, x).$$

Therefore

$$(s_\epsilon)^2/\epsilon \leq u(t+s_\epsilon, x) - u(t, x) \leq 2 \sup_{O_1} |u| = 2m.$$

For part (4), note that by part (3), we have

$$\sup_{(x,t)\in\bar{O}_2} |u_\epsilon(t,x)-u(t,x)| \le \sup\bigl\{|u(t+s,x)-u(t,x)| \bigm| (t,x)\in\bar{O}_2,\ |s|\le\sqrt{2\epsilon m}\bigr\}.$$

By compactness of $\bar{O}_2$ and continuity of u, the right hand side of the inequality above tends uniformly on $\bar{O}_2$ to 0 as $\epsilon\to 0$.

For (5), we choose s_ϵ such that $u_\epsilon(t,x)=u(t+s_\epsilon,x)-(s_\epsilon)^2/\epsilon$. By (3), we have $|s_\epsilon|\le\sqrt{2\epsilon m}$. Therefore, we get

$$|s_\epsilon+t-t'|\le|s_\epsilon|+|t-t'|\le\sqrt{2\epsilon m}+\delta-\sqrt{2\epsilon m}=\delta.$$

Therefore, by the definition of u_ϵ, we obtain

$$u_\epsilon(t',x)\ge u(t'+(s_\epsilon+t-t'),x)-\frac{(s_\epsilon+t-t')^2}{\epsilon}=u(t+s_\epsilon,x)-\frac{(s_\epsilon+t-t')^2}{\epsilon}.$$

Subtracting this inequality from the equality $u_\epsilon(t,x)=u(t+s_\epsilon,x)-(s_\epsilon)^2/\epsilon$ yields

$$\begin{aligned}
u_\epsilon(t,x)-u_\epsilon(t',x) &\le \frac{(s_\epsilon+t-t')^2}{\epsilon}-\frac{(s_\epsilon)^2}{\epsilon}\\
&= \frac{(2s_\epsilon+t-t')(t-t')}{\epsilon}\\
&\le \frac{2|s_\epsilon|+|t-t'|}{\epsilon}|t-t'|\\
&\le \frac{2\sqrt{2\epsilon m}+|t-t'|}{\epsilon}|t-t'|,
\end{aligned}$$

where we used $|s_\epsilon|\le\sqrt{2\epsilon m}$, for the last inequality. By symmetry, we obtain

$$|u_\epsilon(t',x)-u_\epsilon(t,x)|\le\frac{\sqrt{2\epsilon m}+|t-t'|}{\epsilon}|t-t'|. \tag{2-3}$$

Assume t, t', x are such that $[t,t']\times\{x\}\subset O_2$. For every $\eta\in\,]0,\delta-\sqrt{2\epsilon m}[$, we can pick a monotone sequence $t=t_0,t_1,\dots,t_n=t'$, with $|t_{i+1}-t_i|\le\eta$, by applying (2-3) for t_i, t_{i+1} instead of t, t', and adding the inequalities, we obtain

$$|u_\epsilon(t',x)-u_\epsilon(t,x)|\le\frac{2\sqrt{2\epsilon m}+\eta}{\epsilon}|t-t'|.$$

We can then let $\eta\to 0$, to conclude that

$$|u_\epsilon(t',x)-u_\epsilon(t,x)|\le\frac{2\sqrt{2\epsilon m}}{\epsilon}|t-t'|. \qquad \square$$

Proposition 2.2. *Let $H: T^*M\to\mathbb{R}$ be a continuous Hamiltonian. Suppose $u: V\to\mathbb{R}$ is a continuous function, defined on the open subset $V\subset\mathbb{R}\times M$,* *which is a viscosity subsolution on V of the evolutionary Hamilton–Jacobi equation* (1-1).

Then, for every compact subset $K \subset V$, we can find a sequence of continuous functions $\hat{u}_n : K \to \mathbb{R}$ such that $\hat{u}_n \to u$ uniformly on K and, for all n except a finite number, the function $\hat{u}_n$ is a viscosity subsolution on the interior $\mathring{K}$ of K, not only of the evolutionary Hamilton–Jacobi equation (1-1), *but also of*

$$|\partial_t u(t,x)| + H(x, \partial_x u(t,x)) = C\sqrt{n}, \tag{2-4}$$

for some $C < +\infty$ independent of n. In particular, if H is coercive above each compact subset of M, then each $\hat{u}_n$ is locally Lipschitz on $\mathring{K}$.

Proof. We choose O_1, m, δ, and $O_2 \supset K$ like it is done above in the beginning of Proposition 2.1. We set $\hat{u}_n = u_{1/n} : O_2 \to \mathbb{R}$, where $u_{1/n}$ is defined by (2-2) with $\epsilon = 1/n$. Hence

$$\hat{u}_n(t,x) = \min_{s\in[-\delta,+\delta]} u(x,+s) - ns^2.$$

By part (4) of Proposition 2.1, we get the uniform convergence of $\hat{u}_n$ to u.

We pick an integer n_0 such that $\sqrt{2m/n_0} < \delta$. We now check the fact that $\hat{u}_n$ is a viscosity subsolution of both Hamilton–Jacobi equations on O_2, for all $n \geq n_0$. Assume $(t_0, x_0) \in O_2$, and that $\varphi : V \to \mathbb{R}$ is C^1 is such that $\hat{u}_n \leq \varphi$ with equality at (t_0, x_0). Since $\sqrt{2m/n} \leq \sqrt{2m/n_0} < \delta$, by Proposition 2.1(5), we know that $t \mapsto \hat{u}_n(x,t)$ is locally Lipschitz with local Lipschitz constant $\leq 2\sqrt{2mn}$. This implies

$$|\partial_t \varphi(t_0, x_0)| \leq 2\sqrt{2mn}. \tag{2-5}$$

We now choose $s_n \in [-\delta, +\delta]$ such that

$$u(t_0 + s_n, x_0) - ns_n^2 = \hat{u}_n(t_0, x_0) = \varphi(t_0, x_0).$$

For s small enough and y close to x_0, we have $(t_0 + s, y) \in O_2$. Therefore, since $s_n \in [-\delta, +\delta]$, by the definition of $\hat{u}_n$, for s small enough and y close to x_0, we get

$$u(t_0 + s + s_n, y) - ns_n^2 \leq \hat{u}_n(t_0 + s, y) \leq \varphi(t_0 + s, y).$$

Subtracting from this inequality the equality $u(t_0 + s_n, x_0) - ns_n^2 = \varphi(t_0, x_0)$, we get

$$u(y, t_0 + s + s_n) - u(t_0 + s_n, x_0) \leq \varphi(t_0 + s, y) - \varphi(t_0, x_0).$$

Since u is a viscosity subsolution on $O_1 \ni (t_0 + s_n, x_0)$, of (1-1), we must have

$$\partial_t \varphi(t_0, x_0) + H(x_0, \partial_x \varphi(t_0, x_0)) \leq 0. \tag{2-6}$$

Therefore $\hat{u}_n$ is a viscosity subsolution of (1-1). Using the inequalities (2-5) and (2-6), we also obtain

$$|\partial_t\varphi(t_0, x_0)| + H(x_0, \partial_x\varphi(t_0, x_0)) \le 4\sqrt{2mn}.$$

Therefore $\hat{u}_n$ is a viscosity solution of (2-4) with $C = 4\sqrt{2m}$. □

Corollary 2.3. *Let $H : T^*M \to \mathbb{R}$ be a continuous Hamiltonian that is coercive above each compact subset of M and convex in the momentum p; i.e., for each $x \in M$, the map $T_x^*M \to \mathbb{R}, p \mapsto H(x, p)$ is convex. Let $u : V \to \mathbb{R}$ be a continuous functions defined on the open subset $V \subset \mathbb{R} \times M$ which is a viscosity subsolution of the evolutionary Hamilton–Jacobi equation* (1-1).

For every open set $V' \subset V$ whose closure $\bar{V}'$ is compact and contained in V, we can approximate uniformly u on V' by a C^∞ subsolution of the evolutionary Hamilton–Jacobi equation (1-1).

Proof. By Proposition 2.2 above, we can make a first approximation by a subsolution $u_1 : V' \to \mathbb{R}$ of (1-1) that is locally Lipschitz on V'. The function $u_2 : V' \to \mathbb{R}, (t, x) \to u_1(t, x) - \epsilon t$ is therefore a locally Lipschitz viscosity subsolution of

$$\partial_t v + H(x, \partial_x v) = -\epsilon.$$

Note also that the variable t is bounded on the compact subset $\bar{V}'$ of $\mathbb{R} \times M$. Therefore, by choosing appropriately ϵ, we can assume u_2 uniformly as close to u_1 as we wish. We can now consider the Hamiltonian $\bar{H} : T^*(\mathbb{R} \times M)$ defined by

$$\bar{H}(t, s, x, p) = s + H(x, p),$$

where we use the identification $T^*(\mathbb{R} \times M) = T^*\mathbb{R} \times T^*M = \mathbb{R} \times \mathbb{R} \times T^*M$. The function u_2 is a locally Lipschitz viscosity subsolution of

$$\bar{H}(t, x, d_{(t,x)}v(t, x)) = -\epsilon.$$

The Hamiltonian $\bar{H}$ is convex in the momentum (s, p). We can now invoke [7, Theorem 10.6, page 1219] to approximate uniformly u_2 on V' by a C^∞ viscosity subsolution $u_3 : V' \to \mathbb{R}$ of

$$\bar{H}(t, x, d_{(t,x)}vu(t, x)) = 0.$$

This means that u_3 is both a uniform approximation of u and a viscosity subsolution of the evolutionary Hamilton–Jacobi equation (1-1). □

Corollary 2.4. *Let $H : T^*M \to \mathbb{R}$ be a continuous Hamiltonian that is coercive above each compact subset of M and convex in the momentum p; i.e., for each $x \in M$, the map $T_x^*M \to \mathbb{R}, p \mapsto H(x, p)$ is convex. If $u_1 : V \to \mathbb{R}$ and*

$u_2 : V \to \mathbb{R}$ are continuous functions defined on the open subset $V \subset \mathbb{R} \times M$ which are viscosity subsolutions of

$$\partial_t v + H(x, \partial_x v) = 0, \tag{2-7}$$

then $u = \min(u_1, u_2)$ is also a viscosity subsolution on V of (2-7).

Proof. Since H is convex, the corollary is well known when u_1 and u_2 are locally Lipschitz. In fact, since u_1 and u_2 are locally Lipschitz, they are differentiable almost everywhere and satisfy for almost every $(t, x) \in V$, the inequalities

$$\partial_t u_1(t, x) + H(x, \partial_x u_1(t, x)) \leq 0 \text{ and } \partial_t u_2(t, x) + H(x, \partial_x u_2(t, x)) \leq 0.$$

But the subset $D \subset V$ where the three locally Lipschitz functions u, u_1, u_2 are differentiable is of full measure and, for every $(t, x) \in D$, we have either $d_{(t,x)}u = d_{(t,x)}u_1$ or $d_{(t,x)}u = d_{(t,x)}u_2$. Therefore, $\partial_t u(t, x) + H(x, \partial_x u_(t, x)) = 0$ almost everywhere on V. Since the Hamiltonian $\bar{H}(t, x, s, p) = s + H(x, p)$ is convex in (t, p) by [7, Theorem 10.2, page 1217], we conclude that $u = \min(u_1, u_2)$ is also a viscosity subsolution on V of (2-7), when both u_1 and u_2 are locally Lipschitz.

The result for general continuous functions follows from this locally Lipschitz case and the stability of viscosity solutions (see [7, Theorem 6.1, page 1209], for example) using the approximation result obtained in Proposition 2.2. □

Corollary 2.5. *Let $H : T^*M \to \mathbb{R}$ be a continuous Hamiltonian that is coercive above each compact subset of M and convex in the momentum p; i.e., for each $x \in M$, the map $T_x^*M \to \mathbb{R}$, $p \mapsto H(x, p)$ is convex. Suppose the family of functions $u_i : V \to M$, $i \in I$, where $V \subset \mathbb{R} \times M$ is an open subset, is such that its infimum $u = \inf_{i \in I} u_i$ is continuous and everywhere finite on V. If each u_i, $i \in I$ is a viscosity subsolution* (*resp. solution*) *of the evolutionary Hamilton–Jacobi*

$$\partial_t v + H(x, \partial_x v) = 0. \tag{2-8}$$

on V, then u is also a viscosity subsolution (*resp. solution*) *of the evolutionary Hamilton–Jacobi* (2-8) *on V.*

Proof. Since the space of continuous functions $\mathcal{C}(V, \mathbb{R})$ endowed with the compact-open topology is metric and separable, we can find a sequence $(i_n)_{n \in \mathbb{N}}$, with $i_n \in I$, such that the sequence $(u_{i_n})_{n \in \mathbb{N}}$ is dense in the subset $\{u_i \mid i \in I\} \subset \mathcal{C}(V, \mathbb{R})$ for the compact open topology. Therefore

$$u = \inf_{i \in I} u_i = \inf_{n \in \mathbb{N}} u_{i_n}.$$

For $m \in \mathbb{N}$, let us define $U_m : V \to \mathbb{R}$ by

$$U_m = \min_{0 \leq n \leq m} u_{i_n}.$$

If each u_i, $i \in I$ is a viscosity subsolution of (2-8) on V, Corollary 2.4 implies that each U_m is also a subsolution of (2-8) on V. Note that U_m is nonincreasing in m and $U_m \searrow u$. Since we are assuming that u is finite and continuous on V, by Dini's theorem, the nonincreasing convergence $U_m \searrow u$ is uniform on every compact subset of V. Therefore by the stability theorem for viscosity solutions, the function u is a viscosity solution of (1-1) on V.

If each u_i, $i \in I$ is a viscosity solution of (2-8) on V, then $u = \inf_{i \in I} u_i$ is a supersolution of (2-8) on V; see for example [7, Proposition 8.1, page 1213]. □

2.2. *Maximum principle.*

Theorem 2.6 (maximum principle). *Let $H : T^*M \to \mathbb{R}$ be a Hamiltonian that is continuous, coercive above each compact subset of M and convex in the momentum p. For $a < b \in \mathbb{R}$ and $K \subset M$ a compact subset, if the continuous functions $u, v : [a, b] \times K \to \mathbb{R}$ are respectively a subsolution and a supersolution of the evolutionary Hamilton–Jacobi equation* (1-1) *on $]a, b[\times \mathring{K}$ then the maximum of $u - v$ on $[a, b] \times K$ is achieved on $[a, b] \times \partial K \cup \{a\} \times K$. Therefore*

$$\max_{[a,b]\times K} u - v = \max_{[a,b]\times\partial K\cup\{a\}\times K} u - v.$$

Proof. It is not difficult to see that by the approximation result of Proposition 2.2, we can assume u locally Lipschitz in $\mathring{K} \times]a, b[$. As usual, for $\epsilon, \delta > 0$, we introduce the function $u_{\epsilon,\delta} : [a, b[\times K \to \mathbb{R}$ by

$$u_{\epsilon,\delta}(t, x) = u(t, x) - \epsilon(t - a) - \frac{\delta}{b - t}.$$

Note that $u_{\epsilon,\delta} \le u$ and that $u_{\epsilon,\delta}(t, x) \to -\infty$ as $t \to b$, uniformly in $x \in K$. Since $t \mapsto -\epsilon(t - a) - \delta/(b - t)$ is C^1, with derivative $t \mapsto -\epsilon - \delta/(b - t)^2 \le -\epsilon$, the function $u_{\epsilon,\delta}$ is a viscosity subsolution of

$$\partial_t u_{\epsilon,\delta} + H(x, \partial_x u_{\epsilon,\delta}) = -\epsilon, \tag{2-9}$$

on $]a, b[\times \mathring{K}$. Therefore by the doubling of variables argument (see [7, Theorem 7.1, page 1210], for example), using that $u_{\epsilon,\delta}$ is locally Lipschitz on $]a, b[\times \mathring{K}$, we conclude that $u_{\epsilon,\delta} - v$ cannot have a local maximum in $]a, b[\times \mathring{K}$. Since $u_{\epsilon,\delta}(t, x) \to -\infty$ as $t \to b$, the function $u_{\epsilon,\delta} - v$ attains its maximum at a point in $[a, b[\times \partial K \cup \{a\} \times K$. Using that $u_{\epsilon,\delta} \le u$, we obtain

$$u_{\epsilon,\delta} - v \le \max_{[a,b]\times\partial K\cup\{a\}\times K} u - v$$

on $K \times [a, b[$. Letting $\delta, \epsilon \to 0$, we obtain $u - v \le \max_{[a,b]\times\partial K\cup\{a\}\times K} u - v$ on $K \times [a, b[$. Continuity of both u and v yields

$$\max_{K\times[a,b]} u - v \le \max_{[a,b]\times\partial K\cup\{a\}\times K} u - v. \qquad \square$$

For viscosity solutions, we obtain:

Corollary 2.7. *Let $H : T^*M \to \mathbb{R}$, $(x, p) \mapsto H(x, p)$ Hamiltonian that is continuous, coercive above each compact subset of M and convex in the momentum p. For $a < b \in \mathbb{R}$ and $K \subset M$ a compact subset, assume that the two continuous functions $u, v : [a, b] \times K \to \mathbb{R}$ are viscosity solutions of the evolutionary Hamilton–Jacobi equation* (1-1) *on $]a, b[\times \mathring{K}$. If $u = v$ on $[a, b] \times \partial K \cup \{a\} \times K$, then $u = v$ on $[a, b] \times K$.*

3. Tonelli Hamiltonians and their Lagrangians

Definition 3.1. A Tonelli Hamiltonian H on the complete Riemannian manifold (M, g) is a function $H : T^*M \to \mathbb{R}$ satisfying the following conditions:

(1*) The function H is C^2.

(2*) (uniform superlinearity) For every $K \geq 0$, we have

$$C^*(K) = \sup_{(x,p)\in T^*M} K\|p\|_x - H(x, p) < \infty.$$

(3*) (uniform boundedness in the fibers) For every $R \geq 0$, we have

$$A^*(R) = \sup\{H(x, p) \mid \|p\| \leq R\} < +\infty.$$

(4*) (C^2 strict convexity in the fibers) For every $(x, p) \in T^*M$, the second derivative along the fibers, $\partial^2 H/\partial p^2(x, p)$, is (strictly) positive definite.

Note that both A^* and C^* are nondecreasing functions, and that (2*) implies

$$\forall (x, p) \in T^*M,\ H(x, p) \geq K\|p\| - C^*(K).$$

If M is compact, the third condition is automatically satisfied, and the second condition is equivalent to

$$\frac{H(x, p)}{\|p\|_x} \to +\infty \quad \text{as } \|p\|_x \to +\infty.$$

We thus recover the usual definition of a Tonelli Hamiltonian in the case of M compact.

We note that the uniform superlinearity implies that a Tonelli Hamiltonian is coercive.

We should emphasize that, in the noncompact case, the Tonelli condition depends on the choice of the complete Riemannian metric on M.

Example 3.2. (1) The easiest example of a Tonelli Hamiltonian is $H_0 : T^*M \to \mathbb{R}$ defined by

$$H_0(x, p) = \tfrac{1}{2}\|p\|_x^2.$$

In fact, in this case,

$$\begin{aligned}
A_0^*(R) &= \sup\{H_0(x,p) \mid \|p\|_x \le R\} = \tfrac{1}{2}R^2,\\
C_0^*(K) &= \sup_{(x,p)\in T^*M} K\|p\|_x - H_0(x,p) = \sup_{(x,p)\in T^*M} K\|p\|_x - \tfrac{1}{2}\|p\|_x^2 = \tfrac{1}{2}K^2.
\end{aligned}$$

(2) Let $V : M \to \mathbb{R}$ be a C^2 function and let $X : M \to TM$ be a C^2 vector field on M. We define the Hamiltonian $H_{X,V} : T^*M \to \mathbb{R}$ by

$$H_{X,V}(x,p) = \tfrac{1}{2}\|p\|_x^2 + p(X(x)) + V(x).$$

For every $x \in M$, we have

$$\sup_{\substack{p\in T_x^*M\\ \|p\|_x=R}} H_{X,V}(x,p) = \tfrac{1}{2}R^2 + R\|X(x)\|_x + V(x).$$

Therefore

$$A_{X,V}^*(R) = \tfrac{1}{2}R^2 + \sup_{x\in M}(R\|X(x)\|_x + V(x)).$$

In particular, we get

$$A_{X,V}^*(0) = \sup_{x\in M} V(x) \text{ and } \sup_{x\in M}\|X(x)\|_x + \inf_{x\in M} V(x) \le A_{X,V}^*(1).$$

For every $x \in M$, we have

$$\begin{aligned}
\sup_{\substack{p\in T_x^*M\\ \|p\|_x=R}} K\|p\|_x - H_{X,V}(x,p) &= \sup_{\substack{p\in T_x^*M\\ \|p\|_x=R}} K\|p\|_x - \tfrac{1}{2}\|p\|_x^2 - p(X(x)) - V(x)\\
&= KR - \tfrac{1}{2}R^2 + R\|X(x)\|_x - V(x).
\end{aligned}$$

Therefore, for every $x \in M$, we have

$$\sup_{p\in T_x^*M} K\|p\|_x - H_{X,V}(x,p) = \tfrac{1}{2}(K + \|X(x)\|_x)^2 - V(x),$$

and

$$C_{X,V}^*(K) = \sup_{x\in M} K\|p\|_x - H_{X,V}(x,p) = \sup_{x\in M} \tfrac{1}{2}(K + \|X(x)\|_x^2) - V(x).$$

In particular, we get $-\inf_{x\in M} V(x) \le C_{X,V}^*(0)$. Therefore, the Hamiltonian $H_{X,V}$ is Tonelli if and only if $\|V\|_\infty = \sup_{x\in M}|V(x)| < +\infty$ and $\|X\|_\infty = \sup_{x\in M}\|X(x)\|_x < +\infty$.

In the sequel, we will assume that $H : T^*M \to \mathbb{R}$ is a Tonelli Hamiltonian on the complete Riemannian manifold M. We now need to introduce the (Tonelli)

Lagrangian $L : TM \to \mathbb{R}$ associated to the Hamiltonian H. It is defined by the Fenchel formula

$$L(x, v) = \sup_{p \in T_x^* M} p(v) - H(x, p) \tag{3-1}$$

Since H is Tonelli, note that the sup in the definition of L is achieved at the unique point $p \in T_x^* M$, where $v = \partial_p H(x, p)$.

Moreover, from the Fenchel formula (3-1) above, we obtain the Fenchel inequality

$$p(v) \leq L(x, v) + H(x, p) \quad \text{for all } x \in M, v \in T_x M, p \in T_x^* M, \tag{3-2}$$

with equality if and only if $v = \partial_p H(x, p)$.

This Lagrangian L is everywhere finite, and enjoys the same properties as H (see [9], for example):

(1) The Lagrangian L is at least C^2. In fact, it is as smooth as H.

(2) (uniform superlinearity) For every $K \geq 0$, we have

$$C(K) = \sup_{(x,v) \in TM} K\|v\|_x - L(x, v) < \infty. \tag{3-3}$$

(3) (uniform boundedness in the fibers) For every $R \geq 0$, we have

$$A(R) = \sup\{L(x, v) \mid \|v\| \leq R\} < +\infty. \tag{3-4}$$

(4) (C^2 strict convexity in the fibers) For every $(x, v) \in TM$, the second derivative along the fibers, $\partial^2 L / \partial v^2(x, v)$, is (strictly) positive definite.

Again (2) implies

$$\forall (x, v) \in TM, L(x, v) \geq K\|v\| - C(K). \tag{3-5}$$

A Tonelli Lagrangian on the complete Riemannian manifold (M, g) is a function $L : TM \to \mathbb{R}$ which satisfies condition (1) to (4) above. As is well-known, we can define a Hamiltonian $H : T^*M \to \mathbb{R}$ by the same Fenchel formula

$$H(x, p) = \sup_{v \in T_x M} p(v) - L(x, v).$$

Again the supremum above is attained precisely when $p = \partial_v L(x, v)$. This H is a Tonelli Hamiltonian whose associated Lagrangian is precisely L.

Example 3.3. We give the Lagrangians of the Hamiltonians in Example 3.2.

(1) The Lagrangian $L_0 : TM \to \mathbb{R}$ associated to the Tonelli Hamiltonian $H_0 : T^*M \to \mathbb{R}$ is

$$L_0(x, v) = \frac{1}{2}\|v\|_x^2,$$

and $A_0(R) = R^2/2$, $C_0(K) = K^2/2$.

(2) The Lagrangian $L_{X,V} : TM \to \mathbb{R}$ associated to the Hamiltonian $H_{X,V} : T^*M \to \mathbb{R}$ is

$$L_{X,V}(x, v) = \tfrac{1}{2}\|v - X(x)\|_x^2 - V(x) = \tfrac{1}{2}\|v\|_x^2 - \langle v, X(x)\rangle + \tfrac{1}{2}\|X(x)\|_x^2 - V(x).$$

For every $x \in M$, we have

$$\begin{aligned}\sup_{\substack{v\in T_xM\\ \|v\|_x=R}} L_{X,V}(x, v) &= \tfrac{1}{2}R^2 + R\|X(x)\|_x + \tfrac{1}{2}\|X(x)\|_x^2 - V(x)\\ &= \tfrac{1}{2}(R + \|X(x)\|_x)^2 - V(x).\end{aligned}$$

Therefore

$$A_{X,V}(R) \le \tfrac{1}{2}(R + \|X\|_\infty)^2 - \inf_{x\in M} V(x).$$

A similar computation gives

$$\begin{aligned}C_{X,V}(K) &= \tfrac{1}{2}K^2 + \sup_{x\in M}(K\|X(x)\|_x + V(x))\\ &\le \tfrac{1}{2}K^2 + K\|X\|_\infty + \sup_{x\in M} V(x).\end{aligned}$$

4. Action, minimizers, Euler–Lagrange flow

Again in the sequel, we fix a Tonelli Hamiltonian $H : T^*M \to \mathbb{R}$ on the complete Riemannian manifold (M, g) and we will denote by $L : TM \to \mathbb{R}$ its associated Tonelli Lagrangian.

We need to use the calculus of variations for Lagrangians: minimizers, extremals, Euler–Lagrange equation and flow. An introduction to these concepts can be found in [3; 5; 6], for example. We recall certain notions for the convenience of the reader and to fix notation.

Definition 4.1 (length, action). Let $\gamma : [a, b] \to M$ be an absolutely continuous curve.

- Its Riemannian length $\ell_g(\gamma)$ is

$$\ell_g(\gamma) = \int_a^b \|\dot\gamma(s)\|_{\gamma(s)}\, ds.$$

- Its action $\mathbb{L}(\gamma)$ (for L) is

$$\mathbb{L}(\gamma) = \int_a^b L(\gamma(s), \dot\gamma(s))\, ds.$$

Note that since L is bounded below by $-C(0)$ the integral above makes always sense (it can be $+\infty$). In fact, since $L + C(0) \ge 0$, we set

$$\int_a^b L(\gamma(s), \dot\gamma(s))\, ds = -C(0)(b-a) + \int_a^b L(\gamma(s), \dot\gamma(s)) + C(0) ds.$$

From the definition of the distance d on the Riemannian manifold (M, g), we also have

$$d(x, y) = \inf_{\gamma} \ell_g(\gamma),$$

where the inf is taken over all absolutely continuous curves $\gamma : [a, b] \to M$ with $\gamma(a) = x$, $\gamma(b) = y$.

Here are some basic estimates relating action of curves to their length.

Lemma 4.2. *Let $\gamma : [a, b] \to M$ be an absolutely continuous curve. For every $K \in [0, \infty[$, we have*

$$\mathbb{L}(\gamma) \geq K\ell_g(\gamma) - C(K)(b-a) \geq Kd(\gamma(a)\gamma(b)) - C(K)(b-a) \tag{4-1}$$

and

$$d(\gamma(a), \gamma(b)) \leq \ell_g(\gamma) \leq \frac{\mathbb{L}(\gamma) + C(K)(b-a)}{K}. \tag{4-2}$$

In particular, for every $\epsilon > 0$, we have

$$d(\gamma(a), \gamma(b)) \leq \ell_g(\gamma) \leq \epsilon\mathbb{L}(\gamma) + \epsilon C(1/\epsilon)(b-a). \tag{4-3}$$

Proof. We use the inequality (3-5), to obtain

$$L(\gamma(s), \dot\gamma(s)) \geq K\|\dot\gamma(s)\|_{\gamma(s)} - C(K),$$

from which it follows by integration that

$$\mathbb{L}(\gamma) \geq K\ell_g(\gamma) - C(K)(b-a).$$

Both inequalities (4-1) and (4-2) follow easily. Moreover, inequality (4-3) follows from (4-2) with $K = 1/\epsilon$. $\square$

The estimates above yield a modulus of continuity for curves with bounded Lagrangian. Recall that a modulus of continuity is a nondecreasing function $\eta : [0, +\infty[\to [0, +\infty[$ that is continuous at 0 and satisfies $\eta(0) = 0$.

Lemma 4.3. *For every finite $K, T \geq 0$, we can find a modulus of continuity $\eta_{K,T} : [0, +\infty[\to [0, +\infty[$ such that, for every absolutely continuous curve $\gamma : [a, b] \to M$, with $b - a \leq T$ and $\mathbb{L}(\gamma) \leq K$, we have*

$$d(\gamma(t'), \gamma(t)) \leq \ell_g(\gamma\,|\,[t, t']) \leq \eta_{K,T}(|t'-t|) \quad \textit{for all } t, t' \in [a, b].$$

Proof. Since $L \geq -C(0)$, for any curve $\gamma : [a, b] \to M$, and all $a \leq t \leq t' \leq b$, we obtain

$$\begin{aligned}-C(0)(t-a)+\mathbb{L}(\gamma|[t,t'])-C(0)(b-t') &\leq \mathbb{L}(\gamma|[0,t])+\mathbb{L}(\gamma|[t,t'])+\mathbb{L}(\gamma|[t',b])\\ &= \mathbb{L}(\gamma).\end{aligned}$$

Therefore

$$\mathbb{L}(\gamma\,|\,[t,t']) \le \mathbb{L}(\gamma) - C(0)(b-t') - C(0)(t-a) \le \mathbb{L}(\gamma) + |C(0)|(b-a).$$

Hence, by (4-3) of Lemma 4.2, if $\mathbb{L}(\gamma) \le K$ and $b-a \le T$, for every $\epsilon > 0$, we get

$$d(\gamma(t'),\gamma(t)) \le \ell_g(\gamma\,|\,[t,t']) \le \epsilon(K + |C(0)|T) + \epsilon C(1/\epsilon)(t'-t).$$

It is not difficult to see that we can take modulus of continuity the function $\eta_{K,T}$ defined by

$$\eta_{K,T}(s) = \inf_{\epsilon>0} \epsilon(K + |C(0)|T) + \epsilon|C(1/\epsilon)|s. \qquad \square$$

Once action is defined, the notion of minimizer can be introduced.

Definition 4.4 (minimizer). A minimizer (for L) is a curve $\gamma : [a,b] \to M$ such that

$$\mathbb{L}(\delta) = \int_a^b L(\delta(s),\dot\delta(s))\,ds \ge \mathbb{L}(\gamma) = \int_a^b L(\gamma(s),\dot\gamma(s))\,ds,$$

for every absolutely continuous curve $\delta : [a,b] \to M$ such that $\delta(a) = \gamma(a)$ and $\delta(b) = \gamma(b)$.

It is not difficult to show that the restriction to any subinterval $[c,d] \subset [a,b]$ of a minimizer $\gamma : [a,b] \to M$ is itself a minimizer.

Examples 4.5. (1) If $L_0 : TM \to \mathbb{R}$ is given by $L_0(x,v) = \frac{1}{2}\|v\|_x^2$, then $\gamma : [a,b] \to M$ is a minimizer if and only if γ is a geodesic of M with $\ell_g(\gamma) = d(\gamma(a),\gamma(b))$. Such a minimizer satisfies

$$\mathbb{L}(\gamma) = \frac{d(\gamma(a),\gamma(b))^2}{2(b-a)}.$$

(2) (Mañé Lagrangian) Let X be a C^2 vector field on the complete Riemannian manifold M. Define the Lagrangian $L_X : TM \to \mathbb{R}$ by

$$L(x,v) = \tfrac{1}{2}\|v - X(x)\|_x^2.$$

This Lagrangian is Tonelli. Since $L \ge 0$, the solution curves of the vector field X are minimizers. In fact, they are the only minimizers for L_X with zero action.

(3) For a real number $p \ge 4$, if $L_p : TM \to \mathbb{R}$ is given by $L_p(x,v) = \frac{1}{2}\|v\|_x^2 + \frac{1}{p}\|v\|_x^p$, then L is a Tonelli Lagrangian. We note that Lagrangian $\tilde L_p : TM \to \mathbb{R}$ defined by $\tilde L_p(x,v) = \frac{1}{p}\|v\|_x^p$ is not Tonelli since $\partial^2_{v^2} L(x,0)$ is identically 0 for every $x \in M$. If $\gamma : [a,b] \to M$ is a curve, we have

$$\mathbb{L}(\gamma) = \int_a^b \tfrac{1}{2}\|\dot\gamma(s)\|_\gamma^2 + \tfrac{1}{p}\|\dot\gamma(s)\|_\gamma^p\,ds.$$

Since the functions $t \mapsto t^2$ and $t \mapsto t^p$ are strictly convex, Jensen's inequality implies

$$\begin{aligned}\frac{\mathbb{L}(\gamma)}{b-a} &\geq \frac{1}{2}\left(\frac{1}{b-a}\int_a^b \|\dot\gamma(s)\|_{\gamma(s)}\,ds\right)^2 + \frac{1}{p}\left(\frac{1}{b-a}\int_a^b \|\dot\gamma(s)\|_{\gamma(s)}\,ds\right)^p\\ &\geq \frac{1}{2}\left(\frac{d(\gamma(a),\gamma(b))}{b-a}\right)^2 + \frac{1}{p}\left(\frac{d(\gamma(a),\gamma(b))}{b-a}\right)^p,\end{aligned}$$

with equality if and only if $\|\dot\gamma(s)\|_{\gamma(s)}$ identically equals $d(\gamma(a),\gamma(b))/(b-a)$. Hence, the curve γ is a minimizer if and only if it is a length minimizing geodesic of M. Therefore the action of a minimizer $\gamma : [a,b] \to M$ is given by

$$\mathbb{L}(\gamma) = \frac{d(\gamma(a),\gamma(b))^2}{2(b-a)} + \frac{d(\gamma(a),\gamma(b))^p}{p(b-a)^{p-1}}. \qquad \square$$

Minimizers play a crucial role. Like all minima of a function, minimizers must be critical points for the action functional $\mathbb{L}$. These critical points are called extremals.

More precisely, an extremal (for L) is a curve $\gamma : [a,b] \to M$ such that the derivative $D_\gamma \mathbb{L} | \mathcal{E}_\gamma$ at γ vanishes, with

$$\mathcal{E}_\gamma = \{\delta : [a,b] \to M \mid \delta(a) = \gamma(a), \delta(b) = \gamma(b)\}.$$

By the classical calculus of variations, the curve γ is an extremal if and only if it satisfies the Euler–Lagrange equation, given in local coordinates by

$$\frac{d}{dt}\left(\frac{\partial L}{\partial v}(\gamma(t),\dot\gamma(t))\right) = \frac{\partial L}{\partial x}(\gamma(t),\dot\gamma(t)). \tag{4-4}$$

This last ODE (4-4) defines a second order ODE on M. Therefore there exists a flow φ_t on TM, called the Euler–Lagrange flow, such that $\gamma : [a,b] \to M$ is an extremal if and only if its speed curve $s \mapsto (\gamma(t),\dot\gamma(t))$ is an orbit of φ_t. Moreover, for any $(x,v) \in TM$, the projected curve $\gamma_{x,v}(t) = \pi\varphi_t(x,v)$, where $\pi : TM \to M$ is the canonical projection, is an extremal with $(\gamma_{x,v}(t), \dot\gamma_{x,v}(t)) = \varphi_t(x,v)$. Hence, if two extremals have the same position and speed at a time t, then they coincide on their common interval of definition.

We now state Tonelli's theorem; see [3; 5; 6] for a proof.

Theorem 4.6 (Tonelli). *Suppose $L : TM \to \mathbb{R}$ is a Tonelli Lagrangian on the complete Riemannian manifold M. For every $t > 0$ and every $x, y \in M$, there exists an absolutely continuous curve $\gamma : [0,t] \to M$, with $\gamma(0) = x$, $\gamma(t) = y$ which is a minimizer.*

Any minimizer is as smooth as L and is a solution of the Euler–Lagrange equation.

There is a fundamental relation between the Euler–Lagrange flow for the Lagrangian $L : TM \to \mathbb{R}$ and the Hamiltonian flow of the associated Hamiltonian $H : T^*M \to \mathbb{R}$ of L. Recall that L is obtained from H by (3-1). As we already observed, it is also true, in the Tonelli case, that H can be obtained in the same way from L

$$H(x, p) = \sup_{v \in T_x M} p(v) - L(x, v). \tag{4-5}$$

Again, since L is Tonelli, the supremum in the definition of $H(x, p)$ is attained at the unique $v \in T_x M$ such that $p = \partial_v L(x, v)$. In particular, we have

$$H\,(x, \partial_v L(x, v)) = \partial_v L(x, v)(v) - L(x, v).$$

Recall that the Hamiltonian flow of H is the flow φ_t^* on T^*M obtained from the ODE on T^*M given in local coordinates by

$$\dot{x} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial x}.$$

The Hamiltonian H is invariant under the flow φ_t^*.

In fact the flow φ_t on TM and φ_t^* on T^*M are conjugated by the Legendre transformation $\mathcal{L} : TM \to T^*M$ given by

$$\mathcal{L}(x, x) = (x, \partial_v L(x, v)).$$

In particular, the function $H \circ \mathcal{L}$ in invariant by the Euler–Lagrange flow. Expressed in the variables (x, v), it is called the energy of the Lagrangian.

Definition 4.7. The energy $E : TM \to \mathbb{R}$ of the Lagrangian $L : TM \to \mathbb{R}$ is defined by

$$\begin{aligned} E(x, v) &= H \circ \mathcal{L}(x, v) \\ &= H(x, \partial_v L(x, v)) \\ &= \sup\nolimits_{u \in T_x M} \langle \partial_v L(x, v), u \rangle - L(x, u) \\ &= \partial_v L(x, v)(v) - L(x, v). \end{aligned} \tag{4-6}$$

As said above, E is constant along any orbit of the Euler–Lagrange flow.

Definition 4.8. Let $\gamma : [a, b] \to M$ be an extremal of L. Its energy $E(\gamma(s), \dot{\gamma}(s))$, $s \in [a, b]$, is constant along its speed curve. Therefore, we can define the energy $E(\gamma)$ for the extremal $\gamma : [a, b] \to M$ by $E(\gamma) = E(\gamma(s), \dot{\gamma}(s))$, for any $s \in [a, b]$.

We will give later estimates for speeds of extremals. We first define the minimal action to join x to y in time t.

Definition 4.9 (minimal action h_t). For $x, y \in M$ and $t > 0$, we define the minimal action $h_t(x, y)$ to join x to y in time t by

$$h_t(x, y) = \inf_{\gamma} \int_0^t L(\gamma(s)\dot{\gamma}(s))\, ds,$$

where the infimum is taken over all absolutely continuous curves $\gamma : [0, t] \to M$, with $\gamma(0) = x$ and $\gamma(t) = y$.

We will also set $h_0(x, x) = 0$ and $h_0(x, y) = +\infty$, for $x \neq y$. These last two definitions are the natural ones in view of Lemma 4.11.

It is useful to introduce the function $\mathcal{H} : [0, +\infty[\times M \times M \to \mathbb{R}$ defined by

$$\mathcal{H}(t, x, y) = h_t(x, y).$$

Since L is bounded from below by $-C(0)$, we obtain that $\mathcal{H}(t, x, y) = h_t(x, y)$ is always finite, for $t > 0$.

By Tonelli's theorem (Theorem 4.6), for $t > 0$, the infimum in the definition of h_t is always attained. We can also use the definition of h_t to give a characterization of minimizers:

Proposition 4.10. *For any $x, y \in M$ and every $t > 0$, we can find an absolutely continuous curve $\gamma : [0, t] \to M$, with $\gamma(0) = x$, $\gamma(t) = y$ and*

$$h_t(x, y) = \mathbb{L}(\gamma) = \inf_{\gamma} \int_0^t L(\gamma(s)\dot{\gamma}(s))\, ds.$$

Any such curve is a minimizer. Moreover, an absolutely continuous curve $\delta : [a, b] \to M$ is a minimizer if and only if

$$h_{b-a}(\delta(a), \delta(b)) = \int_a^b L(\delta(s), \dot{\delta}(s))\, ds.$$

A first estimate of $h_t(x, y)$ is given by the next lemma.

Lemma 4.11. *For every $t > 0$, every $x, y \in M$ and every $K \geq 0$, we have*

$$-C(K)t + Kd(x, y) \leq h_t(x, y) \leq tA(d(x, y)/t). \tag{4-7}$$

In particular, we have $-C(0)t \leq h_t(x, y)$, $h_t(x, x) \leq A(0)t$, and $h_{d(x,y)}(x, y) \leq A(1)d(x, y)$.

Proof. A minimizing geodesic $\gamma_{x,y} : [0, t] \to M$ joining x to y has length $\ell_g(\gamma_{x,y}) = d(x, y)$ and a speed of constant norm. But integrating the speed yields the length; hence

$$\|\dot{\delta}(s)\|_{\delta(s)} = d(x, y)/t \quad \text{for } s \in [a, b].$$

By the uniform boundedness of L in the fibers (inequality (3-4)), we thus get

$$L(\gamma_{x,y}(s), \dot{\gamma}_{x,y}(s)) \leq A\,(d(x, y)/t) \quad \text{for every } s \in [a, b],$$

and again by integration

$$\mathbb{L}(\gamma) \leq t A\left(\frac{d(x, y)}{t}\right).$$

Therefore, we also obtain second inequality in (4-7).

For the first inequality of (4-7), we now observe that, by inequality (4-1) of Lemma 4.2, for any absolutely continuous curve $\gamma : [0, t] \to M$, with $\gamma(0) = x$ and $\gamma(t) = y$, we have

$$K d(x, y) - C(K)t \leq \mathbb{L}(\gamma).$$

Taking the infimum of the above inequality over all such curves γ yields the desired inequality. □

Examples 4.12. We estimate the function h_t for some examples.

(1) If $L_0 : TM \to \mathbb{R}$ is given by $L_0(x, v) = \frac{1}{2}\|v\|_x^2$, from Example 4.5(1), we obtain

$$h_t(x, y) = \frac{d(x, y)^2}{2t}.$$

(2) For a real number $p \geq 4$, if $L_p : TM \to \mathbb{R}$ is given by $L_p(x, v) = \frac{1}{2}\|v\|_x^2 + \frac{1}{p}\|v\|_x^p$, from of Example 4.5(1), we obtain

$$h_t(x, y) = \frac{d(x, y)^2}{2t} + \frac{d(x, y)^p}{pt^{p-1}}.$$

(3) If $L_{X,V} : TM \to \mathbb{R}$ is given by

$$L_{X,V}(x, p) = \tfrac{1}{2}\|v - X(x)\|_x^2 - V(x) = \tfrac{1}{2}\|v\|_x^2 - \langle v, X(x)\rangle + \tfrac{1}{2}\|X(x)\|_x^2 - V(x),$$

where $V : M \to \mathbb{R}$ is a C^2 function and X is a C^2 vector field on M. From Example 3.3(2), we know that

$$A_{X,V}(R) \leq \tfrac{1}{2}(R + \|X\|_\infty)^2 - \inf_{x\in M} V(x).$$

Therefore by Lemma 4.11, we get

$$h_t(x, y) \leq \frac{(d(x, y) + t\|X\|_\infty)^2}{2t} - t \inf_{x\in M} V(x).$$

Again by Example 3.3(2), we know that

$$C_{X,V}(K) \leq \tfrac{1}{2}K^2 + K\|X\|_\infty + \sup_{x\in M} V(x).$$

Therefore by inequality (4-1) of Lemma 4.2, we have

$$h_t(x,y) \geq Kd(x,y) - \tfrac{1}{2}tK^2 - tK\|X\|_\infty - t\sup_{x\in M} V(x).$$

Since this is true for every $K \geq 0$, taking the supremum over all $K \geq 0$ yields

$$h_t(x,y) \geq \begin{cases} -t\sup_{x\in M} V(x) & \text{if } d(x,y) \leq t\|X\|_\infty,\\ \dfrac{(d(x,y)-t\|X\|_\infty)^2}{2t} - t\sup_{x\in M} V(x) & \text{otherwise.}\end{cases}$$

We now give some more properties of $h_t(x,y)$.

Proposition 4.13. (1) *For every $t, t' > 0$ and every $x, y \in M$, we have*

$$h_{t+t'}(x,y) = \inf_{z\in M} h_t(x,z) + h_{t'}(y,z),$$

and this infimum is attained.

(2) *If $\gamma : [a,b] \to M$ is a minimizer, for every $a', b' \in [0,t]$, with $a' < b'$, we have*

$$h_{b'-a'}(\gamma(a'),\gamma(b')) = \int_{a'}^{b'} L(\gamma(s),\dot\gamma(s))\,ds.$$

(3) *If $\gamma : [a,b] \to M$ is a minimizer, we have*

$$\begin{aligned} h_{b-a}(\gamma(a),\gamma(b)) &\geq K\ell_g(\gamma) - C(K)(b-a)\\ &\geq Kd(\gamma(a),\gamma(b)) - C(K)(b-a) \end{aligned} \tag{4-8}$$

and

$$d(\gamma(a),\gamma(b)) \leq \ell_g(\gamma) \leq \frac{h_{b-a}(\gamma(a),\gamma(b)) + C(K)(b-a)}{K}. \tag{4-9}$$

In particular, for every $\epsilon > 0$,

$$d(\gamma(a),\gamma(b)) \leq \ell_g(\gamma) \leq \epsilon h_{b-a}(\gamma(a),\gamma(b)) + \epsilon C(1/\epsilon)(b-a). \tag{4-10}$$

Proof. Part (1) follows from the following facts:

- If $\gamma : [0, t+t'] \to M$,

$$\mathbb{L}(\gamma) = \mathbb{L}(\gamma\,|\,[0,t]) + \mathbb{L}(\gamma\,|\,[t,t+t']).$$

- If $\gamma_1 : [0,t] \to M$ and $\gamma_2 : [0,t'] \to M$ are curves with $\gamma_1(t) = \gamma_2(0)$, the concatenation $\gamma_2 * \gamma_1 : [0, t+t'] \to M$, defined by

$$\gamma_2 * \gamma_1(s) = \begin{cases} \gamma_1(s) \text{ for } 0 \leq s \leq t,\\ \gamma_2(s-t) \text{ for } t \leq s \leq t+t',\end{cases}$$

is a curve joining $\gamma_1(0)$ to $\gamma_2(t')$ whose action $\mathbb{L}(\gamma_2 * \gamma_1)$ equals $\mathbb{L}(\gamma_1) + \mathbb{L}(\gamma_2)$.

Part (2) follows from Proposition 4.10, since we already observed (after Definition 4.4) that $\gamma\,|\,[a', b']$ is also a minimizer.

Parts (3) and (4) follow from inequalities (4-1), (4-2) and (4-3) in Lemma 4.2 and Proposition 4.10. □

To estimate the speed of extremals, we start with two lemmas, providing first an estimate of the partial derivative of L with respect to v, and then of the energy (Lemma 4.15).

Lemma 4.14. *For every $K \geq 0$ and every $(x, v) \in TM$, we have*

$$\|\partial_v L(x, v)\|_x \leq A(\|v\|_x + 1) + C(0),$$
$$\|\partial_v L(x, v)\|_x \|v\|_x \geq K\|v\|_x - C(K) - A(0).$$

Therefore $D(R) \to +\infty$ as $R \to +\infty$, where $D : [0, +\infty[\to [0, +\infty[$ is the function defined by

$$D(R) = \inf\bigl\{\|\partial_v L(x, v)\|_x \bigm| v \in T_x M,\ \|v\|_x \geq R\bigr\}.$$

The function D is nondecreasing and $D(0) = 0$. Moreover, we have

$$\|\partial_v L(x, v)\|_x \geq D(\|v\|_x),$$

for every $(x, v) \in TM$.

Proof. By convexity of $L(x, v)$ in v, we have

$$L(x, v + u) - L(x, v) \geq \partial_v L(x, v)(u). \tag{4-11}$$

taking the sup over u with $\|u\|_x \leq 1$, we obtain

$$\|\partial_v L(x, v)\|_x \leq \max_{\|u\|_x \leq 1} L(x, v + u) - L(x, v).$$

But we know that $L \geq -C(0)$ and $\max_{\|u\|_x \leq 1} L(x, v + u) \leq A(\|v\|_x + 1)$, by inequality (3-4). Therefore we get

$$\|\partial_v L(x, v)\|_x \leq A(\|v\|_x + 1) + C(0).$$

Setting $u = -v$ in (4-11), we obtain

$$L(x, 0) - L(x, v) \geq -\partial_v L(x, v)(v),$$

from which we get

$$\begin{aligned}
\|\partial_v L(x, v)\|_x \|v\|_x &\geq \partial_v L(x, v)(v) \\
&\geq L(x, v) - L(x, 0) \\
&\geq K\|v\|_x - C(K) - A(0),
\end{aligned}$$

where we again used (3-4) and (3-5).

The function D is obviously nondecreasing. We then note that

$$D(0) = \inf_{(x,v)\in TM} \|\partial_v L(x, v)\| \geq 0.$$

Since L is superlinear in v, for every $x \in M$, the function $L(x, \cdot)$ achieves a minimum on $T_x M$, at which $\partial_v L(x, \cdot)$ vanishes. Therefore $D(0) = 0$.

We now show that $D(R) \to +\infty$ as $R \to +\infty$. Since D is nondecreasing $\lim_{R\to+\infty} D(R)$ exists in $\mathbb{R} \cup \{+\infty\}$.

Given $K \geq 0$, for any $v \in T_x M$, with $\|v\|_x \geq R$, we have

$$\|\partial_v L(x, v)\|_x \geq K - \frac{C(K) + A(0)}{\|v\|_x} \geq K - \frac{|C(K) + A(0)|}{R}.$$

Therefore $D(R) \geq K - |C(K) + A(0)|/R$, and $\lim_{R\to+\infty} D(R) \geq K$. Since $K \geq 0$ is arbitrary, we indeed get $\lim_{R\to+\infty} D(R) = +\infty$. □

Lemma 4.15. *We have*

$$A(2\|v\|_x) + 2C(0) \geq E(x, v) \geq \|\partial_v L(x, v)\|_x - A(1).$$

Therefore $E(x, v) \geq D(\|v\|_x) - A(1)$, *where* D *is the nondecreasing function defined in Lemma 4.14.*

Proof. We use again the convexity of L expressed by (4-11), with $u = v$ to obtain

$$L(x, 2v) - L(x, v) \geq \partial_v L(x, v)(v).$$

Subtracting $L(x, v)$ from both sides, we get

$$L(x, 2v) - 2L(x, v) \geq \partial_v L(x, v)(v) - L(x, v) = E(x, v).$$

Since $L(x, v) \geq -C(0)$ and $L(x, 2v) \leq A(2\|v\|_x)$, we obtain

$$E(x, v) \leq A(2\|v\|_x) + 2C(0).$$

Since $E(x, v) = \sup_{u\in T_x M} \partial_v L(x, v)(u) - L(x, u)$, we have

$$E(x, v) \geq \sup_{\|u\|_x \leq 1} \partial_v L(x, v)(u) - L(x, u).$$

This last inequality, together with $L(x, u) \leq A(1)$, valid for $\|u\|_x \leq 1$, yields $E(x, v) \geq \|\partial_v L(x, v)\|_x - A(1)$. □

We now give the estimate on the speed of an extremal. It uses the preservation of energy along a solution of the Euler–Lagrange equation.

Proposition 4.16. *Suppose $L : TM \to \mathbb{R}$ is a given Tonelli Lagrangian. There exists a nondecreasing function $\eta : [0, +\infty[\to [0, +\infty[$ such that for every curve $\gamma : [a, b] \to M$ which satisfies the Euler–Lagrange equation, we have*

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)} \le \eta\Big(\inf_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)}\Big).$$

Therefore

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)} \le \eta[\ell_g(\gamma)/(b-a)].$$

Proof. Consider the nondecreasing function D introduced in Lemma 4.14. Since $D(0) = 0$, we can introduce a nondecreasing function ζ defined on $[0, +\infty[$ by

$$\zeta(\rho) = \sup\{R \ge 0 \mid D(R) \le \rho\}.$$

Since $D(R) \to +\infty$ as $R \to +\infty$, the function ζ is finite everywhere. We also have $\zeta(D(R)) \ge R$, since $\zeta(D(R)) = \sup\{R' \mid D(R') \le D(R)\}$.

Consider now a solution $\gamma : [a, b] \to M$ of the Euler–Lagrange equation. Define $s_{\min}, s_{\max} \in [a, b]$ by

$$\|\dot\gamma(s_{\min})\|_{\gamma(s_{\min})} = \inf_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)},$$
$$\|\dot\gamma(s_{\max})\|_{\gamma(s_{\max})} = \sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)}.$$

By Lemma 4.15, we get

$$A(2\|\dot\gamma(s_{\min})\|_{\gamma(s_{\min})}) + 2C(0) \ge E[\gamma(s_{\min}), \dot\gamma(s_{\min})]$$

and

$$E[\gamma(s_{\max}), \dot\gamma(s_{\max})] \ge D\left(\|\dot\gamma(s_{\max})\|_{\gamma(s_{\max})}\right) - A(1).$$

We have $E[\gamma(s_{\min}), \dot\gamma(s_{\min})] = E\,(\gamma(s_{\max}), \dot\gamma(s_{\max}))$, by the conservation of energy. Therefore

$$A(2\|\dot\gamma(s_{\min})\|_{\gamma(s_{\min})}) + 2C(0) + A(1) \ge D\left(\|\dot\gamma(s_{\max})\|_{\gamma(s_{\max})}\right).$$

Since ζ is nondecreasing and $\zeta(D(R)) \ge R$, we obtain

$$\zeta\left(A(2\|\dot\gamma(s_{\min})\|_{\gamma(s_{\min})}) + 2C(0) + A(1)\right) \ge \|\dot\gamma(s_{\max})\|_{\gamma(s_{\max})}.$$

To finish the proof of the first inequality of the proposition, it suffices to define the nondecreasing everywhere finite function $\eta : [0, +\infty[\to [0, +\infty[$ by $\eta(R) = \zeta(A(2R) + 2C(0) + A(1))$.

The second inequality follows from the nondecreasing character of η and

$$(b-a) \min_{s\in[a,b]} \|\dot\gamma(s)\|_{\gamma(s)} \le \int_a^b \|\dot\gamma(s)\|_{\gamma(s)}\, ds = \ell_g(\gamma). \qquad \square$$

Corollary 4.17. *If $L : TM \to \mathbb{R}$ is a given Tonelli Lagrangian, we can find nondecreasing functions $\bar\eta, \tilde\eta : [0, +\infty[\to [0, +\infty[$ such that any minimizer $\gamma : [a, b] \to M$ satisfies*

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)} \le \bar\eta\left(\frac{h_{b-a}(\gamma(a), \gamma(b))}{b-a}\right)$$

and

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)} \le \tilde\eta\left(\frac{d(\gamma(a), \gamma(b))}{b-a}\right).$$

Proof. By (4-9), we have

$$\ell_g(\gamma) \le h_{b-a}(\gamma(a), \gamma(b)) + C(1)(b-a).$$

Therefore, using the function η from Proposition 4.16, since a minimizer satisfies the Euler–Lagrange equation, we obtain

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)} \le \eta\left(C(1) + \frac{h_{b-a}(\gamma(a), \gamma(b))}{b-a}\right).$$

This finishes the proof of the first inequality, with $\bar\eta(s) = \eta(s + C(1))$.

To prove the second one, we recall, from (4-7) in Lemma 4.11, that

$$\frac{h_{b-a}(\gamma(a), \gamma(b))}{b-a} \le A\left(\frac{d(\gamma(a), \gamma(b))}{b-a}\right).$$

Therefore

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(t)} \le \bar\eta\left(A\left(\frac{d(\gamma(a), \gamma(b))}{b-a}\right)\right).$$

The function $t \mapsto \tilde\eta(t) = \bar\eta \circ A(t)$ is finite everywhere and nondecreasing. □

For a subset $S \subset M$, recall that its diameter $\operatorname{diam} S$, for the Riemannian distance d on M, is defined by

$$\operatorname{diam} S = \sup\{d(x, y) \mid x, y \in S\}.$$

The next result, a straightforward consequence of Corollary 4.17, provides us with the criterion for compactness of a set of minimizers.

Proposition 4.18. *Suppose $S \subset M$, with* diam *S finite, and $t_0 > 0$. Any minimizer $\gamma : [a, b] \to M$ such that $\gamma(a), \gamma(b) \in S$ and $b - a \ge t_0$ satisfies*

$$\sup_{t\in[a,b]} \|\dot\gamma(t)\|_{\gamma(s)} \le \tilde\eta(\operatorname{diam} S/t_0),$$

where $\tilde\eta$ is the nondecreasing everywhere finite function from Corollary 4.17. Therefore, the set of minimizers $\gamma : [a, b] \to M$ such that $\gamma(a), \gamma(b) \in S$ and $b - a \ge t_0$ is equi-Lipschitz.

An important property of $h_t(x, y)$, namely its local semiconcavity in (x, y), is proved in [8, Theorem B.19, page 50]. It is not difficult, using the proof of Theorem B.19 in [8], to show that $\mathcal{H}(t, x, y)$ is locally semiconcave in (t, x, y) on $]0, +\infty[\times M \times M$.

Proposition 4.19. *The function $\mathcal{H}$ is locally semiconcave on $]0, +\infty[\times M \times M$. Moreover, for every compact subset $C \subset M \times M$, and every $t_0 > 0$, the family of functions $h_t : C \to \mathbb{R}$, $t \geq t_0$ is equi-semiconcave.*

Another useful reference on semiconcavity and the Hamilton–Jacobi equation is [4].

Example 4.20. If $L_0 : TM \to \mathbb{R}$ is given by $L_0(x, v) = \frac{1}{2}\|v\|_x^2$, from part (1) of Example 4.12, we obtain

$$\mathcal{H}(t, x, y) = \frac{d(x, y)^2}{2t}.$$

Therefore, from the previous proposition we obtain that d^2 is locally semiconcave on $M \times M$. Moreover, since $s \mapsto \sqrt{s}$ is C^∞ on $]0, +\infty[$, we obtain that d is locally semiconcave on $M \times M \setminus \Delta_M$, where $\Delta_M = \{(x, x) \mid x \in M\}$ is the diagonal in $M \times M$.

Since $\mathcal{H}$ is locally semiconcave, it is locally Lipschitz. Therefore, it has a derivative almost everywhere in $]0, +\infty[\times M \times M$. We proceed to express this derivative.

We need to use the notion of upper and lower differentials (called also upper and lower derivatives)–see [2; 1; 4; 6; 7] for more details on this notion and its relationship with viscosity solutions.

Notation 4.21. If $w : N \to \mathbb{R}$ is a function on the manifold N and $n \in N$, the set of upper-differentials (resp. lower-differentials) of w at N is denoted by $D^+w(n) \subset T_n^*N$ (resp. $D^-w(n) \subset T_n^*N$).

Proposition 4.22. *Since $\mathcal{H}$ is locally semiconcave on $]0, +\infty[\times M \times M$, for every $(t, x, y) \in]0, +\infty[\times M \times M$ the set of superderivatives $D^+\mathcal{H}(t, x, y) \subset T^*_{(t,x,y)}(]0, +\infty[\times M \times M = \mathbb{R} \times T_x^*M \times T_y^*M$ is not empty. If $\gamma : [0, t] \to M$ is a minimizer, with $\gamma(0) = x$ and $\gamma(t) = y$, we have*

$$(-E(\gamma), -\partial_v L(\gamma(0), \dot\gamma(0)), \partial_v L(\gamma(t), \dot\gamma(t))) \in D^+\mathcal{H}(t, x, y),$$

where $E(\gamma) = E(\gamma(s), \dot\gamma(s))$, $s \in [0, t]$ is the energy of the minimizer γ.

In particular, we have

$$\begin{aligned} -E(\gamma) &\in D_t^+\mathcal{H}(t, x, y), \\ -\partial_v L(\gamma(0), \dot\gamma(0)) &\in D_x^+\mathcal{H}(t, x, y), \\ \partial_v L(\gamma(t), \dot\gamma(t)) &\in D_y^+\mathcal{H}(t, x, y). \end{aligned} \tag{4-12}$$

The proof that $(-\partial_v L(\gamma(0), \dot\gamma(0)), \partial_v L(\gamma(t), \dot\gamma(t))) \in D^+ h_t(x, y)$ is given in [8, Theorem B.20, page 53]. We leave it to the reader to check the superderivative in t.

Corollary 4.23. *For $(t, x, y) \in]0, +\infty[\times M \times M$, the function $\mathcal{H}$ is differentiable at $(t, x, y) \in]0, +\infty[\times M \times M$ if and only if there exists a unique minimizer $\gamma : [0, t] \to M$, with $\gamma(0) = x$ and $\gamma(t) = y$.*

Moreover, for each $(t, x, y) \in]0, +\infty[\times M \times M$, the set of superderivatives $D^+\mathcal{H}(t, x, y)$ is the convex hull of the set of covectors

$$\bigl(-E(\gamma), -\partial_v L(\gamma(0), \dot\gamma(0)), \partial_v L(\gamma(t), \dot\gamma(t))\bigr),$$

where $\gamma : [0, t] \to M$ is an arbitrary minimizer with $\gamma(0) = x$ and $\gamma(t) = y$.

Proof. If $\mathcal{H}$ is differentiable at $(t, x, y) \in]0, +\infty[\times M \times M$ and $\gamma : [0, t] \to M$ is a minimizer, with $\gamma(0) = x$ and $\gamma(t) = y$, then, by Proposition 4.22 above $\partial_y \mathcal{H}(t, x, y) = \partial_v L(\gamma(t), \dot\gamma(t))$, since L is strictly convex the speed $\dot\gamma(t)$ is completely determined by $\partial_y \mathcal{H}(t, x, y)$. Therefore, since a minimizer satisfies the Euler–Lagrange equation, the curve γ is completely determined by $\partial_y \mathcal{H}(t, x, y)$.

This proves half of the first statement of the corollary. To prove the second part, we recall that $D^+\mathcal{H}(t, x, y)$ is the convex hull of $\partial\mathcal{H}(t, x, y)$ where any point in $\partial\mathcal{H}(t, x, y)$ is a limit of a sequence of derivatives $D\mathcal{H}(t_i, x_i, y_i)$, where $(t_i, x_i, y_i) \to (t, x, y)$ as $i \to \infty$, and $\mathcal{H}$ is differentiable at each (t_i, x_i, y_i). By Proposition 4.22, the derivative $D\mathcal{H}(t_i, x_i, y_i)$ is given by a minimizer $\gamma_i : [0, t_i] \to M$ with $\gamma(0) = x_i$ and $\gamma(t_i) = y$. If $\tilde\eta$ is the nondecreasing finite everywhere function obtained in Corollary 4.17, we have

$$\|\dot\gamma_i(s)\|_{\gamma_i(s)} \le \tilde\eta\left(\frac{d(\gamma(0), \gamma(t_i))}{t_i}\right) \quad \text{for all } s \in [0, t_i].$$

Since $(t_i, x_i, y_i) \to (t, x, y)$, with $t > 0$, we have $\sup_i d(\gamma(0), \gamma(t_i))/t_i < +\infty$.

Let C be the value of this supremum. We see that the norm of the speed $\|\dot\gamma_i(s)\|_{\gamma_i(s)}$ is bounded by $\tilde\eta(C)$, independently of i and $s \in [0, t_i]$. Extracting a subsequence if necessary, we can assume that $(\gamma_i(0), \dot\gamma_i(0))$ converges to some (x, v) with $v \in T_x M$. If we call γ the solution of the Euler–Lagrange equation with $(\gamma(0), \dot\gamma(0)) = (x, v)$, we obtain that $\gamma : [0, t] \to M$ is a minimizer, with $\gamma(0) = x$ and $\gamma(t) = y$. But we have

$$D\mathcal{H}(t_i, x_i, y_i) = \bigl(-E(\gamma_i), -\partial_v L(\gamma_i(0), \dot\gamma_i(0)), \partial_v L(\gamma_i(t), \dot\gamma_(t_i))\bigr),$$

which tends to $\bigl(-E(\gamma), -\partial_v L(\gamma(0), \dot\gamma(0)), \partial_v L(\gamma(t), \dot\gamma(t))\bigr)$. This proves the last part of the corollary.

To finish the proof of the corollary, it suffices to show that if there is a unique minimizer $\gamma : [0, t] \to M$, with $\gamma(0) = x$ and $\gamma(t) = y$, then $\mathcal{H}$ is differentiable at (t, x, y). By what we just proved, this uniqueness condition implies that $D^+\mathcal{H}(t, x, y) = \partial\mathcal{H}(t, x, y)$ is reduced to one point. Since $\mathcal{H}$ is semiconcave, this implies that $\mathcal{H}$ is differentiable at (t, x, y). □

Corollary 4.24. *For $(t, x, y) \in]0, +\infty[\times M \times M$, the following statements are equivalent*:

(i) *The function $\mathcal{H}$ is differentiable at (t, x, y).*

(ii) *The partial derivative $\partial_x\mathcal{H}(t, x, y)$ exists.*

(iii) *The partial derivative $\partial_y\mathcal{H}(t, x, y)$ exists.*

(iv) *There exists a unique minimizer $\gamma : [0, t] \to M$, with $\gamma(0) = x$ and $\gamma(t) = y$.*

If any one of these statements is true, *we have*

$$\begin{aligned}
\partial_t\mathcal{H}(t, x, y) &= -E(\gamma),\\
\partial_x\mathcal{H}(t, x, y) &= -\partial_v L(\gamma(0), \dot\gamma(0)),\\
\partial_y\mathcal{H}(t, x, y) &= \partial_v L(\gamma(t), \dot\gamma(t))),
\end{aligned} \tag{4-13}$$

where $\gamma : [0, t] \to M$ is the unique minimizer with $\gamma(0) = x$ and $\gamma(t) = y$.

Proof. Of course (i) implies (ii) and (iii). From Corollary 4.23, statements (i) and (iv) are equivalent. To finish proving that (i), (ii), (iii) and (iv) are all equivalent, it remains to show that (ii) or (iii) imply (iv). We will show that (ii) implies (iv). In fact, if $\partial_x\mathcal{H}(t, x, y)$ exists and $\gamma : [0, t] \to M$ is a minimizer with $\gamma(0) = x$ and $\gamma(t) = y$, by equality (4-12) of Proposition 4.22, we have $\partial_x\mathcal{H}(t, x, y) = -\partial_v L(\gamma(0), \dot\gamma(0))$. Therefore not only the position at time 0 of γ is unique, but also its speed $\dot\gamma(0)$ is unique. Since such a minimizer γ satisfies Euler–Lagrange, we conclude that γ is unique.

The last part of the corollary follows from (4-12). □

Corollary 4.25. *We can find a nondecreasing everywhere finite function θ : $[0, +\infty[\to [0, +\infty[$ such that at every point $(t, x, y) \in]0, +\infty[\times M \times M$, where the derivative $D\mathcal{H}(t, x, y)$ exists, it is bounded in norm by $\theta(\mathcal{H}(t, x, y)/t)$.*

Proof. We first estimate $\partial_x\mathcal{H}(t, x, y)$. By Proposition 4.22, if $\gamma : [0, t] \to M$ is a minimizer, with $\gamma(0) = x$ and $\gamma(t) = y$, we have $\partial_x\mathcal{H}(t, x, y) = \partial_v L(\gamma(0), \dot\gamma(0))$. Therefore by Lemma 4.15, we get

$$\|\partial_x\mathcal{H}(t, x, y)\|_x \le A(\|\dot\gamma(0)\|_{\gamma(0)} + 1) + C(0).$$

Combining with Corollary 4.17, since $\mathbb{L}(\gamma) = \mathcal{H}(t, x, y)$, we obtain

$$\|\partial_x\mathcal{H}(t, x, y)\|_x \le A(\bar\eta[\mathcal{H}(t, x, y)/t] + 1) + C(0).$$

Therefore if we define the nondecreasing function $\theta_1 : [0, +\infty[\to [0, +\infty[$ by

$$\theta_1(R) = \max\left(0, A(\bar\eta[R] + 1) + C(0)\right),$$

we obtain

$$\|\partial_x \mathcal{H}(t,x,y)\|_x \le \theta_1(\mathcal{H}(t,x,y)/t).$$

In the same way, we obtain

$$\|\partial_y \mathcal{H}(t,x,y)\|_x \le \theta_1(\mathcal{H}(t,x,y)/t).$$

To estimate $\partial_t \mathcal{H}(t,x,y) = -E(\gamma(s),\dot\gamma(s))$, we use Lemma 4.15 and Corollary 4.17:

$$\begin{aligned}|\partial_t \mathcal{H}(t,x,y)| &= |E(\gamma(0),\dot\gamma(0))|\\ &\le \max\big(A(1),\, A(2\|\dot\gamma(0)\|_{\gamma(0)}) + 2C(0)\big)\\ &\le \max\big(A(1),\, A(2\bar\eta[\mathcal{H}(t,x,y)/t]) + 2C(0)\big).\end{aligned}$$

Hence, if we define the nondecreasing function $\theta_2 : [0,+\infty[\, \to [0,+\infty[$ by

$$\theta_2(R) = \max\big(0,\, A(1),\, A(2\bar\eta[R]) + 2C(0))\big),$$

we obtain

$$|\partial_t \mathcal{H}(t,x,y)| \le \theta_2(\mathcal{H}(t,x,y)/t).$$

Therefore

$$\|D\mathcal{H}(t,x,y)\|^2_{(t,x,y)} \le 2\theta_1(\mathcal{H}(t,x,y)/t)^2 + \theta_2(\mathcal{H}(t,x,y)/t)^2.$$

Since the functions θ_1 and θ_2 are both finite everywhere, nonnegative and nondecreasing, so is the function θ defined by

$$\theta(R) = \sqrt{2\theta_1(R)^2 + \theta_2(R)^2}.$$

This function satisfies the inequality $\|D\mathcal{H}(t,x,y)\|_{(t,x,y)} \le \theta(\mathcal{H}(t,x,y)/t)$. $\square$

Proposition 4.26. *If we fix $y \in M$, the function $\mathcal{H}_y :]0,+\infty[\times M$, defined by*

$$\mathcal{H}_y(t,x) = \mathcal{H}(t,y,x) = h_t(y,x),$$

is a viscosity solution of

$$\partial_t \mathcal{H}_y + H(y, \partial_y \mathcal{H}_y) = 0.$$

Proof. From Proposition 4.19, we know that $\mathcal{H}_y$ is locally semiconcave. Therefore, since the Hamiltonian H is convex in p, it suffices to check the evolutionary Hamilton–Jacobi equation at every point (t,x) where $\mathcal{H}_y$ is differentiable. If (t,x) is such a point and $\gamma : [0,t] \to M$ is a minimizer with $\gamma(0) = y$, $\gamma(t) = x$, by Corollary 4.24, we have

$$\begin{aligned}\partial_x \mathcal{H}_y(t,x) &= \partial_x \mathcal{H}(t,y,x) = \partial_v L(\gamma(t),\dot\gamma(t))\\ \partial_t \mathcal{H}_y(t,x) &= \partial_t \mathcal{H}(t,y,x) = -E(\gamma(t),\dot\gamma(t)) = -H(\gamma(t), \partial_v L(\gamma(t),\dot\gamma(t))).\end{aligned}$$

Therefore

$$\begin{aligned}\partial_t \mathcal{H}_y(t,x) + H(y, \partial_y \mathcal{H}_y(t,x)) \\ &= -H(\gamma(t), \partial_v L(\gamma(t), \dot\gamma(t))) + H(\gamma(t), \partial_v L(\gamma(t), \dot\gamma(t))) \\ &= 0. \qquad \square\end{aligned}$$

5. Action and viscosity (sub)solutions

Again in the sequel, we fix a Tonelli Hamiltonian $H : T^*M \to \mathbb{R}$ on the complete Riemannian manifold (M, g) and we will denote by $L : TM \to \mathbb{R}$ its associated Tonelli Lagrangian.

A first relation between action and viscosity subsolution is given in the next Proposition 5.5. To state it, it is convenient to recall the notion of evolution domination by a Lagrangian introduced in [7, Definition 14.2, page 1232].

To do it in an appropriate way, we first recall that for a curve $\gamma : I \to M$, where I is an interval in $\mathbb{R}$, the graph $\mathrm{Graph}(\gamma) \subset \mathbb{R} \times M$ of γ is

$$\mathrm{Graph}(\gamma) = \{(t, \gamma(t)) \mid t \in I\}.$$

Definition 5.1 (evolution domination by a Lagrangian). We will say that the function $U : S \to [-\infty, +\infty]$, where $S \subset \mathbb{R} \times M$ is evolution-dominated by L on S, if, for every absolutely continuous curve $\gamma : [a, b] \to M$ with $a < b \in \mathbb{R}$ and $\mathrm{Graph}(\gamma) \subset S$ whose action $\mathbb{L}(\gamma) = \int_a^b L(\gamma(s), \dot\gamma(s))\, ds$ is finite, we have

$$U(b, \gamma(b)) \le U(a, \gamma(a)) + \int_a^b L(\gamma(s), \dot\gamma(s))\, ds. \tag{5-1}$$

We will say that such a $U : S \to [-\infty, +\infty]$ is *strongly* evolution-dominated by L on S, if for every $(t, x), (t', x') \in S$, with $t < t'$, it satisfies the stronger condition

$$U(t', x') \le U(t, x) + h_{t'-t}(x, x'). \tag{5-2}$$

Remark 5.2. (1) If $U(a, \gamma(a))$ is finite, the inequality (5-1) is equivalent to

$$U(b, \gamma(b)) - U(a, \gamma(a)) \le \mathbb{L}(\gamma) = \int_a^b L(\gamma(s), \dot\gamma(s))\, dt.$$

(2) If $S \subset \mathbb{R} \times M$ is of the form $S = I \times M$, where I is an interval in $\mathbb{R}$, then $U : I \times M \to [-\infty, +\infty]$ is evolution-dominated by L if and only if it is *strongly* evolution-dominated by L.

Proposition 5.3. *Let $U : S \to [-\infty, +\infty]$ be evolution-dominated by L on the subset $S \subset \mathbb{R} \times M$.*

(1) *Assume* $\gamma : [a, b] \to M$ *is an absolutely continuous function curve, with* $\mathrm{Graph}(\gamma) \subset S$, *whose action is finite. If* $U(t_0, \gamma(t_0)) < +\infty$ (*resp.* $U(t_0, \gamma(t_0)) > -\infty$), *then* $U(t, \gamma(t)) < +\infty$ *for* $t \in [t_0, b]$ (*resp.* $U(t, \gamma(t)) > -\infty$ *for* $t \in [a, t_0]$).

(2) *Let* $S \subset \times\mathbb{R} \to M$ *be such that* $S = I \times W$, *where* I *is an interval in* $\mathbb{R}$ *and* $W \subset M$ *is open and connected. If for some* $(x_0, t_0) \in I \times M$ *we have* $U(x_0, t_0) < +\infty$ (*resp.* $U(x_0, t_0) > -\infty$) *then* $U < +\infty$ *everywhere on* $(I \cap]t_0, +\infty[) \times W$ (*resp.* $U > -\infty$ *everywhere on* $(I \cap]-\infty, t_0[) \times W$).

(3) *If* $U : S \to [-\infty, +\infty]$ *is* ***strongly*** *evolution-dominated by* L *on* S *and, for some* $(x_0, t_0) \in S$, *we have* $U(x_0, t_0) < +\infty$ (*resp.* $U(x_0, t_0) > -\infty$) *then* $U < +\infty$ *everywhere on* $S \cap (]t_0, +\infty[\times M)$ (*resp.* $U > -\infty$ *everywhere on* $S \cap (]-\infty, t_0[\times M)$).

Proof. For part (1) we note that the evolution domination of U by L on S, for $t \in]t_0, b]$, we get

$$U(t, \gamma(t)) \leq U(t_0, \gamma(t_0)) + \int_t^{t_0} L(\gamma(s), \dot\gamma(s))\, ds.$$

Since $\int_t^{t_0} L(\gamma(s), \dot\gamma(s))\, ds$ is finite, the inequality $U(t_0, \gamma(t_0)) < +\infty$ implies $U(t, \gamma(t)) < +\infty$ for $t \in]t_0, b]$.

For part (2), since W is open and connected in the manifold M, given $t > t_0$ and $x \in$, we can find a smooth curve $\gamma : [t_0, t] \to W$ with $\gamma(t_0) = x_0$ and $\gamma(t) = x$. Since L is continuous and γ is C^1, the action $\mathbb{L}(\gamma)$ of γ is finite. Moreover $\mathrm{Graph}(\gamma) \subset I \times W$, the evolution domination condition implies $U(t, x) \leq U(t_0, x_0) + \mathbb{L}(\gamma) < +\infty$.

For part (3), it suffices to observe that, for $(t, x) \in S \cap (]t_0, +\infty[\times M)$, we have $|h_{t-t_0}(x_0, x)| < +\infty$ and the strong L domination implies $U(t, x) \leq U(t_0, x_0) + h_{t-t_0}(x_0, x)$. □

Proposition 5.4. *Suppose* $U : O \to \mathbb{R}$ *is finite-valued and evolution-dominated by* L *on the open subset* $O \subset \mathbb{R} \times M$. *Then* U *is locally bounded on* O. *The function* U *is locally strongly evolution-dominated by* L; *that is, for every* $(t_0, x_0) \in O$ *there exists a neighborhood* $V \subset O$ *of* (t_0, x_0) *such that the restriction* $U\,|\,V$ *is strongly evolution-dominated by* L *on* V.

Proof. Fix a compact neighborhood of the form $[t_0-2\delta, t_0+2\delta] \times \bar B(x_0, 3r) \subset O$ of $(t_0, x_0) \in O$. For any $x \in \bar B(x_0, 2r)$ and $t \in [t_0 - \delta, t_0 + \delta]$, the minimizing geodesic $\gamma_{x_0,x} : [t_0 - 2\delta, t] \to M$ joining x_0 to x is contained in $\bar B(x_0, 2r)$ and, by Lemma 4.11, its action $\mathbb{L}(\gamma_{x_0,x})$ is less than

$$\big(t - (t_0 - 2\delta)\big) A\left(\frac{d(x_0, x)}{t - (t_0 - 2\delta)}\right) \leq 3\delta A\left(\frac{2r}{\delta}\right).$$

Since the function is evolution-dominated by L on $O \supset [t_0 - 2\delta, t_0 + 2\delta] \times \bar{B}(x_0, 3r)$, we obtain

$$U(t, x) \le U(t_0 - 2\delta, x_0) + \mathbb{L}(\gamma_{x_0,x}) \le U(t_0 - 2\delta, x_0) + 3\delta A(2r/\delta).$$

This shows that U is bounded above on the compact neighborhood of (t_0, x_0) given by $[t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, 2r)$. In the same way the minimizing geodesic $\gamma_{x,x_0} : [t, t_0 + 2\delta] \to M$ joining x to x_0 is contained in $\bar{B}(x_0, 2r)$ and has action $\mathbb{L}(\gamma_{x,x_0})$ less than $(t_0 + 2\delta - t)A(d(x, x_0)/(t_0 + 2\delta - t)) \le 3\delta A(2r/\delta)$. Therefore

$$U(t_0 + 2\delta, x_0) \le U(t, x) + 3\delta A(2r/\delta),$$

which implies that U is bounded below on $[t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, 2r)$. We then set

$$K = 2 \sup\bigl\{|U(t, x)| \bigm| (t, x) \in [t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, 2r)\bigr\} < +\infty.$$

Fix $(t, x), (t', x') \in [t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, 2r)$, with $t' < t$.
We obviously get

$$U(t', x') - U(t, x) \le K \le h_{t'-t}(x, x') \quad \text{for } h_{t'-t}(x, x') \ge K. \tag{5-3}$$

If $h_{t'-t}(x, x') \le K$, pick a minimizer $\gamma : [t, t'] \to M$, with $\gamma(t) = x$, $\gamma(t') = x'$ and $h_{t'-t}(x, x') = \mathbb{L}(\gamma) \le K$, since $|t' - t| \le 2\delta$, from Lemma 4.3, we obtain

$$\ell_g(\gamma \,|\, [t, t']) \le \eta_{K,2\delta}(|t' - t|),$$

where $\eta_{K,2\delta} : [0, +\infty[\,\to [0, +\infty[$ is a modulus of continuity; i.e., the function $\eta_{K,2\delta}$ is continuous at 0 and $\eta_{K,2\delta}(0) = 0$. Therefore, we can find $\epsilon > 0$, with $\epsilon < \delta$, such that $\eta_{K,2\delta}(s) \le r$ for all $s \le 2\epsilon$. Hence, if we further assume that

$$(t, x), (t', x') \in [t_0 - \epsilon, t_0 + \epsilon] \times \bar{B}(x_0, r),$$

we obtain $\ell_g(\gamma \,|\, [t, t']) \le r$ and $\gamma([t, t']) \subset \bar{B}(x_0, 2r)$. Since the graph of γ is contained in $[t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, 2r) \subset O$ and U is evolution-dominated by L on O, we get

$$U(t', x') - U(t, x) \le h_{t'-t}(x, x').$$

Together with (5-3), this shows that U is *strongly* evolution-dominated by L on $[t_0 - \epsilon, t_0 + \epsilon] \times \bar{B}(x_0, r)$. □

The reader will notice that the proof of the next proposition, giving the connection between evolution domination and viscosity subsolution, is very similar to the (standard) proof of Proposition 14.3 in [7], once we have Corollary 2.3. We provide a complete proof for the reader's convenience.

Proposition 5.5. *Let H be a Tonelli Hamiltonian on the complete Riemannian manifold M. Suppose $U : O \to \mathbb{R}$ is a continuous function defined on the open subset O. Then U is a viscosity subsolution of*

$$\partial_t U + H(x, \partial_x U) = 0, \tag{5-4}$$

on O if and only if it is evolution-dominated by L on O.

Proof. Assume that U is a viscosity subsolution of (5-4). We prove that

$$U(b, \gamma(b)) - U(a, \gamma(a)) \leq \int_a^b L(\gamma(s), \dot{\gamma}(s))\, dt, \tag{5-5}$$

holds for an absolutely continuous curve $\gamma : [a, b] \to M$, with $\mathrm{Graph}(\gamma) \subset O$.

If U is smooth, the Fenchel inequality (3-2) between L and H yields

$$\partial_x U(t, x)(v) \leq L(x, v) + H(x, \partial_x U(t, x)) \quad \text{for all } v \in T_x M.$$

Since the viscosity subsolution U of (5-4) is smooth on O, we have

$$\partial_t U(t, x) + H\,(x, \partial_x U(t, x)) \leq 0 \text{ everywhere on } O.$$

We combine the two inequalities to obtain

$$\partial_t U(t, x) + \partial_x U(t, x)(v) \leq L(x, v) \quad \text{for all } (t, x, v) \text{ with } (t, x) \in O,\ v \in T_x M.$$

Therefore, since $\mathrm{Graph}(\gamma) \subset O$ and γ is absolutely continuous, we obtain

$$\partial_t U(t, \gamma(t)) + \partial_x U(t, \gamma(t))(\dot{\gamma}(t)) \leq L(\gamma(t), \dot{\gamma}(t)) \quad \text{for almost all } s \in [a, b].$$

By integration, this proves the desired inequality.

For U just continuous, since $\gamma([a, b])$ is a compact subset, we can use Corollary 2.3 to reduce, by an approximation argument, this continuous case to the smooth case.

Let us now assume that U satisfies (5-5) for every absolutely continuous curve $\gamma : [a, b] \to M$, with $\mathrm{Graph}(\gamma) \subset O$. To prove that U is a viscosity subsolution of (5-4), consider a C^1 function $\Phi : O \to \mathbb{R}$, with $\Phi \geq U$ and $\Phi(t, x) = U(t, x)$, for some $(t, x) \in O$. If $v \in T_x M$, let $\gamma : [t - 1, t] \to M$ be a smooth curve with $\gamma(t) = x$ and $\dot{\gamma}(t) = v$. Since γ is continuous and O is open for $\epsilon > 0$ small enough, we have $\mathrm{Graph}(\gamma \mid [t - \epsilon, t]) \subset O$. Using $\Phi \geq U$ and inequality (5-5), we get

$$\begin{aligned}\Phi(t, \gamma(t)) - \Phi(t - \epsilon, \gamma(t - \epsilon)) &\leq U(t, \gamma(t)) - U(t - \epsilon, \gamma(t - \epsilon)) \\ &\leq \int_{t-\epsilon}^{t} L(\gamma(s), \dot{\gamma}(s))\, dt.\end{aligned}$$

Dividing by ϵ and letting $\epsilon \to 0$ yields

$$\partial_t \Phi(t, x) + \partial_x \Phi(t, x)[v] \leq L(x, v),$$

or equivalently

$$\partial_t \Phi(t, x) + \partial_x \Phi(t, x)[v] - L(x, v) \leq 0.$$

Taking the supremum over all $v \in T_x M$, we obtain

$$\partial_t \Phi(t, x) + H(x, \partial_x \Phi(t, x)) \leq 0. \qquad \square$$

6. A construction of viscosity solutions

Again in the sequel, we fix a Tonelli Hamiltonian $H : T^*M \to \mathbb{R}$ on the complete Riemannian manifold (M, g) and we will denote by $L : TM \to \mathbb{R}$ its associated Tonelli Lagrangian.

We will give a rather general way to obtain viscosity solutions on open subsets of $\mathbb{R} \times M$ of the Hamilton–Jacobi equation (1-1).

We start with a nonempty subset $K \subset \mathbb{R} \times M$. Besides being nonempty, we do not impose any other property on K. We set

$$t_{K,\inf} = \inf\{t \mid (t, x) \in K\},$$

We consider a function $U : K \to [-\infty, +\infty[$. We do not assume U continuous or even measurable; the only restriction (for convenience) is that U does not take the value $+\infty$. See Remark 6.1(1), however. We can define the function $\hat{U}$ on $]t_{K,\inf}, +\infty[\times M \to [-\infty, +\infty[$ by

$$\hat{U}(t, x) = \inf\{U(\tilde{t}, \tilde{x}) + h_{t-\tilde{t}}(\tilde{x}, x) \mid (\tilde{t}, \tilde{x}) \in K \text{ and } \tilde{t} \leq t\}. \tag{6-1}$$

Note that this definition makes sense for $t > t_{K,\inf}$, since for such a t the set $\{\tilde{t} \mid (\tilde{t}, \tilde{x}) \in K \text{ and } \tilde{t} \leq t\}$ is not empty.

Remark 6.1. (1) Suppose that we have a function $U : K \to [-\infty, +\infty]$, which may assume the value $+\infty$. If U is not identically $+\infty$, define K_f as

$$K_f = \{(t, x) \mid U(t, x) \neq +\infty\}.$$

Then K_f is not empty and $U_f = U \mid K_f$ never takes the value $+\infty$. We can then define $\hat{U}_f :]t_{\inf}(K_f), +\infty[\times M \to [-\infty, +\infty[$ as above by

$$\hat{U}_f(t, x) = \inf\{U(\tilde{t}, \tilde{x}) + h_{t-\tilde{t}}(\tilde{x}, x) \mid (\tilde{t}, \tilde{x}) \in K_f \text{ and } \tilde{t} \leq t\}.$$

If $t_{K,\inf} = t_{K_f,\inf}$ or equivalently

$$t_{K,\inf} = \inf\{t \mid (t, x) \in K \text{ and } U(t, x) \neq +\infty\}, \tag{6-2}$$

then we have

$$\hat{U}_f(t,x) = \hat{U}(t,x) = \inf\{U(\tilde{t},\tilde{x}) + h_{t-\tilde{t}}(\tilde{x},x) \mid (\tilde{t},\tilde{x}) \in K \text{ and } \tilde{t} \leq t\}.$$

(2) A special case of the construction above is the Lax–Oleinik evolution; see Definition 8.2 and Remark 8.4(3) below.

Theorem 6.2. *Let $U : K \to [-\infty, +\infty[$ be a function defined on the subset $K \subset \mathbb{R} \times M$.*

Define the function $\hat{U}$ on $]t_{\inf,K}, +\infty[\times M \to [-\infty, +\infty[$ by

$$\hat{U}(t,x) = \inf\{U(\tilde{t},\tilde{x}) + h_{t-\tilde{t}}(\tilde{x},x) \mid (\tilde{t},\tilde{x}) \in K \text{ and } \tilde{t} \leq t\}, \tag{6-3}$$

where $t_{K,\inf} = \inf\{t \mid (t,x) \in K\}$. This function $\hat{U}$, is strongly evolution-dominated by L on $]t_{\inf,K}, +\infty[\times M$. Moreover, if $\hat{U}(T,X)$ is finite for some $X \in M$ and some $T \in]t_{K,\inf}, +\infty[$, then the function $\hat{U}$ is

(i) *finite everywhere on $]t_{K,\inf}, T[\times M$;*

(ii) *bounded on every compact subset of $]t_{\inf,K}, T[\times M$;*

(iii) *continuous, locally semiconcave on $]t_{K,\inf}, T[\times M \setminus \bar{K}$;*

(iv) *a viscosity solution of the evolutionary Hamilton–Jacobi* (1-1) *on*

$$]t_{K,\inf}, T[\times M \setminus \bar{K}.$$

Proof. To prove the strong evolution domination, note that for $(t,x), (t',x') \in]t_{\inf,K}, +\infty[\times M$, with $t' < t$, if $\tilde{t} \leq t'$, then $\tilde{t} \leq t$. Therefore, for $(\tilde{t},\tilde{x}) \in K$, with $\tilde{t} \leq t'$, from (6-1), we get

$$\hat{U}(t,x) \leq U(\tilde{t},\tilde{x}) + h_{t-\tilde{t}}(\tilde{x},x) \leq U(\tilde{t},\tilde{x}) + h_{t'-\tilde{t}}(\tilde{x},x') + h_{t-t'}(x',x).$$

Again from (6-1), taking the inf over all $(\tilde{t},\tilde{x}) \in K$, with $\tilde{t} \leq t'$, we obtain

$$\hat{U}(t,x) \leq \hat{U}(t',x') + h_{t-t'}(x',x),$$

which means that $\hat{U}$ is strongly evolution-dominated by L on $]t_{\inf,K}, +\infty[\times M$.

For the rest of the proof, we assume that $\hat{U}(T,X)$ is finite for some $X \in M$ and $T \in]t_{K,\inf}, +\infty[$.

Property (i) is a consequence of (ii). We now prove (ii). Let C be a nonempty compact subset of $]t_{\inf,K}, T[\times M$. By the strong L evolution domination on $]t_{K,\inf}, T[\times M$, we have

$$\hat{U}(T,X) \leq \hat{U}(t,x) + h_{T-t}(x,X) \quad \text{for } t \in]t_{\inf,K}, T[.$$

Since $(t,x) \mapsto h_{T-t}(x,X)$ is finite and continuous on $]\tilde{t}, T[\times M$, which implies that it is bounded from above on the compact subset $C \subset]\tilde{t}, T[\times M$. We conclude that $\hat{U}$ is bounded from below on C.

It remains to show that $\hat{U}$ is bounded from above on C. By compactness of C, we have $t_{\inf,C} = \inf\{t \mid (t,x) \in C\} > t_{\inf,K}$. In particular, we can find $(\tilde{t}, \tilde{x}) \in K$ with $t_{\inf,C} > \tilde{t} \geq t_{\inf,K}$. From (6-1)

$$\hat{U}(t,x) \leq U(\tilde{t},\tilde{x}) + h_{t-\tilde{t}}(\tilde{x},x) \quad \text{for } t > \tilde{t}.$$

Note that we are assuming that U does not take the value $+\infty$, hence $U(\tilde{t},\tilde{x}) < +\infty$. Since C is a compact set contained in $]\tilde{t}, T[\times M$ and $(t,x) \mapsto h_{t-\tilde{t}}(\tilde{x},x)$ is finite and continuous on $]\tilde{t}, +\infty[\times M$, this function $(t,x) \mapsto h_{t-\tilde{t}}(\tilde{x},x)$ is bounded on the compact set C. Hence $\hat{U}(t,x)$ is bounded from above on C.

To prove (iii) and (iv), we first prove a lemma.

Lemma 6.3. *Under the hypothesis of Theorem 6.2, suppose that $\hat{U}(T,X)$ is finite for some $X \in M$ and $T \in]t_{K,\inf}, +\infty[$. Assume that $\delta > 0$ and $(t_0,x_0) \in]t_{\inf,K}, T[\times M$ are such that*

$$[t_0-\delta, t_0+\delta] \times \bar{B}(x_0,\delta) \subset]t_{\inf,K}, T[\times M \setminus \bar{K}.$$

We can find $\epsilon > 0$, with $2\epsilon < \delta$, such that, for all $(t,x) \in [t_0-\epsilon, t_0+\epsilon] \times \bar{B}(x_0,\epsilon)$, we have

$$\hat{U}(t,x) = \inf\{\hat{U}(t',x') + h_{t-t'}(x',x) \mid (t',x') \in [t_0-\delta, t_0-2\epsilon] \times \bar{B}(x_0,\delta)\}.$$

Proof. For all $\epsilon > 0$, with $2\epsilon < \delta$, the inequality

$$\hat{U}(t,x) \leq \inf\{\hat{U}(t',x') + h_{t-t'}(x',x) \mid (t',x') \in [t_0-\delta, t_0-2\epsilon] \times \bar{B}(x_0,\delta)\}$$

follows from the just established strong L domination of $\hat{U}$. Therefore, it suffices to show that, we can find $\epsilon > 0$, with $2\epsilon < \delta$, such that, for all $(t,x) \in [t_0-\epsilon, t_0+\epsilon] \times \bar{B}(x_0,\epsilon)$ and all $\eta \in]0,1]$, we have

$$\inf\{\hat{U}(t',x') + h_{t-t'}(x',x) \mid (t',x') \in [t_0-\delta, t_0-2\epsilon] \times \bar{B}(x_0,\delta)\} \leq \hat{U}(t,x) + \eta.$$

From the already established part (ii), the function $\hat{U}$ is bounded on the compact subset $[t_0-\delta, t_0+\delta] \times \bar{B}(x_0,\delta)$ of $]t_{\inf,K}, T[\times M \setminus \bar{K}$. Therefore

$$A = 1 + 2\sup\{|\hat{U}(t,x)| \mid [t_0-\delta, t_0+\delta] \times \bar{B}(x_0,\delta)\} < +\infty. \tag{6-4}$$

Denote by $\eta_{A,2\delta}$ the continuity modulus provided by Lemma 4.3. Hence, for every absolutely continuous curve $\gamma : [a,b] \to M$, with $b-a \leq 2\delta$ and $\mathbb{L}(\gamma) \leq A$, we have

$$d(\gamma(t'), \gamma(t)) \leq \ell_g(\gamma \mid [t,t']) \leq \eta_{A,2\delta}(|t'-t|) \quad \text{for all } t, t' \in [a,b]. \tag{6-5}$$

Since $\eta_{A,2\delta}$ is a modulus of continuity, we can pick $\epsilon > 0$, with $3\epsilon < \delta$ such that

$$\eta_{A,2\delta}(\alpha) < \delta/3 \quad \text{for } 0 \leq \alpha \leq 3\epsilon. \tag{6-6}$$

Fix now $(t, x) \in\in [t_0 - \epsilon, t_0 + \epsilon] \times \bar{B}(x_0, \epsilon)$ and $\eta \in]0, 1]$. By the definition of $\hat{U}$, (6-1), we can find $(\tilde{t}, \tilde{x}) \in K$ such that

$$U(\tilde{t}, \tilde{x}) + h_{t-\tilde{t}}(\tilde{x}, x) \leq \hat{U}(t, x) + \eta. \tag{6-7}$$

Pick a minimizer $\gamma : [\tilde{t}, t] \to M$, with $\gamma(\tilde{t}) = \tilde{x}$ and $\gamma(t) = x$. Since $(\tilde{t}, \gamma(\tilde{t})) \in K$, which is disjoint from $[t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, \delta)$, and $(t, \gamma(t)) \in [t_0 - \epsilon, t_0 + \epsilon] \times \bar{B}(x_0, \epsilon) \subset]t_0 - \delta, t_0 + \delta[\times \mathring{B}(x_0, \delta)$, we can find $s \in]\tilde{t}, t[$ with $(s, \gamma(s)) \in \partial\big([t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, \delta)\big)$. We have

$$t_0 - \delta \leq s \leq t \leq t_0 + \epsilon < t_0 + \delta \text{ and } \gamma(s) \in \bar{B}(x_0, \delta). \tag{6-8}$$

Since γ is a minimizer and $\gamma(\tilde{t}) = \tilde{x}$, $\gamma(t) = x$, we have

$$\begin{aligned} h_{t-\tilde{t}}(\tilde{x}, x) &= h_{t-\tilde{t}}(\gamma(\tilde{t}), \gamma(t)) \\ &= h_{s-\tilde{t}}(\gamma(\tilde{t}), \gamma(s)) + h_{t-s}(\gamma(s), \gamma(t)) \\ &= h_{s-\tilde{t}}(\tilde{x}, \gamma(s)) + h_{t-s}(\gamma(s), x), \end{aligned}$$

which, by (6-7), implies

$$U(\tilde{t}, \tilde{x}) + h_{s-\tilde{t}}(\tilde{x}, \gamma(s)) + h_{t-s}(\gamma(s), \gamma(t)) \leq \hat{U}(t, x) + \eta.$$

But, again by the definition (6-1) of $\hat{U}$, we have

$$\hat{U}(s, \gamma(s)) \leq U(\tilde{t}, \tilde{x}) + h_{s-\tilde{t}}(\tilde{x}, \gamma(s)).$$

Combining the last two inequalities, we obtain

$$\hat{U}(s, \gamma(s)) + h_{t-s}(\gamma(s), \gamma(t)) \leq \hat{U}(t, x) + \eta, \tag{6-9}$$

<u>*Claim*</u> We have $s \leq t_0 - 2\epsilon$.

From this claim, we can finish the proof of the Lemma.

In fact, combining the claim and (6-8), we have $(s, \gamma(s)) \in [t_0 - \delta, t_0 - 2\epsilon] \times \bar{B}(x_0, \delta)$. Therefore, using (6-9), we obtain

$$\begin{aligned} \inf\big\{\hat{U}(t', x') + h_{t-t'}(x', \gamma(t)) \mid (t', x') \in [t_0 - \delta, t_0 - 2\epsilon] \times \bar{B}(x_0, \delta)\big\} \\ \leq \hat{U}(s, \gamma(s)) + h_{t-s}(\gamma(s), \gamma(t)) \\ \leq \hat{U}(t, x) + \eta. \end{aligned}$$

It remains to prove the claim. Since $(s, \gamma(s)) \in \partial\big([t_0 - \delta, t_0 + \delta] \times \bar{B}(x_0, \delta)\big)$ and $s < t_0 + \delta$, either $s = t_0 - \delta$ or $\gamma(s) \in \partial \bar{B}(x_0, \delta)$. In the first case, we get $s = t_0 - \delta < t - 2\epsilon$ and the claim holds. In the second case, we have $d(x_0, \gamma(s)) = \delta$. But $\gamma(t) = y \in \bar{B}(x_0, \epsilon)$, hence, using $3\epsilon < \delta$, we get

$$d(\gamma(t), \gamma(s)) \geq \delta - \epsilon > \delta/3.$$

We now observe that (6-9) implies

$$\mathbb{L}(\gamma\,|\,[s,t]) = h_{t-s}(\gamma(s),\gamma(t)) \le \hat U(t,x) - \hat U(s,\gamma(s)) + \eta \le A < +\infty, \tag{6-10}$$

since $\eta \le 1$, both (t,x), $(s,\gamma(s))$ are in $[t_0-\delta, t_0+\delta]\times \bar B(x_0,\delta)$ and A is given by (6-4). Furthermore, we have $s<t$ and $s,t\in[t_0-\delta,t_0+\delta]$, which yields $0<t-s\le 2\delta$. Therefore, by the property (6-5) defining $\eta_{A,2\delta}$, we get

$$d(\gamma(t),\gamma(s)) \le \eta_{A,2\delta}(t-s).$$

Since $d(\gamma(t),\gamma(s)) > \delta/3$, it follows from by the definition of ϵ, (6-6), that $t-s>3\epsilon$, which implies

$$s < t-3\epsilon \le (t_0+\epsilon)-3\epsilon = t_0-2\epsilon. \qquad \square$$

End of the proof of Theorem 6.2. To prove (iii) and (iv), we fix (t_0,x_0) in the open subset $]t_{K,\inf}, T[\,\times M\setminus \bar K$, we then pick $\delta>0$ such that

$$[t_0-\delta,t_0+\delta]\times \bar B(x_0,\delta) \subset\,]t_{\inf,K}, T[\,\times M\setminus \bar K.$$

By Lemma 6.3, we can find $\epsilon>0$ such that

$$\hat U(t,x) = \inf\{\hat U(t',x') + h_{t-t'}(x',x) \mid (t',x')\in[t_0-\delta,t_0-2\epsilon]\times \bar B(x_0,\delta)\}, \tag{6-11}$$

for all $(t,x)\in[t_0-\epsilon,t_0+\epsilon]\times\bar B(x_0,\epsilon)$. The map

$$[(t,x),(t',x')] \mapsto (t-t',x',x)$$

is smooth and takes values in $]0,+\infty[\,\times M\times M$ on the compact set

$$\big([t_0-\epsilon,t_0+\epsilon]\times\bar B(x_0,\epsilon)\big)\times\big([t_0-\delta,t_0-2\epsilon]\times\bar B(x_0,\delta)\big).$$

Since, by Proposition 4.19, the map $(s,x',x)\mapsto h_s(x',x)$ is locally semiconcave on $]0,+\infty[\,\times M\times M$, we conclude that $[(t,x),(t',x')]\mapsto h_{t-t'}(x',x)$ is locally semiconcave on a neighborhood of $\big([t_0-\epsilon,t_0+\epsilon]\times\bar B(x_0,\epsilon)\big)\times\big([t_0-\delta,t_0-2\epsilon]\times\bar B(x_0,\delta)\big)$. Hence, since $[t_0-\delta,t_0-2\epsilon]\times\bar B(x_0,\delta)$ is compact, we conclude that the family of maps

$$(t,x)\mapsto h_{t-t'}(x',x),\ (t',x')\in[t_0-\delta,t_0-2\epsilon]\times\bar B(x_0,\delta)$$

is uniformly locally semiconcave on a neighborhood of the compact set $[t_0-\epsilon, t_0+\epsilon]\times\bar B(x_0,\epsilon)$; see [8, Appendix A]. Therefore, so is the family $(t,x)\mapsto \hat U(t',x')+h_{t-t'}(x',x)$, $(t',x')\in[t_0-\delta,t_0-2\epsilon]\times\bar B(x_0,\delta)$, which by equality (6-11) implies that the finite function $\hat U$ is locally semiconcave (and therefore continuous) on a neighborhood $[t_0-\delta,t_0+\delta]\times\bar B(x_0,r)$. See [8, Proposition A.16, p. 34–35].

We then observe that by Proposition 4.26, since H does not depend on the time t, for each $(t', x') \in [t_0 - \delta, t_0 - 2\epsilon] \times \bar{B}(x_0, \delta)$, the function $(t, x) \mapsto \hat{U}(t', x') + h_{t-t'}(x', x)$ is a viscosity solution of the evolutionary Hamilton–Jacobi (1-1) on $]t_0 - 2\epsilon, +\infty[\times M$. Since we already now that $\hat{U}$ is finite and continuous on a neighborhood of $[t_0 - \epsilon, t_0 + \epsilon] \times \bar{B}(x_0, \epsilon)$, by Corollary 2.5 and equality (6-11), we conclude that $\hat{U}$ is a viscosity solution of the evolutionary Hamilton–Jacobi (1-1) on a neighborhood of $[t_0 - \epsilon, t_0 + \epsilon] \times \bar{B}(x_0, \epsilon)$. □

Proposition 6.4. *Assume $C \subset M$ is a closed subset and $a < b \in \mathbb{R}$. Suppose $U : [a, b] \times C \to \mathbb{R}$ is continuous and strongly evolution-dominated by L on $[a, b] \times C$. Set $K = \{a\} \times C \cup [a, b] \times \partial C \subset \mathbb{R} \times M$. Call $\hat{U}$ the function defined on $]a, +\infty[\times M$ by* (6-1) *using the restriction $U \mid K$:*

$$\hat{U}(t, x) = \inf\{U(t', x') + h_{t-t'}(x', x) \mid (t', x') \in K, t' < t\} \quad \text{for } t > a \text{ and } x \in M. \tag{6-12}$$

The function $\hat{\hat{U}} : [a, b] \times C \to \mathbb{R}$ defined by

$$\hat{\hat{U}}(t, x) = \begin{cases} U(a, x) & \text{for } t = a \text{ and } x \in C, \\ \hat{U}(t, x) & \text{for } t > a \text{ and } x \in C, \end{cases}$$

is continuous, strongly evolution-dominated by L and $\geq U$ on $[a, b] \times C$, with $\hat{\hat{U}} \mid K = \hat{U} \mid K$.

Moreover, this function $\hat{\hat{U}}$ is a locally semiconcave viscosity solution of the evolutionary on Hamilton–Jacobi (1-1) *on $]a, b[\times \mathring{C}$.*

Proof. We first note that the inequality $\hat{U} \geq U$ on $]a, +\infty[\times M$ follows from the definition of $\hat{U}$ and the strongly L evolution domination of U on $[a, b] \times C$. This obviously implies that $\hat{\hat{U}} \geq U$ on $[a, b] \times C$.

Since, by Theorem 6.2, the function $\hat{U}$ is strongly L evolution-dominated on $]a, +\infty[\times M$, we obtain that $\hat{\hat{U}}$ is strongly L evolution-dominated on $]a, b] \times C$. From the definition of $\hat{U}$, we conclude that $\hat{\hat{U}}$ is strongly L evolution-dominated on $[a, b] \times C$.

Since by Theorem 6.2, the function $\hat{U}$ is continuous on $]a, +\infty[\times M \setminus \bar{K} \supset]a, b] \times \mathring{C}$. We have to show continuity at every point of $K = \{a\} \times C \cup [a, b] \times \partial C$. Let us start with continuity at (a, x) with $x \in C$. Using that $\hat{\hat{U}} \geq U$ is strongly L evolution-dominated on $[a, b] \times C$, we get

$$U(t, y) \leq \hat{\hat{U}}(t, y) \leq \hat{\hat{U}}(a, y) + h_{t-a}(y, y) \leq U(a, y) + (t - a)A(0).$$

By continuity of U, we obtain the continuity of $\hat{\hat{U}}$ at every point of $\{a\} \times C$. It remains to show that $\hat{\hat{U}}$ is continuous at (t_0, x_0), with $a < t_0 \leq b$ and $x_0 \in \partial C$. We will show at the same time that $\hat{\hat{U}}(t_0, x_0) = \hat{U}(t_0, x_0)$. Fix $t' \in]a, t_0[$. Since

$\hat{\hat{U}} = \hat{U} \geq U$ on $]a, b] \times C$, for all $(t, x) \in]t', b] \times C$, we have

$$U(t, x) \leq \hat{\hat{U}}(t, x) = \hat{U}(t, x) \leq U(t', x_0) + h_{t-t'}(x_0, x), \tag{6-13}$$

where the last inequality follows from the definition of $\hat{U}$, since $t' < t$ and $(t', x_0) \in]a, t_0[\times \partial C \subset K$. If we apply this inequality with $(t, x) = (t_0, x_0)$, we obtain

$$U(t_0, x_0) \leq \hat{\hat{U}}(t_0, x_0) \leq U(t', x_0) + h_{t_0-t'}(x_0, x_0) \leq U(t', x_0) + A(0)(t_0 - t').$$

If we let $t' \to t_0$, by continuity of U, this last inequality yields $\hat{\hat{U}}(t_0, x_0) = U(t_0, x_0)$.

If, in equality (6-13), we keep $t' \in]a, t_0[$ fixed and we let $(t, x) \to (t_0, x_0)$, by continuity of U and h, we obtain

$$\begin{aligned} U(t_0, x_0) \leq \liminf_{(t,x)\to(t_0,x_0)} \hat{\hat{U}}(t, x) &\leq \limsup_{(t,x)\to(t_0,x_0)} \hat{\hat{U}}(t, x) \\ &\leq U(t', x_0) + h_{t-t'}(x_0, x_0) \leq U(t', x_0) + A(0)(t - t'). \end{aligned}$$

Letting again $t' \to t_0$, we conclude that $\lim_{(t,x)\to(t_0,x_0)} \hat{\hat{U}}(t, x) = U(t_0, x_0) = \hat{\hat{U}}(t_0, x_0)$. Therefore we finished both the proof of the continuity of $\hat{\hat{U}} = \hat{U}$, and the equality $\hat{\hat{U}} \,|\, K = U \,|\, K$.

The fact that $\hat{\hat{U}}$ is a locally semiconcave viscosity solution of the evolutionary Hamilton–Jacobi equation (1-1) on $]a, b[\times \mathring{C}$ follows also from Theorem 6.2, since $\hat{\hat{U}} = \hat{U}$ on $]a, b[\times \mathring{C}$. $\square$

Theorem 6.5. *Suppose $O \subset \mathbb{R} \times M$ is an open subset. If $U : O \to \mathbb{R}$ is a continuous viscosity solution of the evolutionary Hamilton–Jacobi equation* (1-1) *on O, then it is locally semiconcave.*

Moreover, for every $(t, x) \in O$, we can find $(t', x') \in O$, with $t' < t$, such that

$$U(t, x) = U(t', x') + h_{t-t'}(x', x).$$

Proof. Fix $(t_0, x_0) \in O$. Since U is a viscosity solution on O, from Proposition 5.5 we obtain that U is dominated by L on O. By Proposition 5.4, we can find a neighborhood V of (t_0, x_0) in O on which U is strongly dominated by L. Without loss of generality, we can assume that $V = [t_0 - \eta, t_0 + \eta] \times \bar{B}(x_0, \eta) \subset O$, for some $\eta > 0$. We set $\mathfrak{K} = \{t_0 - \eta\} \times \bar{B}(x_0, \eta) \cup [t_0 - \eta, t_0 + \eta] \times \partial \bar{B}(x_0, \eta)$.

By Proposition 6.4, the function $\hat{\hat{U}} : [t_0 - \eta, t_0 + \eta] \times \bar{B}(x_0, r) \to \mathbb{R}$ defined by

$$\hat{U}(t, x) = \begin{cases} U(t, x) & \text{if } t = a \text{ and } x \in \bar{B}(x_0, \eta), \\ \inf\{U(t', x') + h_{t-t'}(x', x) \mid (t', x') \in \mathfrak{K},\, t' < t\} & \\ & \text{if } t > a \text{ and } x \in \bar{B}(x_0, \eta), \end{cases}$$

is continuous, is a locally semiconcave viscosity solution of the evolutionary on Hamilton–Jacobi (1-1) on $]t_0-\eta, t_0+\eta[\times \mathring{B}(x_0,r)$ and satisfies $\hat{\hat{U}}=U$ on $\mathfrak{K}=\{t_0-\eta\}\times\bar{B}(x_0,\eta)\cup[t_0-\eta,t_0+\eta]\times\partial\bar{B}(x_0,\eta)$. Since $\hat{\hat{U}}=U$ on $\mathfrak{K}=\{t_0-\eta\}\times\bar{B}(x_0,\eta)\cup[t_0-\eta,t_0+\eta]\times\partial\bar{B}(x_0,\eta)$, Corollary 2.7 of the maximum principle implies $\hat{\hat{U}}=U$ on $[t_0-\eta,t_0+\eta]\times\bar{B}(x_0,r)$. But, by Proposition 6.4, the function $\hat{\hat{U}}$ is locally semiconcave on $]t_0-\eta,t_0+\eta[\times\mathring{B}(x_0,\eta)$. This proves the first part of the theorem.

To prove the remaining part of the theorem, we use the equality $\hat{\hat{U}}=U$ on $[t_0-\eta,t_0+\eta]\times\bar{B}(x_0,r)$ and the definition of $\hat{\hat{U}}$ to find a sequence $(t'_n,x'_n)\in\mathfrak{K}=\{t_0-\eta\}\times\bar{B}(x_0,\eta)\cup[t_0-\eta,t_0+\eta]\times\partial\bar{B}(x_0,\eta)$, with $t'_n<t_0$, such that

$$U(t_0,x_0)\le U(t'_n,x'_n)+h_{t_0-t'_n}(x'_n,x_0)\to U(t_0,x_0)\quad\text{as } n\to+\infty. \tag{6-14}$$

Since $\mathfrak{K}$ is compact, extracting if necessary, we can assume that $(t'_n,x'_n)\to(t',x')\in\mathfrak{K}$ and

$$U(t'_n,x'_n)+h_{t_0-t'_n}(x'_n,x_0)\le U(t_0,x_0)+1.$$

By continuity of U and convergence of (t'_n,x'_n), we have

$$m=\sup_n U(t_0,x_0)-U(t'_n,x'_n)+1<+\infty.$$

Therefore

$$h_{t-t'_n}(x'_n,x)\le m\quad\text{for all } n.$$

Using the left side of the inequality (4-7) in Lemma 4.11, we obtain

$$-C(K)(t_0-t'_n)+Kd(x_0,x'_n)\le h_{t_0-t'_n}(x'_n,x_0)\le m\quad\text{for all } n \text{ and all } K\ge 0.$$

Taking the limit as $n\to+\infty$ and reshuffling, we get

$$Kd(x_0,x')\le C(K)(t_0-t')+m\quad\text{for all } K\ge 0.$$

We now claim that $t'<t_0$. We already know that $t'\le t_0$, since $t'_n<t_0$, for all n. Suppose then by contradiction that $t'=t_0$. The inequality above then implies

$$Kd(x_0,x')\le m\quad\text{for all } K\ge 0.$$

From $m<+\infty$, we conclude $x_0=x'$. Hence $(t',x')=(t_0,x_0)$. This is a contradiction, since $(t',x')\in\mathfrak{K}=\{t_0-\eta\}\times\bar{B}(x_0,\eta)\cup[t_0-\eta,t_0+\eta]\times\partial\bar{B}(x_0,\eta)$. Now that we know that $t'<t_0$, using the continuity of $(s,x,y)\mapsto h_s(x,y)$ for $(s,x,y)\in]0,+\infty[\times M\times M$ we can pass to the limit in (6-14) to obtain

$$U(t_0,x_0)=U(t',x')+h_{t_0-t'}(x',x_0).$$ □

7. Calibrated curves, backward characteristics and differentiability

We again fix a Tonelli Hamiltonian $H : T^*M \to \mathbb{R}$ on the complete Riemannian manifold (M, g) and denote its associated Tonelli Lagrangian by $L : TM \to \mathbb{R}$.

Definition 7.1 (calibrated curve). Let $U : S \to [-\infty, +\infty]$ be a function defined on the subset $S \subset \mathbb{R} \times M$. A curve $\gamma : [a, b] \to M$ is said to be U-calibrated for the Lagrangian L if it is an absolutely continuous curve, with $\mathrm{Graph}(\gamma) \subset S$, whose action $\mathbb{L}(\gamma) = \int_a^b L(\gamma(s), \dot\gamma(s))\, ds$ is finite and

$$U(b, \gamma(b)) = U(a, \gamma(a)) + \mathbb{L}(\gamma) = U(a, \gamma(a)) + \int_a^b L(\gamma(s), \dot\gamma(s))\, ds.$$

Remark 7.2. (1) For such a U-calibrated curve $\gamma : [a, b] \to M$, since its action is finite, if either $U(a, \gamma(a))$ or $U(b, \gamma(b))$ is infinite they are both equal and infinite.

(2) It is not difficult to check that the property of being calibrated is stable by concatenations of curves; i.e., if $\gamma_1 : [a, b] \to M$ and $\gamma_2 : [b, c] \to M$ are U-calibrated, with $\gamma_1(b) = \gamma_2(b)$, then so is the concatenation $\gamma = \gamma_1 * \gamma_2 : [a, c] \to M$, defined by

$$\gamma(t) = \begin{cases} \gamma_1(t) & \text{for } t \in [a, b], \\ \gamma_2(t) & \text{for } t \in [b, c]. \end{cases}$$

(3) More generally, a curve $\gamma : [a, b] \to M$ is said to be piecewise calibrated if we can find a finite sequence $a = t_0 < t_1 < \cdots < t_\ell = b$ such that each restriction $\gamma \,|\, [t_i, t_{i+1}]$, $i = 0, \dots, \ell - 1$ is U-calibrated. Of course, by part (2), any piecewise U-calibrated is U-calibrated.

(4) Suppose $u : O \to \mathbb{R}$ is a function defined on the subset $O \subset M$ and $c \in \mathbb{R}$. If we define $U : \mathbb{R} \times O \to \mathbb{R}$ by

$$U(t, x) = u(x) - ct,$$

it not difficult to see that the absolutely continuous curve $\gamma : [a, b] \to M$ is U-calibrated if and only if $\gamma([a, b]) \subset O$ and

$$u(\gamma(b)) - u(\gamma(b) = \int_a^b L(\gamma(s), \dot\gamma(s)) + c\, ds;$$

i.e., the curve γ is (u, L, c)-calibrated as defined, for example, in [6].

Definition 7.3 (local backward characteristic). Let $U : S \to [-\infty, +\infty]$ be a function defined on the subset $S \subset \mathbb{R} \times M$. A local backward U-characteristic ending at $(t, x) \in S$ is a U-calibrated curve $\gamma : [t - \epsilon, t] \to M$, with $\epsilon > 0$ and $\gamma(t) = x$.

More generally, a curve $\gamma : [a, t] \to M$ is called a local backward U-characteristic if it is a local backward U-characteristic ending at $(t, \gamma(t)) \in S$.

Theorem 6.5 obviously implies the following one:

Theorem 7.4. *Suppose $O \subset\,]0, +\infty[\, \times M$ is an open subset. If $U : O \to \mathbb{R}$ is a continuous viscosity solution of the evolutionary Hamilton–Jacobi equation* (1-1) *on O, then for every $(t, x) \in O$, we can find a local backward U-characteristic ending at (t, x).*

In fact, the notion of U-calibrated curve, or of local backward U-characteristic is useful when U is evolution-dominated as can be seen from Proposition 7.5 below, whose proof is quite similar to the case of stationary solutions of the Hamilton–Jacobi equation. Again the proof is given for the reader convenience. Notice that no continuity assumption has to be made on the function U which is evolution-dominated by L. Note also that by Proposition 5.5, we can apply this proposition when $U : O \to \mathbb{R}$ is continuous and a viscosity subsolution of the evolutionary Hamilton–Jacobi equation (1-1) on the open subset $O \subset \mathbb{R} \times M$.

Proposition 7.5. *Suppose that the function $U : S \to [-\infty, +\infty]$ is evolution-dominated by L on $S \subset \mathbb{R} \times M$ and $\gamma : [a, b] \to M$ is a U-calibrated curve.*

(1) *One of the following statements holds.*
   - $U(t, \gamma(t)) = +\infty$ *for every* $t \in [a, b]$.
   - $U(t, \gamma(t)) = -\infty$ *for every* $t \in [a, b]$.
   - $|U(t, \gamma(t))| < +\infty$ *for every* $t \in [a, b]$.

(2) *For any subinterval $[a', b'] \subset [a, b]$, the restriction $\gamma\,|\,[a', b']$ is also U-calibrated.*

(3) *If S is an open subset of $\mathbb{R} \times M$ and $|U(t, \gamma(t))|$ is not identically $+\infty$, the curve $\gamma : [a, b] \to M$ is a local minimizer of the action and, therefore, an extremal of L.*

Proof. Note that the action of γ is finite (as required in Definition 7.1). To prove (1), assume for example $U(t_0, \gamma(t_0)) = +\infty$ for some $t_0 \in [a, b]$, then by Proposition 5.3, we must have $U(t, \gamma(t)) = +\infty$, for $t \in [a, t_0[$. Therefore $U(a, \gamma(a)) = +\infty$. Since γ is U-calibrated, we also obtain $U(b, \gamma(b)) = +\infty$. Hence $U(t, \gamma(t)) = +\infty$ everywhere on $[a, b[$, again by Proposition 5.3. The case $U(t_0, \gamma(t_0)) = -\infty$ for some $t_0 \in [a, b]$ is similar and leads to $U(t, \gamma(t)) = -\infty$ everywhere on $[a, b]$.

To prove (2) we first observe that, since L is bounded from below, the action $\mathbb{L}(\gamma\,|\,[a', b'])$ is also finite for any subinterval $[a', b'] \subset [a, b]$. In the case where U is identically either $+\infty$ or $-\infty$, this implies the U-calibration of $\gamma\,|\,[a', b']$, for $[a', b'] \subset [a, b]$. By 1), it remains to consider the case $|U(t, \gamma(t))| < +\infty$, for every $t \in [a, b]$. In that case, from the Definition 5.1 of evolution domination, we obtain

$$
\begin{aligned}
U(a', \gamma(a')) - U(a, \gamma(a)) &\le \int_a^{a'} L(\gamma(s), \dot\gamma(s))\, dt,\\
U(b', \gamma(b')) - U(a', \gamma(a')) &\le \int_{a'}^{b'} L(\gamma(s), \dot\gamma(s))\, dt,\\
U(b, \gamma(b)) - U(b', \gamma(b')) &\le \int_{b'}^{b} L(\gamma(s), \dot\gamma(s))\, dt,
\end{aligned}
$$

But if we add the three inequalities above we obtain

$$U(b, \gamma(b) - U(a, \gamma(a)) \le \int_a^b L(\gamma(s), \dot\gamma(s))\, dt,$$

which is an equality. Therefore all three inequalities are equalities.

To prove (3), we observe that, when S is an open subset of $\mathbb{R} \times M$, any curve $\delta : [a, b] \to M$ close enough to γ (in the C^0 topology) has a graph Graph(δ) which is also included in S. If $\delta(a) = \gamma(a)$ and $\delta(b) = \gamma(b)$, the U-calibration of γ and the Definition 5.1 of evolution domination yield

$$U(b, \gamma(b)) - U(a, \gamma(a)) \le \int_a^b L(\delta(s), \dot\delta(s))\, dt,$$

for any absolutely continuous curve $\delta : [a, b] \to M$, with $\delta(a) = \gamma(a)$ and $\delta(b) = \gamma(b)$. But, since γ is U-calibrated, by the definition of calibration, the left side of the inequality is $\int_a^b L(\gamma(s), \dot\gamma(s))\, dt$. This proves the local minimization property. By Tonelli's theorem such a local minimizer is as smooth as L (or H) and is an extremal of L. □

Theorem 7.6. *Suppose $O \subset \mathbb{R} \times M$ is an open subset. If $U : O \to \mathbb{R}$ is a continuous viscosity solution of the evolutionary on Hamilton–Jacobi* (1-1) *on O, then for every $(t, x) \in O$, we can find a U-characteristic extremal $\gamma :]a, t] \to M$ ending at (t, x) and such that either $a = -\infty$ or γ extends to a continuous extremal $\gamma : [a, t] \to M$, with $(a, \gamma(a)) \in \partial O$.*

By Theorem 6.5, we can find a U-calibrated curve $\gamma : [t - \epsilon, t] \to O$, with $\gamma(t) = x$. But this curve γ is an extremal for the Lagrangian L. Therefore, we can extend γ to an extremal $\gamma :]-\infty, +\infty[\to M$. Hence Theorem 7.6 follows from the next lemma.

Lemma 7.7. *Suppose $O \subset]0, +\infty[\times M$ is an open subset. If $U : O \to \mathbb{R}$ is a continuous viscosity solution of the evolutionary Hamilton–Jacobi equation* (1-1) *on O. Assume that the curve $\gamma :]-\infty, +\infty[\to M$ is an extremal for L that is*

U-calibrated on an interval $[t-\epsilon, t]$ for some $\epsilon > 0$, then γ is U-calibrated on the maximal interval $]a, t]$ such that $\operatorname{Graph}(\gamma\,|\,]a, t]) \subset O$.

Proof. Consider the maximal interval $]a, t]$ such that $\operatorname{Graph}(\gamma\,|\,]a, t]) \subset O$. Define b as the infimum of the $s \in\,]a, t]$ such that $\gamma : [s, t]$ is U-calibrated. We have $b \le t-\epsilon$. Suppose that $b > a$, then $(b, \gamma(b)) \in O$, and by continuity of U, the restriction $\gamma\,|\,[b, t]$ is U-calibrated. By Theorem 7.4, there exists a U-calibrated curve $\tilde\gamma : [b-\eta, b] \to M$, with $\eta > 0$ and $\tilde\gamma(b) = \gamma(b)$. By Remark 7.2(2), the concatenation $\tilde\gamma \star \gamma : [b-\eta, t] \to M$ is also U-calibrated. By Proposition 7.5(3), this U-calibrated curve $\tilde\gamma \star \gamma$ is also an extremal for L. Since $\tilde\gamma \star \gamma = \gamma$ on $[t-\epsilon, t]$, with $t-\epsilon < t$, we must have $\tilde\gamma \star \gamma = \gamma$ on $[b-\eta, t]$. This implies that $\gamma\,|\,[b-\eta, t]$ is U-calibrated, which contradicts the definition of b. □

Theorem 7.8 (Lax–Oleinik). *A continuous function $U : [0, T[\, \times M \to \mathbb{R}$ that is a viscosity solution of the evolutionary Hamilton–Jacobi equation* (1-1) *on $]0, T[\, \times M$ satisfies the Lax–Oleinik formula*

$$U(t, x) = \inf_{y \in M} U(0, y) + h_t(y, x),$$

for all $t > 0, x \in M$. The infimum is achieved for all $t > 0, x \in M$.

Proof. Since U is a viscosity solution of the evolutionary Hamilton–Jacobi equation (1-1) on $]0, T[\, \times M$, by Proposition 5.5, it is evolution-dominated by L on $]0, T[\, \times M$. From Remark 5.2(2), it follows that U is strongly evolution-dominated by L on $]0, T[\, \times M$. By continuity of U on $[0, T[\, \times M$, we easily obtain that U is strongly evolution-dominated by L on $[0, T[\, \times M$. Therefore, we have

$$U(t, x) \le \inf_{y \in M} U(0, y) + h_t(y, x),$$

for all $t > 0, x \in M$. To finish the proof of the first part of the theorem, it suffices to show that, for a given $(t, x) \in\,]0, T[\, \times M$, there exists a U-calibrated curve $\gamma : [0, t] \to M$, with $\gamma(t) = x$. Since, for a curve $\gamma :]a, b] \to M$ such that $\operatorname{Graph}(\gamma) \subset\,]0, T[\, \times M$, we must have $a \ge 0$ and $b < T$, by Theorem 7.6 applied to the open set $]0, T[\, \times M$, we can find an extremal $\gamma : [a, t] \to M$ that is U-calibrated on $]a, t]$ with $\gamma(t) = x$ and $(a, \gamma(a)) \in \partial]0, T[\, \times M = \{0\} \times M$. Hence $a = 0$, and the extremal $\gamma : [0, t] \to M$ is U calibrated by continuity of U. □

Corollary 7.9. *Suppose $U, V : [0, T[\, \times M \to \mathbb{R}$ are two continuous functions that are viscosity solutions of the evolutionary Hamilton–Jacobi equation* (1-1) *on $]0, T[\, \times M$. If $U \le V$ on $\{0\} \times M$, then $U \le V$ everywhere on $[0, T[\, \times M$.*

In particular, if $U = V$ on $\{0\} \times M$, then $U = V$ everywhere on $[0, T[\, \times M$.

8. The Lax–Oleinik semigroup and the Lax–Oleinik evolution

Definition 8.1. If $u : M \to [-\infty, +\infty]$ is a function and $t > 0$, the function $T_t^- u : M \to [-\infty, +\infty]$ is defined by

$$T_t^- u(x) = \inf_{y \in M} u(y) + h_t(y, x).$$

We also set $T_0^- u = u$. The (negative) Lax–Oleinik semigroup is T_t^-, $t \geq 0$.

Definition 8.2 (Lax–Oleinik evolution). If $u : M \to [-\infty, +\infty]$, we will denote by $\hat{u} : [0, +\infty[\times M \to [-\infty, +\infty]$ the function defined, for $t > 0$, by

$$\hat{u}(t, x) = T_t^- u(x) = \inf_{y \in M} u(y) + h_t(y, x)$$

and by $\hat{u}(0, x) = u(x)$.

The function $\hat{u}$ is called the (negative) Lax–Oleinik evolution of u. We note that $\hat{u} < +\infty$ on $]0, +\infty[\times M$, if u is not identically $+\infty$.

Proposition 8.3. *For any function $u : M \to [-\infty, +\infty]$, its Lax–Oleinik evolution $\hat{u} : [0, +\infty[\times M \to [-\infty, +\infty]$ is strongly evolution-dominated by L on $[0, +\infty[\times M$.*

Proof. This follows easily from the definition of $\hat{u}$ and Proposition 4.13(1). □

Remark 8.4. (1) If u is not identically $+\infty$, then $\hat{u}(t, x) < +\infty$ for all t in $]0, +\infty[$ and x in M.

(2) If $u(x_0) = -\infty$ for some $x_0 \in M$, then $\hat{u}(t, x) = -\infty$ for all t in $]0, +\infty[$ and x in M.

(3) If u is not identically $+\infty$, then the set $F_u = \{x \in M \mid u(x) \neq +\infty\}$ is not empty. If we set $K = \{0\} \times F_u$ and define $U : K \to [-\infty, +\infty[$ by $U(0, x) = u(x)$, for all $(0, x) \in K$, then $t_{K,\inf} = 0$ and $\hat{U} = \hat{u}$ on $]0, +\infty[\times M$, where $\hat{U}$ is given (see (6-1)) by

$$\begin{aligned}\hat{U}(t, x) &= \inf\{U(\tilde{t}, \tilde{x}) + h_{t-\tilde{t}}(\tilde{x}, x) \mid (\tilde{t}, \tilde{x}) \in K \text{ and } \tilde{t} \leq t\} \\ &= \inf\{u(\tilde{x}) + h_t(\tilde{x}, x) \mid \tilde{x} \in F_u\}.\end{aligned}$$

In particular, all the results given in Section 6 for functions of the type $\hat{U}$ hold for Lax–Oleinik evolutions.

Theorem 8.5. *Assume $u : M \to [-\infty, +\infty]$ is such that $\hat{u}(T, X)$ is finite for some $(T, X) \in]0, +\infty[\times M$. Then $\hat{u}$ is finite, locally semiconcave and a viscosity solution of the evolutionary Hamilton–Jacobi equation*

$$\partial_t \hat{u} + H(x, \partial_x \hat{u}) = 0,$$

on $]0, T[\times M$.

Proof. As explained above, this now follows from Theorem 6.2. □

Examples 8.6. We give some examples of Lax–Oleinik evolution.

(1) For any Tonelli Lagrangian $L : TM \to \mathbb{R}$, we know that $h_t(y, x) \geq -C(0)t$. Therefore $\hat{u}(t, x) \geq \inf_M u - C(0)t$. This implies that $\hat{u}$ is finite everywhere, on $]0, +\infty[\, \times M$, for any function $u : M \to]-\infty, +\infty[$ which is bounded from below and not identically equal to $+\infty$.

(2) For any Tonelli Lagrangian $L : TM \to \mathbb{R}$, if M is compact, we know that $-C(0)t \leq h_t(y, x) \leq A(\operatorname{diam} M/t)$. Since, for any function $u : M \to [-\infty, +\infty]$, we have

$$\hat{u}(t, x) = \inf_{y \in M} u(y) + h_t(y, x),$$

we obtain

$$-C(0)t + \inf_M u \leq \hat{u}(t, x) \leq A(\operatorname{diam} M/t) + \inf_M u.$$

Hence, for a compact manifold $\hat{u}$ is finite everywhere on $]0, +\infty[\, \times M$ if and only if u is bounded from below and not identically $+\infty$. Therefore, for compact M, the class of functions u for which $\hat{u}$ is finite on $]0, +\infty[\, \times M$ does not depend on M.

(3) If $A \subset M$, we define $\Xi_A : M \to \{0, +\infty\}$

$$\Xi_A(x) = \begin{cases} 0 & \text{if } x \in A, \\ \infty & \text{otherwise.} \end{cases}$$

Note that Ξ_M is identically 0, and $\Xi_\varnothing$ is identically $+\infty$. Moreover, the function Ξ_A is not identically $+\infty$ if $A \neq \varnothing$.

For a given Tonelli Lagrangian $L : TM \to \mathbb{R}$, and $A \neq \varnothing$, we obtain, from (1), that $\hat{\Xi}_A$ is finite everywhere on $]0, +\infty[\, \times M$, with

$$\hat{\Xi}_A(t, x) = \inf_{y \in A} h_t(y, x).$$

(4) If $M = \mathbb{R}^n$ with the Euclidean metric, we consider the Lagrangian $L_0(x, v) = \frac{1}{2}\|v\|^2$, where $\|\cdot\|$ is the usual Euclidean metric. We know from Example 4.12(1) that $h_t(x, y) = \|y - x\|^2/2t$. For $\alpha, \beta > 0$, consider the function $u_{\alpha,\beta} : M \to \mathbb{R}$ defined by

$$u_{\alpha,\beta}(x) = -\alpha\|x\|^\beta.$$

Its Lax–Oleinik evolution is given by

$$\begin{aligned} \hat{u}_{\alpha,\beta}(t, x) &= \inf_{y \in \mathbb{R}^n} -\alpha\|y\|^\beta + \frac{\|y - x\|^2}{2t} \\ &= \frac{\|x\|^2}{2t} + \inf_{y \in \mathbb{R}^n} \left(\frac{\|y\|^2}{2t} - \alpha\|y\|^\beta + \frac{\langle y, x \rangle}{t} \right). \end{aligned}$$

Therefore

(i) If $\beta > 2$ then $\hat{u}_{\alpha,\beta}$ is identically $-\infty$.

(ii) If $\beta < 2$ then $\hat{u}_{\alpha,\beta}$ is finite everywhere.

(iii) If $\beta = 2$, for $(t, x) \in M$, we have

$$\hat{u}_{\alpha,2}(t, x) \text{ is } \begin{cases} \text{finite} & \text{if } t < \alpha/2, \\ 0 & \text{if } (t, x) = (\alpha/2, 0), \\ -\infty & \text{otherwise.} \end{cases}$$

(5) If $M = \mathbb{R}^n$ with the Euclidean metric, for a real number $p \geq 4$, we consider the Lagrangian $L_p(x, v) = \frac{1}{2}\|v\|^2 + \frac{1}{p}\|v\|^p$, where $\|\cdot\|$ is the usual Euclidean metric. We know from Example 4.12(2) that $h_t(x, y) = \|y - x\|^2/2t + \|y - x\|^p/pt^{p-1}$. Therefore if, for $\beta > 0$, we consider the function

$$u_\beta(x) = -\|x\|^\beta.$$

In this case, we have

$$\hat{u}_\beta(t, x) = \inf_{y \in M} -\|y\|^\beta + \|y - x\|^2/2t + \|y - x\|^p/pt^{p-1};$$

hence $\hat{u}_\beta$ is finite everywhere if $\beta < p$ and is equal $-\infty$ everywhere for $\beta > p$.

It follows that, for a noncompact manifold M, the class of functions u for which $\hat{u}$ is finite depends on the Lagrangian.

Some of the well-known properties of the Lax–Oleinik semigroup $(T_t^-)_{t \geq 0}$ (see [6]) are given in the following proposition.

Proposition 8.7. (1) (semigroup property) *For every* $t, t \geq 0$, *we have* $T_{t+t'}^- = T_t^- \circ T_{t'}^-$. *In particular, for every* $t, t' \geq 0$ *and* $x, y \in M$,

$$\begin{aligned} T_t^- u(x) &\leq u(x) + h_t(x, x) \leq u(x) + A(0)t, \\ T_{t+t'}^- u(x) &\leq T_{t'}^- u(y) + h_t(y, x), \\ T_{t+t'}^- u(x) &\leq T_{t'}^- u(x) + h_t(x, x) \leq T_{t'}^- u(x) + A(0)t. \end{aligned}$$

(2) *For every* $u : M \to [-\infty, +\infty]$, *and every* $c \in \mathbb{R}$, *we have* $T_t^-(u + c) = T_t^-(u) + c$, *for every* $t \geq 0$.

(3) *For every* $u, v : M \to [-\infty, +\infty]$ *with* $u \leq v$ *everywhere, we have* $T_t^- u \leq T_t^- v$, *for every* $t \geq 0$.

(4) *For every* $u, v : M \to \mathbb{R}$, *we have*

$$-\|u - v\|_\infty + T_t^- v \leq T_t^- u \leq T_t^- v + \|u - v\|_\infty,$$

for every $t \geq 0$.

Here is a further observation on the Lax–Oleinik evolution.

Definition 8.8 (lower semicontinuous regularization). If $u : M \to [-\infty, +\infty]$, we define its lower semicontinuous regularization $u_- : M \to [-\infty, +\infty]$ by

$$u_-(x) = \liminf_{y \to x} u(y) = \sup_V \inf_{y \in V} u(y),$$

where the supremum is taken over all neighborhoods V of x. The function u_- is the largest lower semicontinuous function which is $\leq u$.

Proposition 8.9. *For every function $u : M \to [-\infty, +\infty]$, we have $\hat{u} = \hat{u}_-$ on $]0, +\infty[\times M$.*

Proof. Since $u_- \leq u$, we have $\hat{u}_- \leq \hat{u}$. To prove the converse inequality, it suffices to show that for $(t, x, y) \in]0, +\infty[\times M \times M$, we have

$$u_-(y) + h_t(y, x) \geq \inf_{z \in M} u(z) + h_t(z, x) = \hat{u}(x).$$

By definition of $u_-(y)$, we can find a sequence $y_n \to y$ such that $u(y_n) \to u_-(y)$. Since $h_t(\cdot, x)$ is continuous we obtain

$$u_-(y) + h_t(y, x) = \lim_{n \to +\infty} u(y_n) + h_t(y_n, x) \geq \inf_{z \in M} u(z) + h_t(z, x). \qquad \square$$

We will now consider the Lax–Oleinik evolution of Lipschitz functions.

We start with a lemma connecting the Lipschitz property with the action and the Lax–Oleinik semigroup.

Lemma 8.10. (1) *For a function $u : M \to \mathbb{R}$, and a constant $c \in \mathbb{R}$, the following two conditions are equivalent*:

- $u(x) - u(y) \leq h_s(y, x) + cs$, *for all $s > 0$ and $x, y \in M$.*
- $u \leq T_s^- u + cs$, *for all $s \geq 0$.*

(2) *If a function $u : M \to \mathbb{R}$, for some $c \in M$ satisfies $u \leq T_s^- u + cs$, for all $s \geq 0$, then so does $T_t^- u$ for all $t \geq 0$.*

(3) *If the function $u : M \to \mathbb{R}$ is globally Lipschitz function, with Lipschitz constant $\leq \lambda$, then $u \leq T_t^- u + C(\lambda)t$, for all $t \geq 0$, where $C(\cdot)$ is the function defined in* (3-3).

(4) *If, for some $c \in \mathbb{R}$, the function $v : M \to \mathbb{R}$ satisfies $v \leq T_t^- v + ct$, for all $t > 0$ and $x, y \in M$, then v is Lipschitz, with Lipschitz constant $\leq A(1) + c$, where $A(\cdot)$ is the function defined in* (3-4)

Proof. To prove (1), we note that the condition $u(x) - u(y) \leq h_s(y, x) + cs$ is equivalent to $u(x) \leq u(y) + h_s(y, x) + cs$. Therefore the two conditions in part (1) are equivalent since $T_s^- u(x) = \inf_{y \in M} u(y) + h_s(y, x)$.

Part (2) follows easily from parts (1), (2) and (3) of Proposition 8.7.

To prove (3), using (4-9), we note that

$$u(x) - u(y) \le \lambda d(x, y) \le h_s(y, x) + C(\lambda)s.$$

To prove (4), we note that $h_{d(x,y)}(x, y) \le A(1)d(x, y)$ by Lemma 4.11. Hence

$$v(y) - v(x) \le h_{d(x,y)}(x, y) + cd(x, y) \le [A(1) + c]d(x, y).$$

By symmetry, we conclude that the Lipschitz constant of v is $\le A(1) + c$. □

We recall that a function $u : M \to \mathbb{R}$ is said to be evolution-dominated by $L + c$ if it satisfies the equivalent properties of Lemma 8.10(1).

Proposition 8.11. *The Lax–Oleinik evolution $\hat{u}$ of any (globally) Lipschitz function $u : M \to \mathbb{R}$ is finite everywhere on $[0, +\infty[\times M$.*

Moreover, for every constant $\lambda \in [0, +\infty[$, we can find a constant Λ such that $\hat{u}$ has Lipschitz constant $\le \Lambda$ as soon as u has Lipschitz constant $\le \lambda$.

Proof. Assume that $u : M \to \mathbb{R}$ has Lipschitz constant $\le \lambda$. By Lemma 8.10(3) we have

$$u(x) \le T_s u(x) + C(\lambda)s,$$

for all $s \ge 0$. This implies that $\hat{u}$ is finite everywhere.

Lemma 8.10(2) yields

$$T_t^- u(x) \le T_s^- T_t^- u(x) + C(\lambda)s, \tag{8-1}$$

for all $t, s \in [0, +\infty[$, and $x \in M$. Therefore, by Lemma 8.10(4), the Lax–Oleinik evolution has a Lipschitz constant in x which is $\le A(1) + C(\lambda)$.

To compute the Lipschitz constant in t, we note that, by the semigroup property, we have

$$T_{t+s}^- u(x) \le T_t^- u(x) + h_s(x, x) \le T_t^- u(x) + A(0)s.$$

Combining this last equality with (8-1), we get

$$-C(\lambda)s \le T_{t+s}^- u(x) - T_t^- u(x) \le A(0)s.$$

It follows that the Lipschitz constant in t of $\hat{u}$ is $\le \max\big(|A(0)|, |C(\lambda)|\big)$. This finishes the proof of the existence of the constant Λ. □

We next extend the results obtained above to uniformly continuous function.

Corollary 8.12. *The Lax–Oleinik evolution $\hat{u} : [0, +\infty[\times M \to \mathbb{R}$ of a uniformly continuous function $u : M \to \mathbb{R}$ is finite everywhere and uniformly continuous.*

Proof. By Lemma A.1 in the Appendix, there is a sequence of Lipschitz functions $u_n : M \to \mathbb{R}$ such that $\|u - u_n\|_\infty \to 0$ as $n \to +\infty$. By Proposition 8.7(4), for every $t \ge 0$, and every $n \ge 0$, we have

$$-\|u - u_n\|_\infty + T_t^- u_n \le T_t^- u \le T_t^- u_n + \|u - u_n\|_\infty.$$

Therefore $\hat{u}$ is finite everywhere and $\|\hat{u}-\hat{u}_n\|_\infty \leq \|u-u_n\|_\infty \to 0$ as $n \to +\infty$. By Proposition 8.11, each function $\hat{u}_n$ is Lipschitz. Therefore, again by Lemma A.1, the uniform limit $\hat{u}$ of the Lipschitz functions $\hat{u}_n$ is uniformly continuous. □

We then consider the case when u is Lipschitz in the large; see Definition A.2.

Corollary 8.13. *For any finite constant* $K \geq 0$, *we can find a finite constant* κ *such that any function* $u : M \to \mathbb{R}$ *Lipschitz in the large with constant* K *has a Lax–Oleinik evolution* $\hat{u} : [0, +\infty[\times M \to \mathbb{R}$, *which is finite everywhere and Lipschitz in the large with constant* κ *on* $[0, +\infty[\times M \to \mathbb{R}$.

Proof. By Proposition A.4, we can find a Lipschitz function $\varphi : X \to \mathbb{R}$, with Lipschitz constant K, such that $\|u - \varphi\|_\infty = \sup_{x\in M} |u(x) - \varphi(x)| \leq K/2$.

From Proposition 8.11, the Lax–Oleinik evolution $\hat{\varphi}$ is Lipschitz with a Lipschitz constant $\leq \Lambda(K)$, where $\Lambda(K)$ depends only on K. As in the proof of Corollary 8.12, by Proposition 8.7(4), we have

$$\|\hat{u} - \hat{\varphi}\|_\infty \leq \|u - \varphi\|_\infty \leq K/2.$$

We can now apply again Proposition A.4 of the Appendix, to conclude that $\hat{u} : [0, +\infty[\times M \to \mathbb{R}$ is finite everywhere and Lipschitz in the large with constant $\kappa = \max(\Lambda(K), K)$ on $[0, +\infty[\times M \to \mathbb{R}$. □

Of course, in Corollary 8.13 the Lax–Oleinik evolution $\hat{u}$ of the Lipschitz in the large function $u : M \to \mathbb{R}$ is, as for all Lax–Oleinik evolutions, locally Lipschitz on $]0, +\infty[\times M$, since it is everywhere finite on $]0, +\infty[\times M$. We will show in Theorem 9.5 that $\hat{u}$ is globally Lipschitz on $[t_0, +\infty[\times M$, for every $t_0 > 0$.

Our goal now is the case to give properties of $\hat{u}$ near $\{0\} \times M$ when u is just continuous or merely lower semicontinuous.

We start with a remark.

Remark 8.14. Suppose that $U : [0, +\infty[\times M \to [-\infty, +\infty]$. Denote by U^* the restriction of U to $]0, +\infty[\times M$. If $x \in M$, we can define

$$\liminf_{(t,y)\to(0,x)} U(t, y), \qquad \liminf_{(t,y)\to(0,x)} U^*(t, y) \quad \text{and} \quad \liminf_{y\to x} U(0, y),$$

where in the first case we take $(t, y) \to (0, x)$ with $t \geq 0$ and $y \in M$; in the case of U^* we take $(t, y) \to (0, x)$ with $t > 0$ and $y \in M$; and in the last case $y \to x$ with $y \in M$.

Of course we have

$$\liminf_{(t,y)\to(0,x)} U(t, y) \leq \liminf_{(t,y)\to(0,x)} U^*(t, y),$$

$$\liminf_{(t,y)\to(0,x)} U(t, y) \leq \liminf_{y\to x} U(0, y).$$

Since for any sequence $(t_i, y_i) \to (0, x)$, with $t_i \geq 0$ and $y_i \in M$, either $t_i = 0$ for infinitely many i, or $t_i > 0$ for infinitely many i, we conclude

$$\liminf_{(t,y)\to(0,x)} U(t, y) = \min\Bigl(\liminf_{(t,y)\to(0,x)} U^*(t, y), \liminf_{y\to x} U(0, y)\Bigr). \tag{8-2}$$

Theorem 8.15. *Let $L : TM \to \mathbb{R}$ be a Tonelli Lagrangian. If $u : M \to [-\infty, +\infty]$ is a lower semicontinuous function such that its Lax–Oleinik evolution $\hat{u}$: $[0, +\infty[\times M$, $(t, x) \mapsto T_t^- u(x)$ is finite at some $(T, X) \in]0, +\infty[\times M$, then it satisfies the following properties*:

(i) *For every $x \in M$, we have*

$$\liminf_{(t,y)\to(0,x)} \hat{u}(t, y) = \liminf_{(t,y)\to(0,x)} \hat{u}^*(t, y) = u(x).$$

Therefore the function $\hat{u}$ is lower semicontinuous on $[0, T[\times M$.

(ii) *For every $x \in M$, we have*

$$\limsup_{(t,y)\to(0,x)} \hat{u}(t, y) = \limsup_{y\to x} u(y).$$

Therefore, if u is continuous on M then $\hat{u}$ is continuous on $[0, T[\times M$.

(iii) *For every $x \in M$, both limits* $\lim_{t\to 0} \hat{u}(t, x) = \lim_{t\to 0} \hat{u}^*(t, x)$ *exist and*

$$\lim_{t\to 0} \hat{u}(t, x) = \lim_{t\to 0} \hat{u}^*(t, x) = u(x).$$

For every $x \in M$, the function $t \mapsto \hat{u}(t, x) + A(0)t$ is nondecreasing in t.

Proof. We first note that from Proposition 8.7(1), we have

$$\hat{u}(t, y) \leq u(y) + A(0)t. \tag{8-3}$$

This obviously implies the equality in (ii). By the lower semicontinuity of u, this also implies

$$\liminf_{(t,y)\to(0,x)} \hat{u}^*(t, y) \leq u(x).$$

Therefore, from (8-2), we conclude that

$$\liminf_{(t,y)\to(0,x)} \hat{u}(t, y) = \liminf_{(t,y)\to(0,x)} \hat{u}^*(t, y).$$

To finish the proof of (i), it remains to show that

$$\ell = \liminf_{(t,y)\to(0,x)} \hat{u}^*(t, y) \geq u(x).$$

If $\ell = +\infty$, there is nothing to prove. Therefore we assume that $\ell < +\infty$. We then choose a sequence $(t_i, y_i) \to (0, x)$, with $t_i > 0$ such that

$$\lim_{i\to+\infty} \hat{u}(t_i, y_i) = \ell.$$

We now note, again by Proposition 8.7(1), that for all $(t, y), (t', y') \in [0, +\infty[\times M$, with $t' < t$, we have

$$\hat{u}(t, y) \leq \hat{u}(t', y') + h_{t-t'}(y', y). \tag{8-4}$$

In particular, we get

$$\hat{u}(t, y) \geq \hat{u}(T, X) + h_{T-t}(y, X), \tag{8-5}$$

for all $(t, y) \in [0, T[\times M$. We then use

$$\hat{u}(t_i, y_i) = \inf_{z \in M} u(z) + h_{t_i}(z, y_i)$$

to find a sequence $z_i \in M$ such that

$$\hat{u}(t_i, y_i) \leq u(z_i) + h_{t_i}(z_i, y_i) \to \ell.$$

From (4-7), we know that $h_{t_i}(z, y_i) \geq -C(0)t_i \to 0$. Therefore, if z_i admits x as an accumulation point of the sequence z_i, from the lower semicontinuity of u, we would obtain

$$\ell = \lim_{i \to +\infty} u(z_i) + h_{t_i}(z, y_i) \geq \liminf_{i \to +\infty} u(z_i) \geq u(x).$$

It remains to consider the case when x is not an accumulation point of the sequence z_i. Therefore we can find $\epsilon > 0$ such that

$$d(x, z_i) > \epsilon \quad \text{for all } i. \tag{8-6}$$

Since $y_i \to x$, neglecting the first terms of the sequence, we can assume

$$d(x, y_i) < \epsilon \quad \text{for all } i. \tag{8-7}$$

For every i, we can now find a minimizer $\gamma_i : [0, t_i] \to M$, with $\gamma_i(0) = z_i$ and $\gamma_i(t_i) = y_i$. From (8-6) and (8-7), we can find $t'_i \in]0, t_i[$ such that $d(x, \gamma_i(t'_i)) = \epsilon$, for all i. Since $\gamma_i : [0, t_i] \to M$ is a minimizer, with $\gamma_i(0) = z_i$ and $\gamma_i(t_i) = y_i$, we have

$$h_{t_i}(z_i, y_i) = h_{t'_i}(z_i, \gamma_i(t'_i)) + h_{t_i - t'_i}(\gamma_i(t'_i), y_i).$$

Therefore

$$\begin{aligned} u(z_i) + h_{t_i}(z_i, y_i) &= u(z_i) + h_{t'_i}(z_i, \gamma_i(t'_i)) + h_{t_i - t'_i}(\gamma_i(t'_i), y_i) \\ &\geq \hat{u}(t'_i, \gamma_i(t'_i)) + h_{t_i - t'_i}(\gamma_i(t'_i), y_i). \end{aligned}$$

Since the sequence $\gamma_i(t'_i)$ is contained in the compact ball $\bar{B}(x, \epsilon)$ and $t_i \to 0 < T$, from (8-5), we get

$$\inf_i \hat{u}(t'_i, \gamma_i(t'_i)) = \kappa > -\infty.$$

Hence

$$u(z_i) + h_{t_i}(z_i, y_i) \geq \kappa + h_{t_i - t_i'}(\gamma_i(t_i'), y_i),$$

which implies

$$\ell = \lim_{i\to+\infty} u(z_i) + h_{t_i}(z, y_i) \geq \kappa + \lim_{i\to+\infty} h_{t_i-t_i'}(\gamma_i(t_i'), y_i). \tag{8-8}$$

For $K > 0$, we now use (4-8) and $d(x, \gamma_i(t_i')) = \epsilon$ to obtain

$$\begin{aligned} h_{t_i-t_i'}(\gamma_i(t_i'), y_i) &\geq K d(\gamma_i(t_i'), y_i) - C(K)(t_i - t_i') \\ &\geq K(\epsilon - d(x, y_i)) - C(K)(t_i - t_i'). \end{aligned}$$

Since $y_i \to x$ and $0 < t_i' < t_i \to 0$, we obtain

$$\lim_{i\to+\infty} h_{t_i-t_i'}(\gamma_i(t_i'), y_i) \geq K\epsilon.$$

Since $\epsilon > 0$ and $K > 0$ is arbitrary, we get

$$\lim_{i\to+\infty} h_{t_i-t_i'}(\gamma_i(t_i'), y_i) = +\infty.$$

This contradicts (8-8), since $\ell < +\infty$ and $\kappa > -\infty$. This finishes the proof of the equality in (i). The last part of (i) follows from this equality and the already observed continuity of $\hat{u}$ on the open subset $]0, +T[\, \times M$; see Theorem 8.5. Note that this same continuity of $\hat{u}$ on $]0, +T[\, \times M$, together with (i) and the inequality in (ii), yields also the last part of (ii).

To prove the equality in (iii), we first note, using (i), that

$$u(x) = \liminf_{(t,y)\to(0,x)} \hat{u}(t, y) \leq \liminf_{t\to 0} \hat{u}(t, x) \leq \liminf_{t\to 0} \hat{u}^*(t, x).$$

Moreover, from (8-3), we have

$$\hat{u}(t, x) \leq u(x) + A(0)t,$$

which yields

$$\limsup_{t\to 0} \hat{u}^*(t, x) \leq \limsup_{t\to 0} \hat{u}(t, x) \leq u(x).$$

The above inequalities on the lim inf's and lim sup's imply the equality in (iii). The last statement in (iii) follows from the third inequality in Proposition 8.7(1), which yields

$$\hat{u}(t + t', x) \leq \hat{u}(t, x) + A(0)t' \quad \text{for all } t, t' \geq 0. \qquad \square$$

Corollary 8.16. *Let $u : M \to [-\infty, +\infty]$ be a lower semicontinuous function, such that $\hat{u}(T, X)$ is finite for some $(T, X) \in\,]0, +\infty[\, \times M$. Then for every $(t, x) \in\,]0, T[\, \times M$, we can find a backward $\hat{u}$-characteristic $\gamma : [0, t] \to M$*

ending at (t, x). *In particular, for every* $(t, x) \in\ ]0, T[\, \times M$, *we can find* $y \in M$ *such that*

$$\hat{u}(t, x) = u(y) + h_t(y, x).$$

Proof. Fix $(t, x) \in\ ]0, T[\, \times M$. From Theorem 7.6, we can find an extremal $\gamma : [0, t] \to M$, with $\gamma(t) = x$, which is $\hat{u}$-calibrated on $]0, t]$; i.e., for all $s \in\ ]0, t[$, we have

$$\hat{u}(t, x) = \hat{u}(s, \gamma(s)) + \int_s^t L(\gamma(\sigma), \dot{\gamma}(\sigma))\, d\sigma. \tag{8-9}$$

Since $(s, \gamma(s)) \to (0, \gamma(0))$ as $s \to 0$, from part (i) of Theorem 8.15, we obtain $\liminf_{s\to 0} \hat{u}(s, \gamma(s)) \geq u(\gamma(0)) = \hat{u}(0, \gamma(0))$. Hence, if we let $s \to 0$ in (8-9), we obtain

$$\begin{aligned} \hat{u}(t, x) &= \liminf_{s\to 0} \hat{u}(s, \gamma(s)) + \int_0^t L(\gamma(\sigma), \dot{\gamma}(\sigma))\, d\sigma \\ &\geq \hat{u}(0, \gamma(0)) + h_t(\gamma(0), x) \geq \hat{u}(t, x). \end{aligned}$$

Therefore all inequalities are equalities. Hence γ is $\hat{u}$-calibrated on the closed interval $[0, t]$. □

We conclude this section with a proof that all continuous viscosity solutions of the evolutionary Hamilton–Jacobi equation on an open set $]0, T[\, \times M$ are given by a Lax–Oleinik evolution of a unique lower semicontinuous function.

Theorem 8.17. *Assume* $U :]0, T[\, \times M \to \mathbb{R}$, *with* $T \in\ ]0, +\infty]$ *is a continuous viscosity solution of the evolutionary Hamilton–Jacobi equation*

$$\partial_t U + H(x, \partial_x U) = 0,$$

on $]0, T[\, \times M$. *Then there exists a unique lower semicontinuous function* $u : M \to [-\infty, +\infty]$ *such that* $U = \hat{u}$ *on* $]0, T[\, \times M$. *In fact, we have*

$$u(x) = \liminf_{(t,y)\to(0,x)} U(t, y) = \lim_{t\to 0} U(t, x).$$

Proof. If u exists, it follows from Theorem 8.15 that we must have

$$u(x) = \liminf_{(t,y)\to(0,x)} U(t, y) = \lim_{t\to 0} U(t, x).$$

This implies the uniqueness if u exists. To prove the existence, we define $u : M \to [-\infty, +\infty]$ by

$$u(x) = \liminf_{(t,y)\to(0,x)} U(t, y).$$

This function u is lower semicontinuous. We first show that $\hat{u} \leq U$ on $]0, T[\, \times M$. For this, we fix $(t, x) \in\ ]0, T[\, \times M$. For any $y \in M$, by definition of u, we can find a sequence $(t_i, y_i) \in]0, T[\times M$ with

$$(t_i, y_i) \to (0, y) \text{ and } U(t_i, y_i) \to u(y) \quad \text{as } i \to +\infty.$$

Since U is a viscosity solution on $]0, T[\times M$, we know from Proposition 5.5 and Remark 5.2(2), that U is strongly evolution-dominated by L. Using that $t_i \to 0 < t$, for i large, we must have

$$U(t, x) \leq U(t_i, y_i) + h_{t-t_i}(y_i, x).$$

If we let $i \to +\infty$, we obtain

$$U(t, x) \leq u(y) + h_t(y, x).$$

Since $y \in M$ is arbitrary, we conclude that $U \leq \hat{u}$ on $]0, T[\times M$.

It remains to show that $\hat{u} \leq U$ on $]0, T[\times M$. The argument is almost identical to the proof of last corollary. Fix $(t, x) \in]0, T[\times M$. From Theorem 7.6, we can find an extremal $\gamma : [0, t] \to M$, with $\gamma(t) = x$, which is U-calibrated on $]0, t]$; i.e., for all $s \in]0, t[$, we have

$$U(t, x) = U(s, \gamma(s)) + \int_s^t L(\gamma(\sigma), \dot{\gamma}(\sigma))\, d\sigma. \tag{8-10}$$

Since $(s, \gamma(s)) \to (0, \gamma(0))$ as $s \to 0$, from the definition of u, we obtain $\liminf_{s \to 0} U(s, \gamma(s)) \geq u(\gamma(0))$. Hence, if we let $s \to 0$ in (8-10), we obtain

$$\begin{aligned} U(t, x) &= \liminf_{s \to 0} U(s, \gamma(s)) + \int_0^t L(\gamma(\sigma), \dot{\gamma}(\sigma))\, d\sigma \\ &\geq u(\gamma(0)) + h_t(\gamma(0), x) \geq \hat{u}(t, x). \end{aligned}$$

□

9. Differentiability properties of the Lax–Oleinik evolution

Theorem 9.1 (differentiability theorem). *Assume that the function $U : O \to \mathbb{R}$, defined on the open subset O of $\mathbb{R} \times M$, is evolution-dominated by L. If the curve $\gamma : [a, b] \to M$, is U-calibrated for L, we have*:

(i) *If $t \in]a, b]$ then U is upper semicontinuous at $(t, \gamma(t))$ and*

$$(-E(\gamma), \partial_v L(\gamma(t), \dot{\gamma}(t)) \in D^+ U(t, \gamma(t)).$$

(ii) *If $t \in [a, b[$ then U is lower semicontinuous at $(t, \gamma(t))$ and*

$$(-E(\gamma), \partial_v L(\gamma(t), \dot{\gamma}(t)) \in D^- U(t, \gamma(t)).$$

(iii) *For every $t \in [a, b]$, if the function U is differentiable at $(t, \gamma(t))$, then*

$$DU(t, \gamma(t)) = (-E(\gamma), \partial_v L(\gamma(t), \dot{\gamma}(t)) \in T^*_{(t,\gamma(t))} \mathbb{R} \times M = \mathbb{R} \times T^*_{\gamma(t)} M.$$

(iv) *If $t \in]a, b[$, then U is indeed differentiable* (*hence continuous*) *at $(t, \gamma(t))$.*

Proof. To prove (i), fix $t \in\,]a, b]$. By Proposition 5.4, there exists an open subset $O' \subset O$, with $(t, \gamma(t)) \in O'$, such that the restriction $U \mid O'$ is strongly evolution domination by L. By continuity of γ, we can then find $[a', b'] \subset [a, b]$, with $a' < t \leq b'$, and $(s, \gamma(s)) \in O'$, for all $s \in [a', b']$. The strong L evolution domination of $U \mid O'$ implies

$$U(s, x) - U(a', \gamma(a')) \leq h_{s-a'}(\gamma(a'), x) = \mathcal{H}(s - a', \gamma(a'), x), \tag{9-1}$$

for every $(s, x) \in O'$, with $s > a'$. Applying this inequality with $(s, x) = (t, \gamma(t))$, and using that $\gamma \mid [a', t]$ is U-calibrated, we obtain

$$\int_{a'}^{t} L(\gamma(s), \dot{\gamma}(s)) = U(t, \gamma(t)) - U(a', \gamma(a')) \leq \mathcal{H}(t - a', \gamma(a'), \gamma(t)).$$

But $\int_{a'}^{t} L(\gamma(s), \dot{\gamma}(s)) \geq \mathcal{H}(t - a', \gamma(a'), \gamma(t))$. Therefore the inequality above is an equality. Subtracting this equality from the inequality (9-1), we get

$$U(s, x) - U(t, \gamma(t) \leq \mathcal{H}(s - a', \gamma(a'), x) - \mathcal{H}(t - a', \gamma(a'), \gamma(t)). \tag{9-2}$$

Since $\mathcal{H}$ is continuous, we first obtain from this inequality (9-1) the upper semicontinuity. Moreover, inequality (9-1) together with the equality case at $(t, \gamma(t))$ implies

$$D^{+}_{(t,x)}\mathcal{H}(t - c, \gamma(t), \gamma(c)) \subset D^{+}U(t, \gamma(t)).$$

But by Proposition 4.22, we have

$$(-E(\gamma), \partial_v L(\gamma(t), \dot{\gamma}(t)) \in D^{+}_{(t,x)}\mathcal{H}(t - c, \gamma(t), \gamma(c)).$$

The proof of (ii) is similar.

To prove (iii), we recall that if $DU(t, \gamma(t))$ exists then $D^{+}U(t, \gamma(t)) = D^{-}U(t, \gamma(t)) = \{DU(t, \gamma(t))\}$.

To prove (iv), observe that, for $t \in\,]a, b[$, both $D^{+}U(t, \gamma(t)$ and $D^{-}U(t, \gamma(t))$ are nonempty by (i) and (ii). This implies that U is differentiable at (t, x); see for example [7, Proposition 3.3]. □

Corollary 9.2. *Assume $L : TM \to \mathbb{R}$ is a Tonelli Lagrangian. Let $U : [0, T[\, \times M \to \mathbb{R}$ be evolution-dominated by L.*

(i) *If U is differentiable at (t, x), then there is at most one U-calibrated $\gamma : [c, d] \to M$, with $t \in [c, d]$ and $x = \gamma(t)$.*

(ii) *If $\gamma_1 : [c_1, d_1] \to M$ and $\gamma_2 : [c_2, d_2] \to M$ are U-calibrated curves such that $\gamma_1(t) = \gamma_2(t)$, with $t \in [c_1, d_1] \cap [c_2, d_2]$ and either $t \in\,]c_1, d_1[$ or $t \in\,]c_2, d_2[$, then $\gamma_1 = \gamma_2$ on $[c_1, d_1] \cap [c_2, d_2]$.*

(iii) *If $\gamma_1 : [0, c] \to M$ and $\gamma_2 : [0, d] \to M$ are two U-calibrated curves, with $c \le d$ such that $\gamma_1(t) = \gamma_2(t)$, for some $t \in [0, c]$, if γ_1 and γ_2 are not identical on $[0, c]$, then either $t = 0$ or $t = c = d$.*

Proof. Part (i) follows from part (iii) of Theorem 9.1, since for any such minimizer we have

$$\partial_x U(t, x) = \partial_v L(\gamma(t), \dot\gamma(t)) = \partial_v L(x, \dot\gamma(t)),$$

which shows that not only the position of the extremal γ at time t is fixed $(= x)$ but so is its speed at time t.

Part (ii) follows from part (i). In fact, if either $t \in]c_1, d_1[$ or $t \in]c_2, d_2[$, then, by part (iv) of Theorem 9.1, the function U is differentiable at (t, x).

To prove part (iii), we observe that part (ii) implies $t \in \{0, c\}$ and $t \in \{0, d\}$, which implies either $t = 0$ or $t = c = d$. □

The next corollary follows from the previous one applied to backward U-characteristics.

Corollary 9.3. *Assume $L : TM \to \mathbb{R}$ is a Tonelli Lagrangian. Let*

$$U :]0, T[\times M \to \mathbb{R}$$

be evolution-dominated by L.

(i) *If U is differentiable at $(t, x) \in]0, T[\times M$, then there is at most one backward U-characteristic $\gamma :]0, t] \to M$ ending at (t, x).*

(ii) *If $\gamma :]0, a] \to M$ is a backward U-characteristic, then U is differentiable at every $(t, \gamma(t))$, with $t \in]0, a[$.*

Proposition 9.4. *Let $u : M \to [-\infty, +\infty]$ be a lower semicontinuous function such that $\hat u(T, X)$ is finite for some $(T, X) \in]0, +\infty[\times M$. Then $\hat u$ is differentiable at $(t, x) \in]0, T[\times M$ if and only if there is a unique backward U-characteristic ending at (t, x). Moreover, the set of upper differentials $D^+\hat u(t, x)$ is equal to the convex hull of all covectors $(-E(\gamma), \partial_v L(\gamma(t), \dot\gamma(t)))$, with $\gamma : [0, t] \to M$ a backward $\hat u$-characteristic ending at (t, x).*

Proof. By Theorem 6.5, we already know that $\hat u$ is locally semiconcave. We first show that for a backward $\hat u$-characteristic $\gamma : [0, t] \to M$ ending at (t, x), we have $(-E(\gamma), \partial_v L(\gamma(t), \dot\gamma(t)) \in D^+\hat u(t, x)$.

Since γ is calibrating for $\hat u$, it is a minimizer; therefore we have

$$\mathcal{H}(t, \gamma(0), x) = \int_0^t L(\gamma(s), \dot\gamma(s))\, ds,$$

and

$$\hat u(t, x) = u(\gamma(0)) + \mathcal{H}(t, \gamma(0), x).$$

By definition of $\hat{u}$, we also have

$$\hat{u}(t', x) \leq u(\gamma(0)) + \mathcal{H}(t', \gamma(0), x'),$$

for all $(t', x') \in]0, +\infty[\times M$. This implies that $D^+_{(t,x)}\mathcal{H}(t, \gamma(0), x) \subset D^+\hat{u}(t, x)$. But by Proposition 4.22, we have $(-E(\gamma), \partial_v L(\gamma(t), \dot{\gamma}(t)) \in D^+_{(t,x)}\mathcal{H}(t, \gamma(0), x)$.

The rest of the proof is similar to the proof of Corollary 4.23. □

We now apply the results above to Lipschitz in the large functions; see A.2 for the definition.

Theorem 9.5. *Assume that $L : TM \to \mathbb{R}$ is a Tonelli Lagrangian. For every finite constant $K, t_0 > 0$, we can find a constant $\lambda < +\infty$ such that for any $u : M \to \mathbb{R}$ Lipschitz in the large with constant K, its Lax–Oleinik evolution $\hat{u}$ is finite everywhere and (globally) Lipschitz on $[t_0, +\infty[\times M$, with Lipschitz constant $\leq \lambda$.*

Proof. Since $\hat{u} = \hat{u}_-$ on $]0, +\infty[\times M$, where u_- is the lower semicontinuous regularization of u and u_- is Lipschitz in the large with the same constant by Lemma A.3, without loss of generality, we can assume that u is lower semicontinuous.

Since, from Corollary 8.13, the Lax–Oleinik evolution $\hat{u}$ is finite everywhere, from Theorem 6.5, we obtain that it is locally semiconcave. Hence, the Lax–Oleinik evolution $\hat{u}$ locally Lipschitz on $]0, +\infty[\times M$. Therefore, we need to show that the norm of derivative of $\hat{u}$ is bounded almost everywhere, on $[t_0, +\infty[\times M$, by a constant that depends only on K and t_0, but not on u.

From Corollary 8.16, for every $(t, x) \in]0, +\infty[\times M$, we can find $y \in M$ such that

$$\hat{u}(t, x) = u(y) + h_t(y, x) = u(y) + \mathcal{H}(t, y, x). \tag{9-3}$$

Since

$$\mathcal{H}(t, y, x) = h_t(y, x) \leq u(x) - u(y) + A(0)t \leq K + Kd(x, y) + A(0)t.$$

We now use the fact that $2Kd(x, y) - C(2K)t \leq h_t(y, x) = \mathcal{H}(t, y, x)$, to get $Kd(x, y) \leq \frac{1}{2}[\mathcal{H}(t, y, x) + C(2K)t]$. Combining with the inequality above, we obtain

$$\mathcal{H}(t, y, x) \leq K + \tfrac{1}{2}[\mathcal{H}(t, y, x) + C(2K)t] + A(0)t.$$

Since $\mathcal{H}(t, y, x) = h_t(y, x)$, the inequality above is equivalent to

$$\mathcal{H}(t, y, x) \leq 2K + C(2K)t + 2A(0)t.$$

Therefore, we get

$$\frac{\mathcal{H}(t, y, x)}{t} = \frac{h_t(y, x)}{t} \leq \frac{2K}{t} + C(2K) + 2A(0) \leq \frac{2K}{t_0} + C(2K) + 2A(0). \tag{9-4}$$

By its definition, the Lax–Oleinik evolution $\hat{u}$ is strongly evolution-dominated by L, as before, we have

$$\hat{u}(t', x') \leq u(y) + \mathcal{H}(t', y, x') \quad \text{for all } (t', x') \in]0, +\infty[\times M.$$

Subtracting from this last inequality the equality (9-3), we obtain

$$\hat{u}(t', x') - \hat{u}(t, x) \leq \mathcal{H}(t', y, x') - \mathcal{H}(t, y, x) \quad \text{for all } (t', x') \in]0, +\infty[\times M.$$

If $\hat{u}$ is differentiable at (t, x), since $\mathcal{H}$ is locally semiconcave, the inequality above implies that $(t', x') \mapsto \mathcal{H}(t', y, x')$ is differentiable at (t, x), with

$$\partial_t \hat{u}(t, x) = \partial_t \mathcal{H}(t, y, x) \text{ and } \partial_x \hat{u}(t, x) = \partial_x \mathcal{H}(t, y, x).$$

By Corollary 4.24, this implies that $\mathcal{H}$ is differentiable at (t, y, x). But by Corollary 4.25 and (9-4), the derivative $D\mathcal{H}(t, y, x)$ is bounded in norm by a constant depending only on $2Kt_0^{-1} + C(2K) + 2A(0)$. Therefore, the same is true for the derivative of $\hat{u}$ at (t, x). □

Appendix: Uniformly continuous and Lipschitz in the large functions

The following lemma is well-known.

Lemma A.1. *Let N be a Riemannian manifold (not necessarily complete or without boundary). Denote by d the distance on N associated to the Riemannian metric. For any function $u : M \to \mathbb{R}$, the following conditions are equivalent:*

(1) *The function u is uniformly continuous (with respect to d).*

(2) *For every $\epsilon > 0$, we can find $\lambda_\epsilon < +\infty$ such that*

$$|u(x) - u(y)| \leq \epsilon + \lambda_\epsilon d(y, x).$$

(3) *There exists a sequence of Lipschitz (for d) functions $u_n : M \to \mathbb{R}$, $n \in \mathbb{N}$ such that $u_n \to u$ uniformly on M; that is, the norm $\|u - u_n\|_\infty$ approaches 0 as $n \to +\infty$.*

Proof. The implication (3) $\Longrightarrow$ (1) is well-known.

We now prove (1) $\Longrightarrow$ (2). Since u is uniformly continuous, we can find $\alpha > 0$ such that

$$d(x, y) \leq \alpha \Longrightarrow |u(y) - u(x)| \leq \epsilon.$$

For $x, y \in N$ fixed, we can find $n \in \mathbb{N}$ such that $n\alpha \leq d(x, y) < (n+1)\alpha$. By definition of the Riemannian distance, we can find a curve $\gamma : [0, \ell] \to M$, parametrized by arc-length and such that $\gamma(0) = x$, $\gamma(\ell) = y$, and $d(x, y) \leq \ell < (n+1)\alpha$. We set $x_i = \gamma(i\alpha)$, for $i = 0, \dots, n$, and $x_{n+1} = y$. Since $d(x_i, x_{i+1}) \leq \ell_g(\gamma \,|\, [i\alpha, (i+1)\alpha]) = \alpha$, for $i = 0, \dots, n-1$, and $d(x_n, x_{n+1}) \leq$

$\ell_g(\gamma\,|\,[n\alpha,\ell]) = \ell - n\alpha < \alpha$, we get $|u(x_i) - u(x_{i+1})| \le \epsilon$, for $i = 0, \dots, n$. Using $n \le d(x,y)/\alpha$, this yields

$$\begin{aligned}|u(x) - u(y)| &= \left|\sum_{i=0}^{n} u(x_i) - u(x_{i+1})\right| \le \sum_{i=0}^{n} |u(x_i) - u(x_{i+1})| \\ &\le (n+1)\epsilon \le \epsilon + \frac{\epsilon}{\alpha} d(x,y).\end{aligned}$$

This proves (2) with $\lambda_\epsilon = \epsilon/\alpha$.

It remains to prove (2) $\implies$ (3). From (2), we get

$$u(x) - \epsilon \le u(y) + \lambda_\epsilon d(y,x).$$

Taking the infimum over y, we get

$$u(x) - \epsilon \le \inf_{y \in M} u(y) + \lambda_\epsilon d(y,x) \le u(x).$$

The function $u_\epsilon : M \to \mathbb{R}$ defined by $u_\epsilon(x) = \inf_{y\in M} u(y) + \lambda_\epsilon d(y,x)$ has Lipschitz constant $\le \lambda_\epsilon$, and satisfies $\|u_\epsilon - u\|_\infty \le \epsilon$. ☐

We now recall the definition of Lipschitz in the large for a function, see [12, Definition A.5].

Definition A.2. Let X be a metric space with distance d. A function $u : X \to \mathbb{R}$ is said to be Lipschitz in the large if there exists a constant $K < +\infty$ such that

$$|u(y) - u(x)| \le K + Kd(x,y) \quad \text{for every } x, y \in X. \tag{A-1}$$

When the inequality above is satisfied, we say that u is Lipschitz in the large with constant K.

Lemma A.3. *Let X be a metric space with distance d. If $u : X \to \mathbb{R}$ is Lipschitz in the large with constant K, its lower semicontinuous regularization u_- is finite-valued, Lipschitz in the large with the same constant K, and $|u(x) - u_-(x)| \le K$, for every $x \in X$.*

Proof. We can find a sequence $x_i \to x$ such that $u(x_i) \to u_-(x)$. Taking the limit in inequality (A-1), with $y = x_i$, yields $|u(x) - u_-(x)| \le K$. We can also find a sequence $y_i \to y$ such that $u(y_i) \to u_-(y)$. Taking the limit in inequality (A-1), with $y = y_i$ and $x = x_i$, yields $|u_-(y) - u_-(x)| \le K + Kd(x,y)$. ☐

Proposition A.4. *Let X be a metric space with distance d. For any function $u : X \to \mathbb{R}$ and any finite constant $K \ge 0$, the following two statements are equivalent:*

- *The function u is Lipschitz in the large with constant K.*
- *There exists a Lipschitz function $\varphi : X \to \mathbb{R}$, with Lipschitz constant K, such that $\|u - \varphi\|_\infty = \sup_{x\in M} |u(x) - \varphi(x)| \le K/2$.*

Proof. If u satisfies $|u(y)-u(x)| \leq K + Kd(x, y)$, for every $x, y \in X$. We get $-K + u(y) \leq u(x) + Kd(x, y)$. If we define the function $\varphi : X \to \mathbb{R}$ by

$$\varphi(y) = \inf_{x \in M} u(x) + \frac{K}{2} + Kd(x, y),$$

we get $-K/2 + u(y) \leq \varphi(y) \leq u(y) + K/2$. Therefore φ is finite everywhere. It is also Lipschitz with Lipschitz constant $K < +\infty$, and $\|u - \varphi\|_\infty \leq K/2$.

To prove the converse, assume $\varphi : X \to \mathbb{R}$ has Lipschitz constant $\leq K$, and $\|u - \varphi\|_\infty \leq K/2$, we have

$$\begin{aligned} |u(y) - u(x)| &\leq |u(y) - \varphi(y)| + |\varphi(y) - \varphi(x)| + |\varphi(x) - u(x)| \\ &\leq \frac{K}{2} + Kd(x, y) + \frac{K}{2} = K + Kd(x, y). \end{aligned}$$

□

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albert.fathi@math.gatech.edu *School of Mathematics, Georgia Institute of Technology, Atlanta, GA, United States*

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Holonomy and vortex structures in quantum hydrodynamics

MICHAEL S. FOSKETT AND CESARE TRONCI

We consider a new geometric approach to Madelung's quantum hydrodynamics (QHD) based on the theory of gauge connections. Our treatment comprises a constant curvature thereby endowing QHD with intrinsic nonzero holonomy. In the hydrodynamic context, this leads to a fluid velocity which no longer is constrained to be irrotational and allows instead for vortex filaments solutions. After exploiting the Rasetti–Regge method to couple the Schrödinger equation to vortex filament dynamics, the latter is then considered as a source of geometric phase in the context of Born–Oppenheimer molecular dynamics. Similarly, we consider the Pauli equation for the motion of spin particles in electromagnetic fields and we exploit its underlying hydrodynamic picture to include vortex dynamics.

1. Introduction

1.1. ***The role of geometric phases.*** In his seminal work [5], Berry discovered that after undergoing an adiabatic cyclic evolution, a quantum system attains an additional phase factor independent of the dynamics and depending solely on the geometry of the evolution, since referred to as *Berry's phase*. This discovery opened up an entire field of study of the more general concept of *geometric phase* which has since been found to comprise the underlying mechanism behind a wide

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variety of physical phenomena, in both the classical and quantum domains. A key example of each is the Pancharatnam phase in classical optics, [72], which has been experimentally verified using experiments involving laser interferometry [6] and the celebrated Aharonov–Bohm effect of quantum mechanics, discovered in 1959 [3] and experimentally verified in the late 1980s [94], which was given a geometric phase interpretation in [5]. One particular discipline which has benefited greatly from the understanding of geometric phase is quantum chemistry, in which the separation of the molecular wavefunction into nuclear and electronic components gives rise to geometric phase effects in an array of phenomena [67], perhaps most famously including the Jahn–Teller effect [49; 59]. To this day there is extensive research into the role of the geometric phase in quantum systems and in particular the application to molecular dynamics in quantum chemistry [1; 2; 33; 67; 78; 80; 81; 82].

Originally considered by Simon [87], the geometric interpretation of Berry's phase hinges on the gauge theory of principal bundles. The latter serves as a unifying mathematical framework so that the geometric phase identifies the *holonomy* associated to the choice of *connection* on the bundle. In this picture one considers a base manifold M with fibers isomorphic to a Lie group G which can be put together in such a way to create a globally nontrivial topology. The external parameters provide the coordinates on the base space, whilst the fibers are given simply by the $U(1)$ phase factor (not the phase itself!) of the wavefunction. Then, when one considers an adiabatic cyclic evolution of the external parameters, forming a closed loop in the base manifold, the corresponding curve in the $U(1)$-bundle (specified uniquely by a choice of connection) need not form a closed loop, with the extent of the failure to do so called the holonomy or Berry phase. This geometric picture on a principal bundle serves as the setting for all such geometric phase effects, with the base and fibers given by the problem under consideration. As mentioned before, holonomy manifests also in many classical systems, for example that discovered by Hannay [37], with perhaps the most famous physical example being the Foucault pendulum [86]. Such classical examples have led to much further study of these ideas, for example using reduction theory and geometric mechanics [63] as well as applications to the n-body problem [58] and guiding center motion [57].

Recently, a gauge theoretical description of quantum hydrodynamics in terms of connections has been suggested [88], using the Madelung transform [60; 61] to write the wavefunction in exponential form of an amplitude-phase product, $\psi = \mathrm{R}e^{i\hbar^{-1}S}$. This change of variables has the well-known effect of transforming the Schrödinger equation into a hydrodynamical system upon defining a fluid velocity through the relation $\boldsymbol{v} = m^{-1}\nabla S$. Whilst the hydrodynamic picture of quantum mechanics dates back to Madelung [60; 61], it was Takabayasi [90;

92] who first realized that the circulation of the fluid velocity $\oint \boldsymbol{v} \cdot \mathrm{d}\boldsymbol{x}$ must be quantized to ensure that the total wavefunction is single-valued, a fact which was later rediscovered by Wallstrom [98]. As shown in [88], the Madelung transform naturally allows one to consider a principal $U(1)$-bundle over $\mathbb{R}$ associated to the phase of the wavefunction. In this picture, the quantization condition of the circulation is in fact another example of holonomy, now corresponding to the connection $\mathrm{d}S$. More specifically, as the curvature of the connection vanishes everywhere except at those points for which S is not single-valued, this is in fact a type of *monodromy*, with the exact value depending on the winding number of the loop surrounding the singularity.

Here we consider an alternative approach to holonomy in QHD, using the Euler–Poincaré framework [45] to introduce a nonflat differentiable $U(1)$ connection whose constant curvature can be set as an initial condition. This results in holonomy with trivial monodromy as well as corresponding to a nonzero vorticity in the hydrodynamic setting. The key feature of this new approach to QHD is that it allows us to include geometric phase effects without entertaining double-valued functions or singular connections. Indeed, while the latter are still allowed as special cases, thereby leading to quantum vortex structures [90; 93; 92; 8; 9], here we shall apply the present construction to incorporate also nonquantized hydrodynamic vortex filaments, which are then coupled to the equations of quantum hydrodynamics. In this way, we provide an alternative approach to capture geometric Berry phases in the Born–Oppenheimer approximation or in the Aharonov–Bohm effect. We then consider the applications of this new approach to adiabatic molecular dynamics as well as extend the approach to include particles with spin by considering the Pauli equation. Motivated by the latter we then present the framework for introducing our connection in nonabelian systems.

The remainder of this introduction is devoted to presenting a more detailed exposition of the necessary background material and mathematical formalism to set the scene within which we present our results. Section 1.2 commences by outlining the necessary geometric structures of quantum mechanics used throughout this paper, including the Dirac–Frenkel variational principle and Hamiltonian structure of quantum mechanics, before switching to the hydrodynamic picture by introducing the Madelung transform and demonstrating the Lie–Poisson structure of QHD by using momentum map techniques. Section 1.3 presents the geometric interpretation of Wallstrom's quantization condition in terms of the holonomy of the multivalued phase connection. Finally, we conclude the Introduction with an outline of the rest of the paper in Section 1.4, presenting a summary of the results in each subsequent section.

1.2. ***Hamiltonian approach to quantum hydrodynamics.*** In this section we provide the conventional geometric setting for quantum mechanics and its hydrodynamic formulation. As customary in the standard quantum mechanics of pure states, we consider a vector $\psi(t) \in \mathscr{H}$ in a Hilbert space $\mathscr{H}$. Then, the Schrödinger equation $i\hbar\dot{\psi} = \widehat{H}\psi$ [85] can be derived from the Dirac–Frenkel (DF) variational principle [26]

$$0 = \delta \int_{t_1}^{t_2} \langle \psi, i\hbar\dot{\psi} - \widehat{H}\psi \rangle \,\mathrm{d}t\,, \tag{1-1}$$

where the bracket $\langle \psi_1, \psi_2 \rangle$ denotes the real part of the Hermitian inner product $\langle \psi_1 | \psi_2 \rangle$. For the case of square-integrable wavefunctions $\mathscr{H} = L^2(\mathbb{R}^3)$, we have $\langle \psi_1 | \psi_2 \rangle = \int \psi_1^* \psi_2 \,\mathrm{d}^3x$. The variational principle (1-1) can be generalized upon suitable redefinition of the total energy $h(\psi)$, which in the standard case considered here is simply given as the expectation of the Hamiltonian operator $\widehat{H}$, that is $h(\psi) = \langle \psi | \widehat{H}\psi \rangle$. In fact, the Schrödinger equation also admits a canonical Hamiltonian structure. For an arbitrary Hamiltonian $h(\psi)$, the generalized Schrödinger equation reads

$$\frac{\partial \psi}{\partial t} = -\frac{i}{2\hbar}\frac{\delta h}{\delta \psi} =: X_h(\psi)\,, \tag{1-2}$$

in which X_h is the corresponding Hamiltonian vector field. It can be checked that $h(\psi) = \langle \psi | \widehat{H}\psi \rangle$ recovers the standard Schrödinger evolution. Then, the Hamiltonian structure arises from the symplectic form

$$\Omega(\psi_1, \psi_2) = 2\hbar \ \mathrm{Im}\,\langle \psi_1 | \psi_2 \rangle \tag{1-3}$$

on $\mathscr{H}$. It can then be readily verified that the corresponding Poisson bracket returns (1-2) upon considering the relation $\dot{f} = \Omega(X_f, X_h)$. In the standard interpretation of quantum mechanics, $\mathscr{H} = L^2(\mathbb{R}^3)$ and the wavefunction identifies the probability density $D = |\psi|^2$ which evolves according to

$$\frac{\partial D}{\partial t} = \frac{2}{\hbar}\,\mathrm{Im}(\psi^* \widehat{H}\psi)\,. \tag{1-4}$$

In the case of spin-less particles, the Hamiltonian operator $\widehat{H}$ is constructed out of the canonical observables $\widehat{Q} = \boldsymbol{x}$ and $\widehat{P} = -i\hbar\nabla$ satisfying $[\widehat{Q}_i, \widehat{P}_j] = i\hbar\delta_{ij}$, so that $\widehat{H} = \widehat{H}(\widehat{Q}, \widehat{P})$. As we shall now show, for the particular case of the physical Hamiltonian $\widehat{H} = \widehat{P}^2/2m + V(\widehat{Q})$, an equivalent hydrodynamic formulation of the theory emerges by rewriting the wavefunction in its polar form (*Madelung transform*) $\psi(\boldsymbol{x}, t) = \sqrt{D(\boldsymbol{x}, t)}e^{iS(\boldsymbol{x},t)/\hbar}$. Upon performing the appropriate substitutions in the DF variational principle (1-1), the latter becomes

$$0 = \delta \int_{t_1}^{t_2} \int D\left(\partial_t S + \frac{|\nabla S|^2}{2m} + \frac{\hbar^2}{8m} \frac{|\nabla D|^2}{D^2} + V \right) \mathrm{d}^3x \, \mathrm{d}t \,, \tag{1-5}$$

leading to

$$\partial_t D + \operatorname{div} \frac{D \nabla S}{m} = 0 \,, \tag{1-6}$$

$$\partial_t S + \frac{|\nabla S|^2}{2m} - \frac{\hbar^2}{2m} \frac{\Delta \sqrt{D}}{\sqrt{D}} + V = 0 \,. \tag{1-7}$$

The first equation is clearly the continuity equation for the probability density $D = |\psi|^2$. The second equation resembles the Hamilton–Jacobi equation of classical mechanics, albeit with an additional term, often referred to as the *quantum potential*

$$V_Q := -\frac{\hbar^2}{2m} \frac{\Delta \sqrt{D}}{\sqrt{D}} \,. \tag{1-8}$$

Madelung's insight was to recognize that, written in terms of the variables (D, S), the equation for conservation of probability takes the form of a fluid continuity equation for a fluid velocity field $\boldsymbol{v} := m^{-1} \nabla S$. Then, upon taking the gradient of the quantum Hamilton–Jacobi equation, both equations can be rewritten in terms of the new variables $(D, \boldsymbol{v})$ and one obtains the hydrodynamical system

$$\partial_t D + \operatorname{div}(D\boldsymbol{v}) = 0 \,, \tag{1-9}$$

$$m(\partial_t + \boldsymbol{v} \cdot \nabla)\boldsymbol{v} = -\nabla(V_Q + V) \,, \tag{1-10}$$

corresponding to the standard Eulerian form of hydrodynamic equations of motion, from here on referred to as the quantum hydrodynamic (QHD) equations. It is important to notice that as $\boldsymbol{v}$ is a potential flow, the vorticity $\boldsymbol{\omega} := \nabla \times \boldsymbol{v}$ of the flow is identically zero unless there are points where S is multiple-valued.

These quantum hydrodynamic equations were the starting point for several further interpretations of quantum mechanics, most notably Bohmian mechanics [10], inspired by earlier works of de Broglie [20], in which one considers a physical particle that is guided by the quantum fluid. Whilst we do not consider the implications of such theories here, we remark that trajectory-based descriptions of quantum mechanics have been used to simulate a wide variety of physical processes [100] and the use of a QHD approach continues to be an active area of research, particularly in the field of quantum chemistry [47]. More recently the geometric approach to QHD was extended to comprise hybrid quantum-classical dynamics [30]. With this in mind we shall consider the application of the fundamental ideas presented in this paper to quantum chemistry in Section 3.

We now turn our attention to the geometric structure underlying QHD [25; 27; 51]. It has long been known that the map $\psi \mapsto (mD\boldsymbol{v}, D) =: (\boldsymbol{\mu}, D)$ is a momentum map for the natural symplectic action of the semidirect-product group $\mathrm{Diff}(\mathbb{R}^3) \circledS \mathcal{F}(\mathbb{R}^3, U(1))$ on the representation space $L^2(\mathbb{R}^3) \simeq \mathrm{Den}^{1/2}(\mathbb{R}^3)$. Here, $\mathrm{Diff}(\mathbb{R}^3)$ denotes diffeomorphisms of physical space, $\mathcal{F}(\mathbb{R}^3, U(1))$ denotes the space of $U(1)$-valued scalar functions, while $\mathrm{Den}^{1/2}(\mathbb{R}^3)$ denotes the space of half-densities on physical space [4]. Then, as described in [27; 25], it can be shown that, for the case of the physical Hamiltonian operator, the total energy $h(\psi) = \mathrm{Re} \int \psi^* \widehat{H} \psi \, \mathrm{d}^3x$ can be expressed as a functional of these momentum map variables $(\boldsymbol{\mu}, D)$ to read

$$h(\boldsymbol{\mu}, D) = \int \left(\frac{|\boldsymbol{\mu}|^2}{2mD} + \frac{\hbar^2}{8m} \frac{|\nabla D|^2}{D} + DV(\boldsymbol{x}) \right) \mathrm{d}^3x \,. \tag{1-11}$$

This process of expressing a Hamiltonian functional in terms of momentum map variables is known as *Guillemin–Sternberg collectivization* [36] and it leads to a Lie–Poisson system which in this case is defined on the dual of the semidirect-product Lie algebra $\mathfrak{X}(\mathbb{R}^3) \circledS \mathcal{F}(\mathbb{R}^3)$, where $\mathfrak{X}(\mathbb{R}^3)$ denotes vector fields on physical space while $\mathcal{F}(\mathbb{R}^3)$ stands for scalar functions. More explicitly, the Lie–Poisson bracket arising from the Madelung momentum map is as follows:

$$\begin{aligned} \{f, g\}(\boldsymbol{\mu}, D) = \int \boldsymbol{\mu} \cdot \left(\left(\frac{\delta g}{\delta \boldsymbol{\mu}} \cdot \nabla \right) \frac{\delta f}{\delta \boldsymbol{\mu}} - \left(\frac{\delta f}{\delta \boldsymbol{\mu}} \cdot \nabla \right) \frac{\delta g}{\delta \boldsymbol{\mu}} \right) \mathrm{d}^3x \\ + \int D \left(\left(\frac{\delta g}{\delta \boldsymbol{\mu}} \cdot \nabla \right) \frac{\delta f}{\delta D} - \left(\frac{\delta f}{\delta \boldsymbol{\mu}} \cdot \nabla \right) \frac{\delta g}{\delta D} \right) \mathrm{d}^3x \,, \end{aligned} \tag{1-12}$$

which coincides with the Lie–Poisson structure for standard barotropic fluid dynamics [46]. A vector calculus exercise [27] shows that Hamilton's equations $\dot{f} = \{f, h\}$ recover the hydrodynamic equations (1-9)–(1-10).

Despite its deep geometric footing, this construction invokes a Lie–Poisson reduction process [46; 62] involving the existence of smooth invertible Lagrangian fluid paths $\eta \in \mathrm{Diff}(\mathbb{R}^3)$, so that $\dot{\boldsymbol{\eta}}(\boldsymbol{x}_0, t) = \delta h / \delta \boldsymbol{\mu}|_{\boldsymbol{x}=\boldsymbol{\eta}(\boldsymbol{x}_0, t)}$. Thus, this description assumes that the phase S is single-valued thereby leading to zero circulation and vorticity. In other words, this geometric formulation of QHD does not capture holonomy. As we shall see in the remainder of this paper, holonomy can still be restored by purely geometric arguments which however involve a different perspective from the one treated here.

1.3. ***Multi-valued phases in quantum hydrodynamics.*** Having previously investigated the geometry of QHD in terms of momentum maps [25], the rest of this paper focuses on an alternative geometric interpretation of QHD in terms of gauge connections. To see their role in QHD, we notice that whilst the equations of motion (1-9), (1-10) had been known since the early days of quantum mechanics, in 1994 Wallstrom [98] demonstrated that the requirement that the wavefunction be single-valued does not actually imply that the QHD equations are equivalent to the Schrödinger equation $i\hbar\partial_t\psi = -(\hbar^2/2m)\Delta\psi + V\psi$, unless one has the following additional condition on the phase of the wavefunction

$$\oint_{c_0} \nabla S \cdot \mathrm{d}\boldsymbol{x} = 2\pi\hbar n\,, \tag{1-13}$$

around any closed loop $c_0 : [0, 1] \to \mathbb{R}^3$ and for $n \in \mathbb{Z}$. This condition, equivalently asserting that the circulation of the fluid flow $\Gamma = \oint_{c_0} \boldsymbol{v} \cdot \mathrm{d}\boldsymbol{x}$ is quantized, is originally due to Takabayasi [90], and arises due to the fact that S can be considered a multivalued function, by which we mean that the replacement

$$S(\boldsymbol{x}) \to S(\boldsymbol{x}) + 2\pi\hbar n \tag{1-14}$$

leaves the wavefunction invariant. Then, the condition (1-13) is nontrivial, that is $n \neq 0$, whenever the curve c_0 encloses regions in which S is multivalued, which itself occurs only at points where the wavefunction vanishes (nodes) [35; 39]. This can easily be seen by inverting the Madelung transform so that

$$S = -i\hbar \ln \frac{\psi}{|\psi|} = \hbar \left(\arctan \frac{\operatorname{Re}\psi}{\operatorname{Im}\psi} + n\pi \right), \tag{1-15}$$

where $n \in \mathbb{Z}$ arises from the multivalued nature of the inverse tangent function. In the hydrodynamic context, examples of this are given by the presence of vortices, a topic which has been studied extensively [8; 9; 90; 93; 92] and which we will turn our attention to in Section 2.4.

In fact, the condition (1-13) can be interpreted geometrically as in [88] by considering the 1-form $\nabla S \cdot \mathrm{d}\boldsymbol{x} = \mathrm{d}S$ as a connection on a $U(1)$-bundle over $\mathbb{R}^3$. This is explained as follows. Firstly, in writing $\psi = \sqrt{D}e^{iS/\hbar}$, we effectively make the decomposition $\mathbb{C} = \mathbb{R}^+ \times U(1)$. We then consider the principal $U(1)$-bundle over $\mathbb{R}^3$, where the object $i\hbar^{-1}\mathrm{d}S$ can be considered as a $\mathfrak{u}(1)$-valued connection 1-form. Furthermore, it can be shown that the exponential of the loop integral in (1-13) is indeed an element of the holonomy group of this bundle. See Chapter II in the standard reference [53] for details on holonomy and principal bundles and [86; 23; 15; 99; 14] for their appearance in mechanical systems. As the curvature of the connection vanishes everywhere except at those points where S is multivalued, the quantization of the circulation can be explained geometrically, simply as the presence of the winding number through monodromy. Following the discovery of the Berry phase [5] and its geometric interpretation due to Simon [87], this concept connecting geometric phases and holonomy via monodromy has been found to arise in a wide variety of situations in quantum mechanics, ranging from QHD to the Aharonov–Bohm effect, and molecular dynamics. In this paper, we shall present a new alternative approach to QHD that features holonomy without monodromy by introducing a nonflat connection.

1.4. ***Outline of paper.*** Section 2 presents the key idea of this paper, providing an alternative framework for understanding holonomy in QHD. Starting with 2.1, we introduce a different method of writing the wavefunction as an amplitude-phase product, allowing us to introduce a phase connection and write the Lagrangian in terms of this new dynamical variable. In deriving the equations of motion, we allow for this connection to possess nontrivial curvature resulting in new terms in phase equation. In Section 2.2 we move to the fluid picture and show how these new terms give rise to a nontrivial circulation theorem and demonstrate that this connection carries nontrivial holonomy without monodromy. In Section 2.3 we reconstruct the Schrödinger equation from the QHD system and see how the nontrivial curvature of the connection appears through minimal coupling, whilst Section 2.4 demonstrates how the nonzero vorticity can sustain solutions corresponding to vortex filaments and presents a coupled system of vortex dynamics within the Schrödinger equation.

In Section 3 we consider the application of these techniques to the Born–Oppenheimer factorization of the molecular wavefunction in adiabatic quantum chemistry. We begin in Section 3.1 by presenting the standard approach used in the literature and derive the QHD version of the equations of motion from the standard exponential polar form applied to the nuclear factor. This section also presents a summary of the key simplifications often used in the nuclear equation to aid simulations. In Section 3.2 we simply apply the formalism developed in Section 2 to the Born–Oppenheimer system and comment on how these novel features may provide alternative viewpoints on key problems, which in the usual case arise due to the multivalued nature of the objects in question. We conclude the section by considering a modified approach which couples a classical nuclear trajectory to a hydrodynamic vortex, incorporating geometric phase effects.

In Section 4 we apply our treatment to exact factorization (EF) systems, in which one considers a wavefunction with additional parametric dependence. We commence in Section 4.1 by considering the time-dependent generalization of the Born–Oppenheimer ansatz, to which the name EF was given in [1], and apply our treatment to this system whilst also demonstrating its variational and Hamiltonian structures. In Section 4.2, we consider the exact factorization in the special case in which the "electronic factor" is given by a two-level system, thus leading us to introduce the spin density vector and accordingly specialize the geometric structures. Finally, as a particular case, we consider the exact factorization of the

Pauli spinor in Section 4.3 and show that this treatment endows the hydrodynamic form of the Pauli equation with our additional holonomy. This section concludes with the coupling of the Pauli equation to vortex filament dynamics.

The method of deriving the QHD phase connection implies that it has vanishing curvature. In Section 5 we show this explicitly and continue to show that in fact any gauge connection (corresponding to any arbitrary Lie group G) introduced in this way must have zero curvature. In this more general (nonabelian) case, we also demonstrate how, for mechanical systems that give rise to connections through this approach, this zero curvature relation can be relaxed at the level of the Lagrangian, instead with the connection allowed to possess constant curvature as an initial condition, exactly as in the abelian case of QHD presented in Section 2.

2. Phase factors in quantum hydrodynamics

Having reviewed the standard approach to quantum hydrodynamics, including the interpretation of the quantized circulation condition as monodromy on a principal bundle, in this section we present an alternative approach in which nontrivial holonomy is built-in as an initial condition through a new dynamical connection. The point of departure is that, since the exponential map in $U(1)$ is not one-to-one, we are motivated to look at phase factors as elementary objects rather than expressing them as exponentials of Lie algebra elements in $\mathfrak{u}(1) = i\mathbb{R}$. As we shall see, this simple step eventually leads to a new method for incorporating holonomy in quantum hydrodynamics.

2.1. ***Hamiltonian approach to connection dynamics.*** Instead of using the standard polar decomposition of the wavefunction, we begin by writing

$$\psi(\boldsymbol{x}, t) = \sqrt{D(\boldsymbol{x}, t)}\,\theta(\boldsymbol{x}, t), \quad \text{with } \theta \in \mathcal{F}(\mathbb{R}^3, U(1)). \tag{2-1}$$

By writing explicitly the $U(1)$ factor θ we avoid using the exponential map, which is not injective and works only with single-valued functions. Furthermore, this expression for the wavefunction has the advantage of making the (gauge) Lie group $U(1)$ appear explicitly, allowing us to use the tools of geometric mechanics [62]. The relation $\theta^* = \theta^{-1}$ allows us to write the Dirac–Frenkel variational principle (1-5) as

$$0 = \delta \int_{t_1}^{t_2}\!\!\int \left(i\hbar D\theta^{-1}\partial_t\theta - \frac{\hbar^2}{2m}\left(\left|\nabla\sqrt{D}\right|^2 + D|\nabla\theta|^2\right) - DV \right) \mathrm{d}^3x\,\mathrm{d}t\,. \tag{2-2}$$

Now, we let the phase factor $\theta(\boldsymbol{x}, t)$ evolve according to the standard $U(1)$ action:

$$\theta(\boldsymbol{x}, t) = \Theta(\boldsymbol{x}, t)\theta_0(\boldsymbol{x}), \quad \text{with } \Theta \in \mathcal{F}(\mathbb{R}^3, U(1)). \tag{2-3}$$

In turn, this allows us to rewrite the time derivative as

$$\partial_t\theta = (\partial_t\Theta\,\Theta^{-1})\theta := \xi\theta\,, \quad \text{where } \xi\in\mathcal{F}(\mathbb{R}^3,\mathfrak{u}(1)), \tag{2-4}$$

so that $\xi(\boldsymbol{x},t)$ is a purely imaginary function. We can further evaluate terms involving the gradient of θ by introducing a connection $\boldsymbol{\nu}$ thus:

$$\begin{aligned}\nabla\theta &= \nabla\Theta\,\theta_0 + \Theta\nabla\theta_0 = \nabla\Theta\,\Theta^{-1}\theta - \Theta\boldsymbol{\nu}_0\theta_0\\ &= -(-\nabla\Theta\,\Theta^{-1}+\boldsymbol{\nu}_0)\theta =: -\boldsymbol{\nu}\theta,\end{aligned} \tag{2-5}$$

where we have $\boldsymbol{\nu}_0 := -\nabla\theta_0/\theta_0$ and $\nu = \boldsymbol{\nu}\cdot \mathrm{d}\boldsymbol{x}\in\mathfrak{u}(1)\otimes\Omega^1(\mathbb{R}^3)$, the factor $\Omega^1(\mathbb{R}^3)$ being the space of differential one-forms on $\mathbb{R}^3$. Such approaches to introducing gauge connections have been used in the geometric mechanics literature before, for example in the study of liquid crystal dynamics [28; 29; 31; 32; 42; 95]. Indeed, we present the general formulation for gauge connections in continuum mechanical systems in Section 5.

Remark 2.1 (trivial and nontrivial connections). As discussed in the next section, the gauge connection introduced in this way must have zero curvature. This is shown by taking the curl of the relation $\nabla\theta = -\boldsymbol{\nu}\theta$. In the present approach, we are exploiting this zero curvature case in order to have a final form of the QHD Lagrangian. Once variations have been taken in Hamilton's principle, the equations will be allowed to hold also in the case of nonzero curvature. This is a common technique used in geometric mechanics to derive new Lagrangians, for example used in [16] to generalize the Dirac–Frenkel Lagrangian to include mixed state dynamics as well as in the study complex fluids [31; 32; 42]. Within the theory of quantum dynamics, a similar approach was also used by Dirac in

In terms of our newly introduced ξ and $\boldsymbol{\nu}$, our variational principle reads

$$0=\delta\int_{t_1}^{t_2}\!\!\int\Big(i\hbar D\xi - \frac{\hbar^2}{2m}\big(D|\boldsymbol{\nu}|^2+\big|\nabla\sqrt{D}\big|^2\big)-DV\Big)\,\mathrm{d}^3x\,\mathrm{d}t\,, \tag{2-6}$$

where we have set $|\boldsymbol{\nu}|^2=\boldsymbol{\nu}^*\cdot\boldsymbol{\nu}$. At this stage noting that both ξ and $\boldsymbol{\nu}$ are purely imaginary, we define their real counterparts

$$\bar{\xi} := i\hbar\xi\,, \quad \bar{\boldsymbol{\nu}} := i\hbar\boldsymbol{\nu}\,, \tag{2-7}$$

so that we can rewrite the variational principle (2-6) as

$$0=\delta\int_{t_1}^{t_2}\!\!\int D\Big(\bar{\xi}-\frac{|\bar{\boldsymbol{\nu}}|^2}{2m}-\frac{\hbar^2}{8m}\frac{|\nabla D|^2}{D^2}-V\Big)\,\mathrm{d}^3x\,\mathrm{d}t =: \delta\int_{t_1}^{t_2}\ell(\bar{\xi},\bar{\boldsymbol{\nu}},D)\,\mathrm{d}t\,. \tag{2-8}$$

After computing $(\delta\bar{\xi}, \delta\bar{\boldsymbol{\nu}}) = (\partial_t \bar{\eta}, -\nabla\bar{\eta})$ with arbitrary $\bar{\eta} := i\hbar\delta\Theta\,\Theta^{-1}$, taking variations with arbitrary δD yields the following general equations of motion:

$$\partial_t\left(\frac{\delta\ell}{\delta\bar{\xi}}\right) - \operatorname{div}\frac{\delta\ell}{\delta\bar{\boldsymbol{\nu}}} = 0, \qquad \partial_t\bar{\boldsymbol{\nu}} + \nabla\bar{\xi} = 0, \qquad \frac{\delta\ell}{\delta D} = 0. \tag{2-9}$$

More specifically, the first equation leads to the continuity equation

$$\partial_t D + \operatorname{div}(m^{-1} D\bar{\boldsymbol{\nu}}) = 0, \tag{2-10}$$

in which we notice how $\tilde{\boldsymbol{\nu}} := m^{-1}\bar{\boldsymbol{\nu}}$ plays the role of a fluid velocity. Next, the third equality in (2-9) becomes

$$\bar{\xi} = \frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V_Q + V, \tag{2-11}$$

where we recall the quantum potential (1-8). Then, the second in (2-9) leads to

$$\partial_t\bar{\boldsymbol{\nu}} + \nabla\left(\frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V_Q + V\right) = 0, \tag{2-12}$$

which formally coincides with the gradient of (1-7).

Remark 2.2 (Lie–Poisson structure I). The new QHD equations (2-10) and (2-12) comprise a Lie–Poisson bracket on the dual of the semidirect-product Lie algebra $\mathcal{F}(\mathbb{R}^3) \circledS \Omega^1(\mathbb{R}^3)$. Specifically, the Lie–Poisson bracket for equations (2-10)–(2-12) reads

$$\{f, h\} = \int\left(\frac{\delta h}{\delta\bar{\boldsymbol{\nu}}}\cdot\nabla\frac{\delta f}{\delta D} - \frac{\delta f}{\delta\bar{\boldsymbol{\nu}}}\cdot\nabla\frac{\delta h}{\delta D}\right)\mathrm{d}^3x, \tag{2-13}$$

while the Hamiltonian is

$$h(D, \bar{\boldsymbol{\nu}}) = \int D\left(\frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + \frac{\hbar^2}{8m}\frac{|\nabla D|^2}{D^2} + V\right)\mathrm{d}^3x.$$

The bracket (2-13) arises from a Lie–Poisson reduction on the semidirect-product group $\mathcal{F}(\mathbb{R}^3, U(1)) \circledS \Omega^1(\mathbb{R}^3, \mathfrak{u}(1))$. Here, $\Omega^1(\mathbb{R}^3, \mathfrak{u}(1))$ denotes the space of differential one-forms with values in $\mathfrak{u}(1) \simeq i\mathbb{R}$, while the semidirect-product structure is defined by the affine gauge action $\boldsymbol{\nu} \mapsto \boldsymbol{\nu} + \Theta^{-1}\nabla\Theta$, where $\Theta \in \mathcal{F}(\mathbb{R}^3, U(1))$ and $\boldsymbol{\nu} \in \Omega^1(\mathbb{R}^3, \mathfrak{u}(1))$. For further details on this type of affine Lie–Poisson reduction, see [28; 42].

Before continuing we specify the three different manifestations of the $U(1)$ connection we use in this paper. Firstly, we introduced the $\mathfrak{u}(1)$-valued connection $\boldsymbol{\nu}$ via the relation $\nabla\theta =: -\boldsymbol{\nu}\theta$. Then, its real counterpart $\bar{\boldsymbol{\nu}}$ was introduced via $\bar{\boldsymbol{\nu}} := i\hbar\boldsymbol{\nu} \in \Omega^1(\mathbb{R}^3)$, which, for $\theta = e^{iS/\hbar}$, coincides with ∇S. Finally, in anticipation of the next section, we define $\tilde{\boldsymbol{\nu}} \in \Omega^1(\mathbb{R}^3)$ by performing a further division by the mass, $\tilde{\boldsymbol{v}} := i\hbar m^{-1}\boldsymbol{v} = m^{-1}\bar{\boldsymbol{v}}$. This, corresponding to $m^{-1}\nabla S$ in the standard approach, will serve as the fluid velocity in the QHD picture.

Note how the usual exponential form $\theta = e^{iS/\hbar}$ in (2-1) returns $\bar{\xi} = -\partial_t S$ and $\bar{\boldsymbol{v}} = \nabla S$, thus transforming equation (2-11) into the standard phase equation (quantum Hamilton–Jacobi equation) (1-7) of QHD. However, in our approach $\bar{\boldsymbol{v}}$ is allowed to have nontrivial curvature, as can be seen from the curl of (2-12):

$$\partial_t(\nabla \times \bar{\boldsymbol{v}}) = 0. \tag{2-14}$$

This relation demonstrates explicitly how, in view of Remark 2.1, the curvature of the connection $\bar{\boldsymbol{v}}$ need not be trivial (unlike ordinary QHD) but is instead preserved in time. This is one of the main upshots of the present approach. We will develop this observation in the next section.

2.2. ***Hydrodynamic equations and curvature.*** In order to reconcile the new QHD equations with the Madelung–Bohm construction, this section discusses the hydrodynamic form of (2-10)–(2-12) in terms of the velocity-like variable $\tilde{\boldsymbol{v}}$. As already seen, the continuity equation is naturally rewritten in terms of $\tilde{\boldsymbol{v}}$ as

$$\partial_t D + \operatorname{div}(D\tilde{\boldsymbol{v}}) = 0. \tag{2-15}$$

Next, we multiply (2-12) by m^{-1} and expand the gradient to obtain the hydrodynamic-type equation

$$m(\partial_t + \tilde{\boldsymbol{v}} \cdot \nabla)\tilde{\boldsymbol{v}} = -\tilde{\boldsymbol{v}} \times (\nabla \times \bar{\boldsymbol{v}}) - \nabla(V + V_Q). \tag{2-16}$$

This equation again clearly demonstrates the importance of not utilizing the exponential form of the phase as we now have the additional Lorentz-force term $-\tilde{\boldsymbol{v}} \times (\nabla \times \bar{\boldsymbol{v}})$, which is absent in the equation (1-10) of standard quantum hydrodynamics. Indeed, one sees that this additional term vanishes exactly when $\tilde{\boldsymbol{v}}$ is a pure gradient. In the Bohmian interpretation, the Lagrangian fluid paths (aka *Bohmian trajectories*) are introduced via the relation $\dot{\boldsymbol{\eta}}(\boldsymbol{x}, t) = \tilde{\boldsymbol{v}}(\boldsymbol{\eta}(\boldsymbol{x}, t), t)$, so that Bohmian trajectories obey the Lagrangian path equation

$$m\ddot{\boldsymbol{\eta}} = -\dot{\boldsymbol{\eta}} \times \nabla \times \bar{\boldsymbol{v}} - \nabla_{\boldsymbol{x}}(V + V_Q)|_{\boldsymbol{x}=\boldsymbol{\eta}(\boldsymbol{x},t)}. \tag{2-17}$$

We observe that a nonzero curvature modifies the usual equation of Bohmian trajectories by the emergence of a Lorentz-force term. Notice that this term persists in the semiclassical limit typically obtained by ignoring the quantum potential contributions.

We continue by writing the fluid equation in terms of the Lie derivative and the sharp isomorphism induced by the Euclidean metric in the fluid kinetic energy term in (2-8). We have

$$m(\partial_t + \pounds_{\tilde{\boldsymbol{v}}^\sharp})\tilde{\boldsymbol{v}} = -\tilde{\boldsymbol{v}}^\sharp \times (\nabla \times \bar{\boldsymbol{v}}) + \tfrac{1}{2}m\nabla|\tilde{\boldsymbol{v}}|^2 - \nabla(V + V_Q). \tag{2-18}$$

Then, we obtain Kelvin's circulation theorem in the form

$$0=\frac{\mathrm{d}}{\mathrm{d}t}\oint_{c(t)}\tilde{\boldsymbol{v}}\cdot\mathrm{d}\boldsymbol{x}+\frac{1}{m}\oint_{c(t)}\tilde{\boldsymbol{v}}^{\sharp}\times(\nabla\times\tilde{\boldsymbol{v}})\cdot\mathrm{d}\boldsymbol{x}=\frac{\mathrm{d}}{\mathrm{d}t}\oint_{c_0}\tilde{\boldsymbol{v}}\cdot\mathrm{d}\boldsymbol{x}. \tag{2-19}$$

Here, $c(t)$ is a loop moving with the fluid velocity $\tilde{\boldsymbol{v}}^{\sharp}$ such that $c(0)=c_0$ and the last equality follows directly from (2-14). In terms of the geometry of principal bundles, the last equality tells us that the holonomy of the connection $\boldsymbol{v}$ must be constant in time. Since no singularities are involved and $\boldsymbol{v}$ is assumed to be differentiable, the last equality in (2-19) is an example of nontrivial holonomy with trivial monodromy.

We conclude this section with a short comment on helicity conservation. By taking the dot product of the second equation in (2-9) with $\nabla\times\tilde{\boldsymbol{v}}$,

$$\partial_t(\tilde{\boldsymbol{v}}\cdot\nabla\times\tilde{\boldsymbol{v}})=-m^{-1}\,\mathrm{div}(\xi\nabla\times\tilde{\boldsymbol{v}}),$$

so that hydrodynamic helicity is preserved in time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\tilde{\boldsymbol{v}}\cdot(\nabla\times\tilde{\boldsymbol{v}})\,\mathrm{d}^3x=0. \tag{2-20}$$

Now that the hydrodynamic Bohmian interpretation has been discussed, it is not yet clear how this construction is actually related to the original Schrödinger equation of quantum mechanics. This is the topic of the next section.

2.3. ***Schrödinger equation with holonomy.*** In this section, we discuss the relation between the new QHD framework given by equations (2-10)–(2-12) and the original Schrödinger equation. As a preliminary step, we consider the Helmholtz decomposition of $\tilde{\boldsymbol{v}}$, that is,

$$\tilde{\boldsymbol{v}}(\boldsymbol{x},t)=\nabla s(\boldsymbol{x},t)+\hbar\nabla\times\boldsymbol{\beta}(\boldsymbol{x}), \tag{2-21}$$

where $\boldsymbol{\beta}$ is a constant function to ensure (2-14). Also, we have added the factor $\hbar$ and fixed the Coulomb gauge div $\boldsymbol{\beta}=0$ for later convenience. Notice that although s appears exactly in the place that S would in the standard Madelung transform from Section 1.2, here we have used the lowercase letter to emphasize that in this case we consider s as a single-valued function. The relation (2-21) is reminiscent of similar expressions for the Bohmian velocity $\tilde{\boldsymbol{v}}$ already appearing in [12], although in the latter case these were motivated by stochastic augmentations of standard quantum theory. One can verify that upon substituting (2-21) into the equations of motion (2-9) and (2-10), the latter become

$$\partial_t s + \frac{|\nabla s + \hbar\nabla\times\boldsymbol{\beta}|^2}{2m} + V + V_Q = 0, \tag{2-22}$$

$$\partial_t D + \operatorname{div}\left(D\,\frac{\nabla s + \hbar\nabla\times\boldsymbol{\beta}}{m}\right) = 0 \tag{2-23}$$

Here, we have discarded numerical integration factors in the first equation. We recognize that these correspond to the standard Madelung equations for a free elementary charge in a magnetic field $\hbar\Delta\boldsymbol{\beta}$.

We will further characterize the Helmholtz decomposition (2-21) of the connection $\boldsymbol{\nu}$ in terms of its defining relation (2-5). In particular, after constructing the Lagrangian (2-8), $\boldsymbol{\nu}$ is then only defined as the solution of $\partial_t\boldsymbol{\nu} = -\nabla\xi$ in (2-9). Combining the latter with $\partial_t\theta = \xi\theta$ leads to $\partial_t(\boldsymbol{\nu} + \theta^{-1}\nabla\theta) = 0$ so that direct integration yields

$$\boldsymbol{\nu} = -\frac{\nabla\theta}{\theta} + i\,\boldsymbol{\Lambda}(\boldsymbol{x}), \tag{2-24}$$

for a constant real function $\boldsymbol{\Lambda}(\boldsymbol{x})$. An immediate calculation then shows that $\nabla\times(\nabla\theta/\theta) = 0$. Then, upon moving to the real-valued variables (2-7), direct comparison to (2-21) yields

$$\nabla s = -i\hbar\frac{\nabla\theta}{\theta}, \qquad \nabla\times\boldsymbol{\beta} = -\boldsymbol{\Lambda}. \tag{2-25}$$

Now that we have characterized the additional terms due to the presence of nonzero curvature in the Madelung equations, we can use the expressions above to reconstruct the quantum Schrödinger equation. As we shall see, this coincides with the equation for $\psi = \sqrt{D}e^{is/\hbar}$, as it arises from the new Madelung equations (2-22)–(2-23). Introducing $R = \sqrt{D}$ in (2-1), we compute

$$\begin{aligned} i\hbar\partial_t\psi &= i\hbar(\partial_t R\,\theta + R\,\partial_t\theta) \\ &= \left[-\frac{i\hbar}{m}\left(\frac{\nabla R}{R}\cdot\bar{\boldsymbol{\nu}}\right) - \frac{i\hbar}{2m}\operatorname{div}\bar{\boldsymbol{\nu}} + \frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V_Q\right]\psi + V\psi, \end{aligned} \tag{2-26}$$

having used the continuity equation in (2-10) to find $\partial_t R$ and (2-4) with (2-7) and (2-11) to find $\partial_t\theta$.

We must still manipulate the kinetic energy term to express everything in terms of ψ. Before continuing we notice that (2-1) leads to

$$\nabla\psi = (R^{-1}\nabla R + \theta^{-1}\nabla\theta)\psi, \tag{2-27}$$

so that, since $\theta^{-1}\nabla\theta$ is purely imaginary,

$$\frac{\nabla R}{R} = \frac{\operatorname{Re}(\psi^*\nabla\psi)}{|\psi|^2}, \qquad \frac{\nabla\theta}{\theta} = \frac{i\,\operatorname{Im}(\psi^*\nabla\psi)}{|\psi|^2}. \tag{2-28}$$

Using (2-24) now leads to $\bar{\boldsymbol{v}} = \hbar\,\mathrm{Im}(\psi^*\nabla\psi)/|\psi|^2 - \hbar\boldsymbol{\Lambda}$, so that the right-hand side of (2-26) can be entirely written in terms of ψ. As shown in Appendix A, lengthy calculations yield

$$\left[-\frac{i\hbar}{m}\frac{\nabla R}{R}\cdot\bar{\boldsymbol{v}} - \frac{i\hbar}{2m}\operatorname{div}\bar{\boldsymbol{v}} + \frac{|\bar{\boldsymbol{v}}|^2}{2m} + V_Q\right]\psi = -\frac{\hbar^2}{2m}\Delta\psi + \frac{i\hbar^2}{m}\boldsymbol{\Lambda}\cdot\nabla\psi + \frac{\hbar^2}{2m}|\boldsymbol{\Lambda}|^2\psi.$$

Putting everything back together we obtain the Schrödinger equation associated to the modified Madelung equations (2-22)–(2-23):

$$i\hbar\partial_t\psi = \left[\frac{(-i\hbar\nabla - \hbar\boldsymbol{\Lambda})^2}{2m} + V\right]\psi\,. \tag{2-29}$$

Notice how $\hbar\boldsymbol{\Lambda}$, corresponding to the constant curvature part of our $U(1)$ connection, appears in the place of a magnetic vector potential in the Schrödinger equation in which $\hbar$ plays the role of a coupling constant. The quantity $\hbar\boldsymbol{\Lambda}$ has been called the *internal vector potential* in quantum chemistry [89] and its role is to incorporate holonomic effects in quantum dynamics. A static version of equation (2-29) also appeared in Dirac's work on singular electromagnetic fields [24].

Remark 2.3 (Lie–Poisson structure II). Going back to Madelung hydrodynamics, we notice that the introduction of the vector potential $\boldsymbol{\Lambda}$ leads to writing the hydrodynamic equation (2-16) in the form

$$m(\partial_t + \tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} = \hbar\tilde{\boldsymbol{v}}\times\nabla\times\boldsymbol{\Lambda} - \nabla(V + V_Q)\,.$$

In turn, upon recalling the density variable $D = R^2$ and by introducing the momentum variable $\boldsymbol{\mu} = mD\tilde{\boldsymbol{v}} + \hbar D\boldsymbol{\Lambda}$, the equation above possesses the alternative Hamiltonian structure (in addition to (2-13)) given by the hydrodynamic Lie–Poisson bracket (1-12), although the Hamiltonian (1-11) is now modified to

$$h(\boldsymbol{\mu}, D) = \int\left(\frac{|\boldsymbol{\mu} - \hbar D\boldsymbol{\Lambda}|^2}{2mD} + \frac{\hbar^2}{8m}\frac{|\nabla D|^2}{D} + DV(\boldsymbol{x})\right)\mathrm{d}^3x\,.$$

At this point topological defects may be incorporated by allowing $\boldsymbol{\Lambda}$ in (2-29) to satisfy

$$\oint_{c_0}\boldsymbol{\Lambda}\cdot\mathrm{d}\boldsymbol{x} = 2\pi n; \tag{2-30}$$

in this case, the present construction reduces to the standard approach to multivalued wavefunctions in condensed matter theory; see, e.g., [52]. In the variational framework, the velocity field $\tilde{\boldsymbol{v}} = \delta h/\delta\boldsymbol{\mu}$ (introduced by the reduced Legendre transform [62]) becomes the fundamental variable, the resulting hydrodynamic

Lagrangian being

$$\ell(\tilde{\boldsymbol{v}}, D) = \int \left(\frac{1}{2} m D |\tilde{\boldsymbol{v}}|^2 + \hbar D \tilde{\boldsymbol{v}} \cdot \boldsymbol{\Lambda} - \frac{\hbar^2}{8m} \frac{|\nabla D|^2}{D} - D V \right) \mathrm{d}^3 x \,. \tag{2-31}$$

Thus, the treatment in this paper may accommodate both geometric and topological features depending on the explicit expression of $\boldsymbol{\Lambda}$.

Motivated by the appearance of the phase connection as a minimal coupling term in the Schrödinger equation (2-29), it may be useful to include the effect of an external magnetic field on the quantum system within this new QHD framework. Then, in the case of a spinless unit charge, the Schrödinger equation with holonomy reads

$$i\hbar \partial_t \psi = \left[\frac{(-i\hbar\nabla - (\hbar\boldsymbol{\Lambda} + \boldsymbol{A}))^2}{2m} + V \right] \psi \,. \tag{2-32}$$

In this instance $\boldsymbol{\Lambda}$ and $\boldsymbol{A}$ are formally equivalent $U(1)$ gauge connections. Setting $\boldsymbol{\Lambda} = 0$ in the Hamiltonian operator of (2-32) yields the Aharonov–Bohm Hamiltonian, in which case again the magnetic potential has a topological singularity. However, despite the apparent equivalence between $\boldsymbol{\Lambda}$ and $\boldsymbol{A}$, they are related to essentially different features: while the holonomy associated to $\boldsymbol{A}$ is associated to the properties of the external magnetic field, the holonomy associated to $\boldsymbol{\Lambda}$ is intrinsically related to the evolution of the quantum state ψ itself. This specific difference is particularly manifest in the case of two spinless unit charges moving within an external magnetic field. Indeed, in that case the 2-particle wavefunction $\psi(\boldsymbol{x}_1, \boldsymbol{x}_2, t)$ leads to defining $\boldsymbol{\Lambda}(\boldsymbol{x}_1, \boldsymbol{x}_2)$ and $\boldsymbol{A}(\boldsymbol{x})$ on different spaces, thereby revealing their essentially different nature. At present, we do not know if this difference plays any role in the two-particle Aharonov–Bohm effect [84], although we plan to develop this aspect in future work.

2.4. ***Schrödinger equation with hydrodynamic vortices.*** In this section, we show how the present setting can be used to capture the presence of vortices in quantum hydrodynamics. While the presence of topological vortex singularities in quantum mechanics has been known since the early days, this problem was considered in the context of the Madelung–Bohm formulation by Takabayasi [90; 93; 92] and later by Białynicki-Birula [8; 9]. In the hydrodynamic context, the vorticity two-form ω is the differential of the Eulerian velocity field so that in our case $\boldsymbol{\omega} := \nabla \times \tilde{\boldsymbol{v}}$. Then, upon using (2-24), one has

$$\boldsymbol{\omega}(\boldsymbol{x}) = -\frac{\hbar}{m} \nabla \times \boldsymbol{\Lambda}(\boldsymbol{x}) \,. \tag{2-33}$$

In this section we wish to introduce the presence of hydrodynamic vortices in Schrödinger quantum mechanics. To this purpose, we consider a hydrodynamic vortex filament of the form

$$\boldsymbol{\omega}(\boldsymbol{x}) = \Gamma \int \boldsymbol{R}_\sigma \, \delta(\boldsymbol{x} - \boldsymbol{R}(\sigma)) \, \mathrm{d}\sigma \,, \tag{2-34}$$

where $\boldsymbol{R}(\sigma)$ is the curve specifying the filament, σ is a parametrization of the curve, $\boldsymbol{R}_\sigma := \partial \boldsymbol{R}/\partial\sigma$, and the number Γ is the vortex strength and the expression $\Gamma = 2n\pi\hbar/m$ recovers the particular case of quantized vortices [92]. For the quantization of three-dimensional vortex filaments, we refer the reader to [34]. Here, in order to avoid problems with boundary conditions, we consider the simple case of vortex rings. Then, inverting the curl operator in (2-33) by using the Biot–Savart law [83] yields

$$\boldsymbol{\Lambda}(\boldsymbol{x}) = \frac{m}{\hbar} \nabla \times \Delta^{-1} \boldsymbol{\omega} = \frac{m\Gamma}{\hbar} \nabla \times \int \boldsymbol{R}_\sigma \, G(\boldsymbol{x} - \boldsymbol{R}) \, \mathrm{d}\sigma \,, \tag{2-35}$$

where $G(\boldsymbol{x} - \boldsymbol{y}) = -|\boldsymbol{x} - \boldsymbol{y}|^{-1}/(4\pi)$ is the convolution kernel for the inverse Laplace operator Δ^{-1} and we have made use of (2-34). Thus, the Schrödinger equation (2-29) becomes

$$i\hbar\partial_t \psi = \frac{1}{2m}\left(-i\hbar\nabla + m\Gamma\nabla \times \int \boldsymbol{R}_\sigma \, G(\boldsymbol{x} - \boldsymbol{R}) \, \mathrm{d}\sigma \right)^2 \psi + V\psi \,, \tag{2-36}$$

where the vortex position appears explicitly. In what follows, we will set $\Gamma = 1$ for simplicity without affecting the general treatment.

Since in the present treatment the vorticity is constant, including the motion of the vortex filament in this description requires the addition of extra features. In quantum mechanics, the dynamics of hydrodynamic vortices has been given a Hamiltonian formulation by Rasetti and Regge [76] and it was later developed in [43; 54; 55; 73; 74; 97]. Then, one can think of exploiting the Rasetti–Regge approach to let the quantum vortex move while interacting with the quantum state obeying (2-36). At the level of Hamilton's variational principle, this method leads to the following modification of the Dirac–Frenkel Lagrangian in (1-1):

$$\begin{aligned} &L(\boldsymbol{R}, \partial_t \boldsymbol{R}, \psi, \partial_t \psi) \\ &\quad = \frac{1}{3} \int \partial_t \boldsymbol{R} \cdot \boldsymbol{R} \times \boldsymbol{R}_\sigma \, \mathrm{d}\sigma \\ &\qquad + \mathrm{Re} \int i\hbar\psi^* \partial_t \psi - \psi^* \left[\frac{1}{2m} \left(-i\hbar\nabla + m\nabla \times \int \boldsymbol{R}_\sigma \, G(\boldsymbol{x} - \boldsymbol{R}) \, \mathrm{d}\sigma \right)^2 + V \right] \psi \, \mathrm{d}^3 x \,, \end{aligned} \tag{2-37}$$

where the expression $\psi^*[\ldots]\psi$ on the last row identifies the Hamiltonian functional $h(\boldsymbol{R}, \psi)$ satisfying $\boldsymbol{R}_\sigma \cdot \delta h/\delta \boldsymbol{R} = 0$ (valid for any Hamiltonian of the form

$h = h(\boldsymbol{\omega})$ [44]) and

$$\boldsymbol{R}_\sigma \times \left(\boldsymbol{R}_\sigma \times \frac{\partial \boldsymbol{R}}{\partial t} - \frac{\delta h}{\delta \boldsymbol{R}} \right) = 0 .$$

Then, one finds

$$\frac{\delta h}{\delta \boldsymbol{R}} = -\frac{m}{\hbar} \boldsymbol{R}_\sigma \times \frac{\delta h}{\delta \boldsymbol{\Lambda}} \bigg|_{\boldsymbol{x}=\boldsymbol{R}} = \hbar \boldsymbol{R}_\sigma \times \mathbb{P} \left(\operatorname{Im}(\psi^* \nabla \psi) - |\psi|^2 \boldsymbol{\Lambda} \right) \big|_{\boldsymbol{x}=\boldsymbol{R}} ,$$

where $\mathbb{P} = \mathrm{Id} - \nabla \Delta^{-1} \operatorname{div}$ is the Leray projection on the divergence-free part. The coupled system reads

$$\partial_t \boldsymbol{R} = \hbar \mathbb{P} \left(\operatorname{Im}(\psi^* \nabla \psi) - |\psi|^2 \boldsymbol{\Lambda} \right) \big|_{\boldsymbol{x}=\boldsymbol{R}} + \kappa \boldsymbol{R}_\sigma , \tag{2-38}$$

$$i\hbar \partial_t \psi = \frac{1}{2m} (-i\hbar \nabla - \hbar \boldsymbol{\Lambda})^2 \psi + V \psi . \tag{2-39}$$

where $\boldsymbol{\Lambda}$ is given as in (2-35) and κ is an arbitrary quantity. We also have that in the presence of vortex filaments the holonomy around a fixed loop c_0 can be expressed as

$$-\hbar \oint_{c_0} \boldsymbol{\Lambda} \cdot \mathrm{d}\boldsymbol{x} = m \int_{S_0} \int \mathrm{d}\sigma \, \delta(\boldsymbol{x} - \boldsymbol{R}(\sigma)) \, \boldsymbol{R}_\sigma \cdot \mathrm{d}\boldsymbol{S} , \tag{2-40}$$

via Stokes' theorem, where S_0 is a surface whose boundary defines the loop $\partial S_0 =: c_0$.

The idea of vortices in quantum mechanics has potentially interesting applications in the field of quantum chemistry. For example, in the Born–Oppenheimer approximation, the curvature of the Berry connection is given by a delta function at the point of conical intersections [50]. Once more, as conical intersections are topological singularities, the vortex structures generated by a singular Berry connection are quantized. After reviewing the general setting of adiabatic molecular dynamics, the next section shows how the construction in this paper can be used to deal with geometric phases in the Born–Oppenheimer approximation.

3. Born–Oppenheimer molecular dynamics

Motivated by the importance of geometric phase effects in quantum chemistry [14; 33; 50; 80; 81; 82], this section applies the formalism outlined in Section 2 to the field of adiabatic molecular dynamics.

We start our discussion by considering the starting point for all quantum chemistry methods, the Born–Oppenheimer ansatz for the molecular wavefunction. As explained in [22; 65], for example, the molecular wavefunction $\Psi(\{\boldsymbol{r}\}, \{\boldsymbol{x}\}, t)$ for a system composed of N nuclei with coordinates $\boldsymbol{r}_i$ and n electrons with coordinates $\boldsymbol{x}_a$ is factorized in terms of a nuclear wavefunction $\Omega(\{\boldsymbol{r}\}, t)$ and a time-independent electronic function $\phi(\{\boldsymbol{x}\};\{\boldsymbol{r}\})$ depending parametrically on the nuclear coordinates $\{\boldsymbol{r}\}_{i=1\dots N}$. In the simple case of a single electron and nucleus, we have $\Psi(\boldsymbol{r},\boldsymbol{x},t)=\Omega(\boldsymbol{r},t)\phi(\boldsymbol{x};\boldsymbol{r})$, so that the normalizations of Ψ and Ω enforce $\int|\phi(\boldsymbol{x};\boldsymbol{r})|^2\,\mathrm{d}^3x=1$. Equivalently, upon making use of Dirac's notation, we denote $|\phi(\boldsymbol{r})\rangle:=\phi(\boldsymbol{x};\boldsymbol{r})$ and write

$$\Psi(t)=\Omega(\boldsymbol{r},t)\,|\phi(\boldsymbol{r})\rangle\,. \tag{3-1}$$

The partial normalization condition becomes $\|\phi(\boldsymbol{r})\|^2:=\langle\phi(\boldsymbol{r})|\phi(\boldsymbol{r})\rangle=1$ and the Hamiltonian operator for the system reads $\widehat{H}=-\hbar^2M^{-1}\Delta/2\,+\widehat{H}_e$. Here, M is the nuclear mass and all derivatives are over the nuclear coordinate $\boldsymbol{r}$. In addition we have that the electronic state is the fundamental eigenstate of the electronic Hamiltonian $\widehat{H}_e$, so that $\widehat{H}_e\,|\phi(\boldsymbol{r})\rangle=E(\boldsymbol{r})\,|\phi(\boldsymbol{r})\rangle$. The motivation for this ansatz comes from the separation of molecular motion into fast and slow dynamics due to the large mass difference between the electron and nucleus, the idea for which goes back to the original work of Born and Oppenheimer [18].

3.1. ***Variational approach to adiabatic molecular dynamics.*** After applying the factorization ansatz (3-1) and following some further manipulation involving integration by parts, the total energy $h=\mathrm{Re}\int\langle\Psi|\widehat{H}\Psi\rangle\,\mathrm{d}^3r$ of the system reads

$$h(\Omega)=\int\bigg(\Omega^*\frac{(-i\hbar\nabla+\boldsymbol{\mathcal{A}})^2}{2M}\Omega+|\Omega|^2\epsilon(\phi,\nabla\phi)\bigg)\,\mathrm{d}^3r\,, \tag{3-2}$$

in which we have introduced the *Berry connection* [5]

$$\boldsymbol{\mathcal{A}}(\boldsymbol{r}):=\langle\phi|-i\hbar\nabla\phi\rangle\in\Omega^1(\mathbb{R}^3)\,, \tag{3-3}$$

and defined the *effective electronic potential*

$$\epsilon(\phi,\nabla\phi):=E+\frac{\hbar^2}{2M}\|\nabla\phi\|^2-\frac{|\boldsymbol{\mathcal{A}}|^2}{2M}\,. \tag{3-4}$$

Here, we have used the eigenvalue equation of $\widehat{H}_e$, while the last two terms correspond to the trace of the so-called *quantum geometric tensor*; see [75] for details. The appearance of the Berry connection is a typical feature of the Born–Oppenheimer method, which is well-known to involve nontrivial Berry phase effects [15; 68; 67]. In order to write the nuclear equation of motion, we use the Dirac–Frenkel Lagrangian $L=\int i\hbar\Omega^*\partial_t\Omega\,\mathrm{d}^3r-h(\Omega)$ and move to a hydrodynamical description. In the standard approach, one writes the nuclear function in the polar form $\Omega(\boldsymbol{r},t)=\sqrt{D(\boldsymbol{r},t)}e^{iS(\boldsymbol{r},t)/\hbar}$. Then, the previous DF Lagrangian becomes

$$L(D,S,\partial_tS)=\int D\bigg(\partial_tS+\frac{|\nabla S+\boldsymbol{\mathcal{A}}|^2}{2M}+\frac{\hbar^2}{8M}\frac{|\nabla D|^2}{D^2}+\epsilon(\phi,\nabla\phi)\bigg)\,\mathrm{d}^3r\,. \tag{3-5}$$

We notice that the Born–Oppenheimer system is formally equivalent to standard quantum mechanics in the presence of an external electromagnetic field. Indeed, the Berry connection $\boldsymbol{\mathcal{A}}$ plays the role of the magnetic vector potential and one has a scalar potential in the form of ϵ. Hence, the standard interpretation is to think of the nuclei evolving in an effective magnetic field generated by the electronic motion. In what follows, we shall adopt Madelung's hydrodynamic picture although an alternative approach using Gaussian wavepackets [56; 38] is reported in Appendix B. Here, we proceed by applying Hamilton's principle $\delta \int_{t_1}^{t_2} L\,\mathrm{d}t = 0$ for arbitrary variations δD and δS, which returns the Euler–Lagrange equations

$$\frac{\partial D}{\partial t} + \operatorname{div}\left(D\,\frac{\nabla S + \boldsymbol{\mathcal{A}}}{M}\right) = 0, \qquad \frac{\partial S}{\partial t} + \frac{|\nabla S + \boldsymbol{\mathcal{A}}|^2}{2M} + V_Q + \epsilon = 0, \tag{3-6}$$

as usual understood as a quantum Hamilton–Jacobi equation for the nuclear phase and a continuity equation for the nuclear density $|\Omega|^2 = D$. Next, we follow the standard approach by introducing $\boldsymbol{v} = M^{-1}\nabla S$. Finally, we write the Madelung equations in hydrodynamic form in terms of the velocity $\boldsymbol{u} := \boldsymbol{v} + M^{-1}\boldsymbol{\mathcal{A}}$:

$$\partial_t D + \operatorname{div}(D\boldsymbol{u}) = 0, \qquad M(\partial_t + \boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\boldsymbol{u}\times\boldsymbol{\mathcal{B}} - \nabla(\epsilon + V_Q), \tag{3-7}$$

where $\boldsymbol{\mathcal{B}} := \nabla \times \boldsymbol{\mathcal{A}}$. Notice how in this frame a Lorentz force becomes apparent.

The last equations above capture the nuclear motion completely; however, in the quantum chemistry literature there are a variety of further specializations that can be made to the nuclear equation of motion, all aiming to alleviate computational difficulty. In the remainder of this section we summarize most of them by considering their subsequent effects on the nuclear fluid equation.

(1) ***Second order coupling:*** In the quantum chemistry literature it is often the case that the second order coupling term, $\langle\phi|\Delta\phi\rangle$, is neglected on the grounds that it has a negligible effect on the nuclear dynamics [96; 64]. As can be verified directly upon expanding the real part, one has $\|\nabla\phi\|^2 = -\operatorname{Re}\langle\phi|\Delta\phi\rangle$; hence such an approximation transforms equation (3-4) to

$$\epsilon(\phi, \nabla\phi) := E - \frac{|\boldsymbol{\mathcal{A}}|^2}{2M},$$

At this stage, one is left with the Lorentz force acting on the nuclei as well as the potential given by the sum of the new effective electronic energy and nuclear quantum potential.

(2) ***Real electronic eigenstate:*** Next, we make the assumption that the electronic eigenstate $\phi(\boldsymbol{r})$ is real-valued, which is valid when the electronic Hamiltonian is nondegenerate [19; 96]. The immediate consequence of the reality of ϕ is that

the Berry connection $\boldsymbol{\mathcal{A}} := \langle\phi| - i\hbar\nabla\phi\rangle$ vanishes since the electronic phase is spatially constant. In this case the nuclear fluid equation becomes

$$(\partial_t + \boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -M^{-1}\nabla(E + V_Q)\,. \tag{3-8}$$

Clearly we still have the nuclear quantum potential as well as the potential energy surface capturing electron-nuclear coupling.

(3) ***Quantum potential:*** As detailed in [25], the quantum potential can also cause difficulties in numerical simulations. If we also consider neglecting the quantum potential term V_Q, the nuclear hydrodynamic equation can be written in its simplest form:

$$(\partial_t + \boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -M^{-1}\nabla E\,. \tag{3-9}$$

The quantum potential is usually neglected by taking the singular weak limit $\hbar^2 \to 0$ of the Lagrangian (3-5). Then, upon considering the single particle solution $D(\boldsymbol{r}, t) = \delta(\boldsymbol{r} - \boldsymbol{q}(t))$, the nuclear equation is equivalent to Newton's second law $M\ddot{\boldsymbol{q}} = -\nabla E$ for a conservative force.

It is only after this extreme level of approximation, neglecting all quantum terms (involving $\hbar$), that one obtains a classical equation of motion for the nuclei, in which one considers the picture of a nucleus evolving on a single potential energy surface [22; 96].

Whilst in this section we have considered adiabatic dynamics in the hydrodynamic picture via the Madelung transform, one can also proceed with an alternative approach in which the nuclear wavefunction is modeled by a frozen Gaussian wavepacket. This idea is presented in Appendix B, where we demonstrate how employing Gaussian coherent states within the variational principle (3-5) provides an alternative approach to regularizing the singularities that are known to arise in Born–Oppenheimer systems.

3.2. ***Holonomy, conical intersections, and vortex structures.*** In the context of the Born–Oppenheimer approximation, our approach to holonomy can be applied by writing the nuclear wavefunction as in (2-1) while leaving the electronic wavefunction unchanged. For a real-valued electronic wavefunction, the Berry connection then vanishes and the Madelung equations (3-6) are replaced by

$$\partial_t D + \operatorname{div}(D\tilde{\boldsymbol{v}}) = 0\,, \tag{3-10}$$

$$M(\partial_t + \tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}} = \hbar\tilde{\boldsymbol{v}}\times\nabla\times\boldsymbol{\Lambda} - \nabla\bigg(E + \frac{\hbar^2}{2M}\|\nabla\phi\|^2 + V_Q\bigg). \tag{3-11}$$

We notice that in the case when the gauge potential $\boldsymbol{\Lambda}$ is singular, these equations correspond to those appearing in the Mead–Truhlar method of adiabatic molecular dynamics [68]. This is a method to deal with the geometric phase arising from double-valued electronic wavefunctions produced by the presence of conical intersections [50; 67; 21]. This is called the *molecular Aharonov–Bohm effect* [66]. As double-valued wavefunctions pose relevant computational difficulties, the Mead–Truhlar method performs a gauge transformation to move the presence of singularities from the wavefunction to the Berry connection.

To illustrate the setting, we first consider the electronic eigenvalue problem

$$\widehat{H}_e\,|\phi_n(\boldsymbol{r})\rangle = E_n(\boldsymbol{r})\,|\phi_n(\boldsymbol{r})\rangle \tag{3-12}$$

and in particular the possibility that the first two separate eigenvalues (known as potential energy surfaces in the chemistry literature) intersect for a given nuclear configuration $\boldsymbol{r}_0$, that is $E_0(\boldsymbol{r}_0) = E_1(\boldsymbol{r}_0)$. In the previous sections, the fundamental eigenvalue E_0 was simply denoted by E. It is well-known that such intersections of the energy surfaces often form the shape of a double cone and are therefore referred to as *conical intersections* in the quantum chemistry literature. The nontrivial Berry phase that arises in such situations corresponds to the fact that the real electronic wavefunction $|\phi_0(\boldsymbol{r})\rangle$ (previously denoted simply by $|\phi(\boldsymbol{r})\rangle$) is double-valued around the point of degeneracy. The Mead–Truhlar method exploits the invariance of the electronic eigenvalue problem under the gauge transformation $|\phi(\boldsymbol{r})\rangle \mapsto |\phi'(\boldsymbol{r})\rangle = e^{i\zeta(\boldsymbol{r})/\hbar}\,|\phi(\boldsymbol{r})\rangle$, thereby redefining the Berry connection according to $\boldsymbol{\mathcal{A}} \mapsto \boldsymbol{\mathcal{A}}' = \boldsymbol{\mathcal{A}} + \nabla\zeta$. Specifically, one selects ζ such that the phase $e^{i\zeta/\hbar}$ exactly compensates the double-valuedness of $|\phi\rangle$ resulting in the new electronic state $|\phi'\rangle$ being single-valued [50; 67] and thus avoiding the need to deal with double-valued functions. However, since $\boldsymbol{\mathcal{A}} = 0$ (because $|\phi\rangle$ is real) and $e^{i\zeta/\hbar}$ must be multivalued, such a transformation has the cost that the corresponding vector potential $\boldsymbol{\mathcal{A}}' = \nabla\zeta$ is singular at the point of the conical intersection. Then, after replacing $|\phi\rangle \to |\phi'\rangle$, one obtains equations (3-10)–(3-11) in the case $\tilde{\boldsymbol{\nu}} = M^{-1}\nabla S$ and $\hbar\boldsymbol{\Lambda} = \nabla\zeta$, so that the problem under consideration becomes equivalent to the Aharonov–Bohm problem, whence the name "molecular Aharonov–Bohm effect".

While conical intersections are essentially topological defects, the physical consistency of these singularities has been recently questioned by Gross and collaborators [70; 78]. In their work, it is argued that the emergence of these topological structures is intrinsically associated to the particular type of adiabatic model arising from the Born–Oppenheimer factorization ansatz. Indeed, the results in [70; 78] and following papers show that these type of singularities are absolutely absent in the exact case of nonadiabatic dynamics. This leads to the question of whether alternative approaches to adiabatic dynamics can be obtained in order to avoid dealing with conical intersections. Notice that the absence of these defects does not imply the absence of a geometric phase. Indeed, as the

Berry connection is not generally vanishing in nonadiabatic dynamics, this leads to nontrivial holonomy which in turn does not arise from topological singularities. In this context, a gauge connection associated to hydrodynamic vortices as in Section 2.4 may be representative of an alternative molecular geometric effect in which the geometric phase depends on the integration loop. In this case, one could drop the quantum potential in (3-11) and select the particle solution $D(\boldsymbol{r},t)=\delta(\boldsymbol{r}-\boldsymbol{q}(t))$ in (3-10).

However, due to (2-33) and (2-34), this approach would produce a δ-like Lorentz force in the nuclear trajectory equation, thereby leading to major difficulties.

The latter may be overcome by finding appropriate closures at the level of Hamilton's principle. For example, one could use Gaussian wavepackets as presented in Appendix B. However, here we adopt a method inspired by previous work in plasma physics [40] and geophysical fluid dynamics [41]. Let us start with the hydrodynamic Lagrangian, of the type (2-31), underlying equations (3-10)–(3-11):

$$\ell(D,\tilde{\boldsymbol{v}})=\int D\left(M|\tilde{\boldsymbol{v}}|^2/2+\hbar\tilde{\boldsymbol{v}}\cdot\boldsymbol{\Lambda}-V_Q-\epsilon\right)\mathrm{d}^3r.$$

Here, the Eulerian variables $D(\boldsymbol{r},t)$ and $\tilde{\boldsymbol{v}}(\boldsymbol{r},t)$ are related to the Lagrangian fluid path $\boldsymbol{\eta}(\boldsymbol{r},t)$ (Bohmian trajectory) by the relations $\dot{\boldsymbol{\eta}}(\boldsymbol{r},t)=\tilde{\boldsymbol{v}}(\boldsymbol{\eta}(\boldsymbol{r},t),t)$ and $D(\boldsymbol{\eta}(\boldsymbol{r},t),t)\,\mathrm{d}^3\eta(\boldsymbol{r},t)=D_0(\boldsymbol{r})\,\mathrm{d}^3r$. If we now restrict the Bohmian trajectory to be of the type $\boldsymbol{\eta}(\boldsymbol{r},t)=\boldsymbol{r}+\boldsymbol{q}(t)$, we have $\tilde{\boldsymbol{v}}(\boldsymbol{r},t)=\dot{\boldsymbol{q}}(t)$ and $D(\boldsymbol{r},t)=D_0(\boldsymbol{r}-\boldsymbol{q}(t))$. Since in this case $\int DV_Q\,\mathrm{d}^3r=\text{const.}$, the Lagrangian $\ell(D,\tilde{\boldsymbol{v}})$ then becomes

$$L(\boldsymbol{q},\dot{\boldsymbol{q}})=\frac{M}{2}|\dot{\boldsymbol{q}}|^2+\int D_0(\boldsymbol{r}-\boldsymbol{q})\big[\hbar\dot{\boldsymbol{q}}\cdot\boldsymbol{\Lambda}(\boldsymbol{r})-\epsilon(\boldsymbol{r})\big]\,\mathrm{d}^3r. \tag{3-13}$$

Here, D_0 is typically a Gaussian distribution and we recall that we are considering the case of a real electronic wavefunction, so that $\boldsymbol{\mathcal{A}}=0$ in the definition of ϵ (3-4). Then, one obtains the Euler–Lagrange equation

$$M\ddot{\boldsymbol{q}}=\hbar\dot{\boldsymbol{q}}\times\nabla\times\int D_0(\boldsymbol{r}-\boldsymbol{q})\boldsymbol{\Lambda}(\boldsymbol{r})\,\mathrm{d}^3r-\nabla\int\epsilon(\boldsymbol{r})D_0(\boldsymbol{r}-\boldsymbol{q})\,\mathrm{d}^3r, \tag{3-14}$$

where $\boldsymbol{\Lambda}$ is given as in (2-35). (This method was recently applied to the Jahn–Teller problem by one of us in [77], where it was shown to recover some recent results obtained from exact nonadiabatic treatments [79].) We see that the nuclear density acts as a convolution kernel regularizing both the connection $\boldsymbol{\Lambda}$ and the potential energy surface appearing in ϵ. For example, this method could be used to regularize topological singularities arising from conical intersections. Then, the geometric phase and the regularized potential energy surface read

$$-\hbar \oint_{c_0} \int \mathrm{d}^3 r' \, D_0(\boldsymbol{r}'-\boldsymbol{r})\boldsymbol{\Lambda}(\boldsymbol{r}') \cdot \mathrm{d}\boldsymbol{r} \quad \text{and} \quad \int \mathrm{d}^3 r' \, D_0(\boldsymbol{r}'-\boldsymbol{r}) E(\boldsymbol{r}').$$

Also, in the present context, the self-consistent vortex evolution may be included upon constructing a Rasetti–Regge type Lagrangian by the replacement $L(\boldsymbol{q},\dot{\boldsymbol{q}}) \to L(\boldsymbol{q},\dot{\boldsymbol{q}}) + \frac{1}{3}\int \partial_t \boldsymbol{R} \cdot \boldsymbol{R} \times \boldsymbol{R}_\sigma \, \mathrm{d}\sigma$, similarly to the approach in Section 2.4. In this case, the vortex evolution equation reads $\partial_t \boldsymbol{R} = M D_0(\boldsymbol{R}-\boldsymbol{q})\dot{\boldsymbol{q}} + \kappa \boldsymbol{R}_\sigma$.

4. Exact wavefunction factorization

4.1. ***Nonadiabatic molecular dynamics.*** While the Born–Oppenheimer approximation has been very successful in the modeling of adiabatic molecular dynamics, many processes in both chemistry and physics involve quantum electronic transitions. In this case, the Born–Oppenheimer approximation breaks down so that nonadiabatic processes require a new modeling framework. In this context, the molecular wavefunction $\Psi(\boldsymbol{r},\boldsymbol{x},t)$ in (3-1) is expanded in the basis provided by the spectral problem (3-12) so that the resulting series expansion is known as *Born–Huang expansion* [17]. While this expansion is the basis for several ab initio methods in nonadiabatic molecular dynamics, an alternative picture, originally due to Hunter [48], has recently been revived by Gross and collaborators [1]. In this alternative picture, the exact solution of the molecular Schrödinger equation is written by allowing the electronic wavefunction in (3-1) to depend explicitly on time, that is

$$\Psi(t) = \Omega(\boldsymbol{r},t)\,|\phi(\boldsymbol{r},t)\rangle\,. \tag{4-1}$$

Going back to von Neumann [71], this type of wavefunction factorization also represents the typical approach to Pauli's equation for charged particle dynamics in electromagnetic fields [91]. In this context, the electronic coordinates are replaced by the spin degree of freedom while the nuclear coordinates are replaced by the particle position coordinate. In more generality, the exact factorization picture is applicable in a variety of multi-body problems in physics and chemistry. In this section, we investigate the role of holonomy in the exact factorization picture. Then, when the holonomy arises from a delta-like curvature, we shall present how the quantum hydrodynamics with spin is modified by the presence of vortex filaments. Before moving on to the Pauli equation, here we shall present the general hydrodynamic equations arising from the exact factorization (4-1).

The typical Hamiltonian for the total system is written as

$$\widehat{H}_{\text{tot}} = -\frac{\hbar^2}{2M}\Delta + \widehat{H}(\boldsymbol{r}) \tag{4-2}$$

so that, after rearrangement, replacing (4-1) in the Dirac–Frenkel Lagrangian

$L = \mathrm{Re} \int \langle \Psi | (i\hbar\partial_t - \widehat{H}_{\mathrm{tot}})\Psi \rangle \, \mathrm{d}^3 r$ leads to the exact factorization Lagrangian

$$L = \mathrm{Re} \int i\hbar\big(\Omega^* \partial_t \Omega + |\Omega|^2 \langle \phi | \partial_t \phi \rangle\big)\, \mathrm{d}^3 r$$
$$- \int \left(\frac{1}{2M} \Omega^* (-i\hbar\nabla + \boldsymbol{\mathcal{A}})^2 \Omega + |\Omega|^2 \left(\langle \phi | \widehat{H} \phi \rangle + \frac{\hbar^2}{2M} \|\nabla \phi\|^2 - \frac{|\boldsymbol{\mathcal{A}}|^2}{2M} \right) \right) \mathrm{d}^3 r, \tag{4-3}$$

where the second line identifies (minus) the expression of the total energy and we recall (3-3). Notice that we have not enforced the partial normalization condition $\|\phi(\boldsymbol{r})\|^2 = 1$ in the variational principle, although this condition can be verified to hold a posteriori after taking variations. When dealing with molecular problems, $|\phi\rangle = \phi(\boldsymbol{x}, t; \boldsymbol{r})$ is a time-dependent electronic wavefunction [1] and $\widehat{H}(\boldsymbol{r})$ is the electronic Hamiltonian in (3-12) from Born–Oppenheimer theory. On the other hand, if we deal with $\frac{1}{2}$-spin degrees of freedom, $|\phi\rangle = |\phi(\boldsymbol{r}, t)\rangle$ is a two-component complex vector parametrized by the coordinate $\boldsymbol{r}$, while $\widehat{H}(\boldsymbol{r})$ is of the form $\widehat{H}(\boldsymbol{r}) = a(\boldsymbol{r}) + \boldsymbol{b}(\boldsymbol{r}) \cdot \hat{\boldsymbol{\sigma}}$ and $\hat{\boldsymbol{\sigma}}$ denotes the array of Pauli matrices $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$.

At this point, the standard approach to QHD requires replacing the polar form of Ω in (4-3). If instead we adopt the method developed in Section 2 and write Ω as in (2-1), we obtain the following hydrodynamic Lagrangian of Euler–Poincaré type [45]:

$$\ell(D, \bar{\xi}, \bar{\nu}, |\phi\rangle) = \int D \left(\bar{\xi} - \frac{|\bar{\boldsymbol{\nu}} + \boldsymbol{\mathcal{A}}|^2}{2M} - \frac{\hbar^2}{8M} \frac{|\nabla D|^2}{D^2} + \Phi \right.$$
$$\left. + \langle \phi | \widehat{H} \phi \rangle - \frac{\hbar^2}{2M} \|\nabla \phi\|^2 + \frac{|\boldsymbol{\mathcal{A}}|^2}{2M} \right) \mathrm{d}^3 r, \tag{4-4}$$

where $\Phi(\boldsymbol{r}) := \langle \phi | i\hbar \partial_t \phi \rangle$. At this stage one can compute the corresponding equations of motion.

Upon introducing the hydrodynamic velocity $\boldsymbol{v}$ and the matrix density $\tilde{\rho}$,

$$\boldsymbol{v}(\boldsymbol{r}, t) = M^{-1}(\bar{\boldsymbol{\nu}} + \boldsymbol{\mathcal{A}}) \quad \text{and} \quad \tilde{\rho}(\boldsymbol{r}, t) = D |\phi\rangle\langle\phi|, \tag{4-5}$$

we obtain the hydrodynamic equations in the form

$$\partial_t D + \mathrm{div}(D\boldsymbol{v}) = 0, \tag{4-6}$$

$$MD(\partial_t + \boldsymbol{v} \cdot \nabla)\boldsymbol{v}$$
$$= \hbar D \boldsymbol{v} \times \nabla \times \boldsymbol{\Lambda} + D \nabla V_Q - \langle \tilde{\rho} | \nabla \widehat{H} \rangle - \frac{\hbar^2}{2M} \partial_j \left(D^{-1} \langle \nabla \tilde{\rho} | \partial_j \tilde{\rho} \rangle \right), \tag{4-7}$$

$$i\hbar(\partial_t \tilde{\rho} + \mathrm{div}(\tilde{\rho}\boldsymbol{v})) = \left[\widehat{H} - \frac{\hbar^2}{2M} \mathrm{div}(D^{-1} \nabla \tilde{\rho}), \tilde{\rho} \right]. \tag{4-8}$$

Here, we have used the notation

$$\langle A(\boldsymbol{r})|B(\boldsymbol{r})\rangle = \mathrm{Tr}(A(\boldsymbol{r})^\dagger B(\boldsymbol{r})),$$

where Tr denotes the matrix trace.

Interestingly, as shown in [25] for an equivalent variant of these equations, this system can also be derived via the standard Euler–Poincaré variational principle for hydrodynamics (as presented earlier in Section 1.2) in which the Eulerian quantities $D(\boldsymbol{r},t)$ and $\boldsymbol{v}(\boldsymbol{r},t)$ are related to the Lagrangian (Bohmian) trajectory $\boldsymbol{\eta}(\boldsymbol{r},t)$ by the relations

$$\dot{\boldsymbol{\eta}}(\boldsymbol{r},t) = \boldsymbol{v}(\boldsymbol{\eta}(\boldsymbol{r},t),t) \quad \text{and} \quad D(\boldsymbol{\eta}(\boldsymbol{r},t),t)\,\mathrm{d}^3\eta(\boldsymbol{r},t) = D_0(\boldsymbol{r})\,\mathrm{d}^3 r.$$

In this instance, as seen before, equations (4-6)–(4-8) correspond to a Lagrangian of the type as given by (2-31), here written as

$$\begin{aligned}&\ell(\boldsymbol{v}, D, \Xi, \tilde{\rho})\\ &= \int\left(\frac{1}{2}MD|\boldsymbol{v}|^2 + \hbar D\boldsymbol{v}\cdot\boldsymbol{\Lambda} + \frac{\hbar^2}{8M}\frac{|\nabla D|^2}{D} + \langle\tilde{\rho}, i\hbar\Xi - \widehat{H}\rangle - \frac{\hbar^2}{4M}\frac{\|\nabla\tilde{\rho}\|^2}{D}\right)\mathrm{d}^3 r,\end{aligned} \tag{4-9}$$

in which $\Xi(\boldsymbol{r},t)$ is defined by the Schrödinger equation

$$\partial_t U(\boldsymbol{r},t) = \Xi(\boldsymbol{\eta}(\boldsymbol{r},t),t)U(\boldsymbol{r},t)$$

for the propagator $U(\boldsymbol{r},t)$ with $\tilde{\rho}(\boldsymbol{\eta}(\boldsymbol{r},t),t)\,\mathrm{d}^3\eta(\boldsymbol{r},t) = U(\boldsymbol{r},t)\tilde{\rho}_0(\boldsymbol{r})U^\dagger(\boldsymbol{r},t)\,\mathrm{d}^3 r$. Then, applying Hamilton's principle by combining the variations

$$\delta D = -\,\mathrm{div}(D\boldsymbol{w}), \qquad \delta\boldsymbol{v} = \partial_t\boldsymbol{w} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{w} - (\boldsymbol{w}\cdot\nabla)\boldsymbol{v}, \tag{4-10}$$

$$\delta\tilde{\rho} = [\Upsilon,\tilde{\rho}] - \mathrm{div}(\tilde{\rho}\boldsymbol{w}), \quad \delta\Xi = \partial_t\Upsilon + [\Upsilon,\Xi] - \boldsymbol{w}\cdot\nabla\Xi + \boldsymbol{v}\cdot\nabla\Upsilon, \tag{4-11}$$

with the auxiliary equations $\partial_t D + \mathrm{div}(D\boldsymbol{v}) = 0$ and $\partial_t\tilde{\rho} + \mathrm{div}(\tilde{\rho}\boldsymbol{v}) = [\Xi,\tilde{\rho}]$ returns equations (4-6)–(4-8). Here, $\boldsymbol{w}$ and Υ are both arbitrary and vanish at the endpoints. In the special case when $\boldsymbol{\Lambda} = 0$, a detailed presentation of this approach can be found in [25].

Remark 4.1 (semidirect product Lie–Poisson structure). Upon defining $\boldsymbol{m} := MD\boldsymbol{v} + \hbar D\boldsymbol{\Lambda}$, equations (4-6)–(4-8) acquire the following Poisson structure:

$$\begin{aligned}\{f,g\}(\boldsymbol{m},D,\tilde{\rho}) = &\int\boldsymbol{m}\cdot\left(\frac{\delta g}{\delta\boldsymbol{m}}\cdot\nabla\frac{\delta f}{\delta\boldsymbol{m}} - \frac{\delta f}{\delta\boldsymbol{m}}\cdot\nabla\frac{\delta g}{\delta\boldsymbol{m}}\right)\mathrm{d}^3 r\\ &-\int D\left(\frac{\delta f}{\delta\boldsymbol{m}}\cdot\nabla\frac{\delta g}{\delta D} - \frac{\delta g}{\delta\boldsymbol{m}}\cdot\nabla\frac{\delta f}{\delta D}\right)\mathrm{d}^3 r\\ &-\int\left\langle\tilde{\rho},\, \frac{i}{\hbar}\left[\frac{\delta f}{\delta\tilde{\rho}},\frac{\delta g}{\delta\tilde{\rho}}\right] + \frac{\delta f}{\delta\boldsymbol{m}}\cdot\nabla\frac{\delta g}{\delta\tilde{\rho}} - \frac{\delta g}{\delta\boldsymbol{m}}\cdot\nabla\frac{\delta f}{\delta\tilde{\rho}}\right\rangle\mathrm{d}^3 r,\end{aligned} \tag{4-12}$$

which is accompanied by the Hamiltonian functional

$$h(\boldsymbol{m}, D, \tilde{\rho}) = \int \left(\frac{|\boldsymbol{m} - \hbar D \boldsymbol{\Lambda}|^2}{2MD} - \frac{\hbar^2}{8M} \frac{|\nabla D|^2}{D} + \langle \tilde{\rho}, \widehat{H} \rangle + \frac{\hbar^2}{4M} \frac{\|\nabla \tilde{\rho}\|^2}{D} \right) \mathrm{d}^3 r . \tag{4-13}$$

We remark here that the change of variables $\tilde{\rho} \to i\hbar\tilde{\rho}$ takes the bracket (4-12) into a Lie–Poisson bracket on the dual of the semidirect-product Lie algebra $\mathfrak{X}(\mathbb{R}^3) \circledS \big(\mathcal{F}(\mathbb{R}^3) \oplus \mathcal{F}(\mathbb{R}^3, \mathfrak{u}(\mathscr{H}_e))\big)$.

4.2. ***Exact factorization for electronic two-level systems.*** Instead of treating infinite-dimensional two-particle systems, the remainder of this paper studies the case in which the electronic state is represented by a two-level system, so that

$$\tilde{\rho}(\boldsymbol{r}, t) = \frac{D(\boldsymbol{r}, t)}{2} \left(\mathbb{1} + \frac{2}{\hbar} \boldsymbol{s}(\boldsymbol{r}, t) \cdot \hat{\boldsymbol{\sigma}} \right) =: \frac{1}{2} \left(D(\boldsymbol{r}, t) \mathbb{1} + \frac{2}{\hbar} \tilde{\boldsymbol{s}}(\boldsymbol{r}, t) \cdot \hat{\boldsymbol{\sigma}} \right),$$

where $\boldsymbol{s}$ is the *spin vector* as described in [7; 13; 11; 91], given by $\boldsymbol{s} = \hbar \langle \phi | \hat{\boldsymbol{\sigma}} \phi \rangle /2$ and satisfying $|\boldsymbol{s}|^2 = \hbar^2/4$, and $\mathbb{1}$ is the 2×2 identity operator. In addition, the Hamiltonian operator reads $\widehat{H} = a(\boldsymbol{r}) \mathbb{1} + \boldsymbol{b}(\boldsymbol{r}) \cdot \hat{\boldsymbol{\sigma}}$. Under these changes of variables, equations (4-6)–(4-8) become

$$\partial_t D + \operatorname{div}(D\boldsymbol{v}) = 0, \tag{4-14}$$

$$MD(\partial_t + \boldsymbol{v} \cdot \nabla)\boldsymbol{v} = \hbar D\boldsymbol{v} \times \nabla \times \boldsymbol{\Lambda} - D\nabla a - \frac{2}{\hbar} \nabla \boldsymbol{b} \cdot \tilde{\boldsymbol{s}} + M^{-1} \partial_j (\tilde{\boldsymbol{s}} \cdot \nabla (D^{-1} \partial_j \tilde{\boldsymbol{s}})), \tag{4-15}$$

$$\hbar M (\partial_t \tilde{\boldsymbol{s}} + \operatorname{div}(\boldsymbol{v}\tilde{\boldsymbol{s}})) = \tilde{\boldsymbol{s}} \times \big(\hbar \operatorname{div}(D^{-1} \nabla \tilde{\boldsymbol{s}}) - 2M\boldsymbol{b}\big). \tag{4-16}$$

For example, in the case of the spin-boson model, one has $a(\boldsymbol{r}) = M\omega^2 r^2/2$ and $\boldsymbol{b}(\boldsymbol{r}) = (\mathcal{D}, 0, \boldsymbol{C} \cdot \boldsymbol{r})/2$, where $\boldsymbol{C}$ and $\mathcal{D}$ are time-independent and spatially constant.

Then, equations (4-14)–(4-16) possess the Euler–Poincaré Lagrangian

$$\ell(\boldsymbol{v}, D, \boldsymbol{\Xi}, \tilde{\boldsymbol{s}}) = \int \left(\frac{1}{2} MD|\boldsymbol{v}|^2 + D(\hbar \boldsymbol{v} \cdot \boldsymbol{\Lambda} - a) + \tilde{\boldsymbol{s}} \cdot \left(\boldsymbol{\Xi} - \frac{2}{\hbar} \boldsymbol{b} \right) - \frac{|\nabla \tilde{\boldsymbol{s}}|^2}{2MD} \right) \mathrm{d}^3 r, \tag{4-17}$$

where $\Xi = -i\, \boldsymbol{\Xi} \cdot \boldsymbol{\sigma}/2$, having used the Lie algebra isomorphism $(\mathfrak{su}(2), [\,\cdot\,,\cdot\,]) \cong (\mathbb{R}^3, \cdot \times \cdot)$ [62], with the variations (4-10) as well as

$$\delta \tilde{\boldsymbol{s}} = \boldsymbol{\Upsilon} \times \tilde{\boldsymbol{s}} - \operatorname{div}(\boldsymbol{w}\tilde{\boldsymbol{s}}), \qquad \delta \boldsymbol{\Xi} = \partial_t \boldsymbol{\Upsilon} + \boldsymbol{\Upsilon} \times \boldsymbol{\Xi} - \boldsymbol{w} \cdot \nabla \boldsymbol{\Xi} + \boldsymbol{v} \cdot \nabla \boldsymbol{\Upsilon}.$$

Here, $\boldsymbol{\Upsilon}(\boldsymbol{r}, t)$ is arbitrary and vanishing at the endpoints. We notice that in using the variable $\tilde{\boldsymbol{s}} := D\boldsymbol{s}$, the quantum potential term has been absorbed in the

Lagrangian and correspondingly no longer appears explicitly in the hydrodynamic equation of motion (4-15).

Analogously, in the case of electronic two-level systems, the Lie–Poisson bracket (4-12) becomes

$$\begin{aligned}\{f, g\}(\boldsymbol{m}, D, \tilde{\boldsymbol{s}}) = &\int \boldsymbol{m}\cdot\left(\frac{\delta g}{\delta \boldsymbol{m}}\cdot\nabla\frac{\delta f}{\delta \boldsymbol{m}} - \frac{\delta f}{\delta \boldsymbol{m}}\cdot\nabla\frac{\delta g}{\delta \boldsymbol{m}}\right)\mathrm{d}^3r\\ &-\int D\left(\frac{\delta f}{\delta \boldsymbol{m}}\cdot\nabla\frac{\delta g}{\delta D} - \frac{\delta g}{\delta \boldsymbol{m}}\cdot\nabla\frac{\delta f}{\delta D}\right)\mathrm{d}^3r\\ &-\int \tilde{\boldsymbol{s}}\cdot\left(\frac{\delta f}{\delta \tilde{\boldsymbol{s}}}\times\frac{\delta g}{\delta \tilde{\boldsymbol{s}}} + \frac{\delta f}{\delta \boldsymbol{m}}\cdot\nabla\frac{\delta g}{\delta \tilde{\boldsymbol{s}}} - \frac{\delta g}{\delta \boldsymbol{m}}\cdot\nabla\frac{\delta f}{\delta \tilde{\boldsymbol{s}}}\right)\mathrm{d}^3r. \end{aligned}\tag{4-18}$$

This is accompanied by the Hamiltonian

$$h(D, \boldsymbol{m}, \tilde{\boldsymbol{s}}) = \int\left(\frac{|\boldsymbol{m}-\hbar D\boldsymbol{\Lambda}|^2}{2MD} + \frac{|\nabla\tilde{\boldsymbol{s}}|^2}{2MD} + \frac{2}{\hbar}\boldsymbol{b}\cdot\tilde{\boldsymbol{s}} + Da\right)\mathrm{d}^3r, \tag{4-19}$$

where we recall the definition $\boldsymbol{m} := MD\boldsymbol{v} + \hbar D\boldsymbol{\Lambda}$.

4.3. ***The Pauli equation with hydrodynamic vortices.*** Having considered a spinless particle in a magnetic field in Section 2.3, here we broaden our treatment to include particles with spin. To do so, one must consider the Pauli equation which captures the interaction of the particle's spin with an external electromagnetic field. Firstly, to describe a spin-$\frac{1}{2}$ particle (of charge $q = 1$, mass M), one considers the two-component spinor wavefunction

$$\Psi(\boldsymbol{r}) = \begin{pmatrix}\Psi_1(\boldsymbol{r})\\ \Psi_2(\boldsymbol{r})\end{pmatrix}, \tag{4-20}$$

where now $\Psi \in L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ and is normalized such that $\int \Psi^\dagger\Psi\,\mathrm{d}^3r = 1$. Then, the dynamics are given by the Pauli equation which amounts to the Schrödinger equation $i\hbar\partial_t\Psi = \widehat{H}_{\text{tot}}\Psi$ with the Hamiltonian operator

$$\widehat{H}_{\text{tot}} = \frac{(-i\hbar\nabla - \boldsymbol{A})^2}{2M} - \frac{\hbar}{2M}\boldsymbol{B}\cdot\hat{\boldsymbol{\sigma}} + V\mathbb{1}, \tag{4-21}$$

in which $\boldsymbol{A}(\boldsymbol{r})$ is the constant magnetic potential, $\boldsymbol{B} := \nabla\times\boldsymbol{A}$ is the magnetic field and $V(\boldsymbol{r})$ is a scalar potential.

In order to proceed with the method proposed in the previous section, we follow the idea outlined in [88; 13; 11] and decompose the spinor wavefunction into the form $\Psi = \sqrt{D(\boldsymbol{r}, t)}\,\theta(\boldsymbol{r}, t)\,|\phi(\boldsymbol{r}, t)\rangle$ (here we use the Dirac notation convention for the "electronic factor"), in which ϕ satisfies the partial normalization condition $\langle\phi(\boldsymbol{r})|\phi(\boldsymbol{r})\rangle =: \|\phi(\boldsymbol{r})\|^2 = 1$. Clearly, we are in the situation described in Sections 4.1 and 4.2 so that, upon absorbing the additional external magnetic field, the fluid velocity (4-5) now reads

$$\boldsymbol{v} = M^{-1}(\bar{\boldsymbol{v}} + \boldsymbol{\mathcal{A}} - \boldsymbol{A}), \tag{4-22}$$

and one can immediately specialize the results from the previous section, so that the Lagrangian (4-17) becomes

$$\begin{aligned}\ell(\boldsymbol{v}, D, \boldsymbol{\Xi}, \tilde{\boldsymbol{s}}) \\ = \int \left(\frac{1}{2} M D |\boldsymbol{v}|^2 + D\boldsymbol{v} \cdot (\hbar \boldsymbol{\Lambda} + \boldsymbol{A}) - DV + \tilde{\boldsymbol{s}} \cdot (\boldsymbol{\Xi} + M^{-1}\boldsymbol{B}) - \frac{|\nabla \tilde{\boldsymbol{s}}|^2}{2MD} \right) \mathrm{d}^3 r.\end{aligned} \tag{4-23}$$

In turn, this produces the equations of motion

$$\partial_t D + \operatorname{div}(D\boldsymbol{v}) = 0, \tag{4-24}$$

$$\begin{aligned} MD(\partial_t + \boldsymbol{v} \cdot \nabla)\boldsymbol{v} \\ = \hbar D \boldsymbol{v} \times \nabla \times \boldsymbol{\Lambda} - D\nabla V + M^{-1} \nabla \boldsymbol{B} \cdot \tilde{\boldsymbol{s}} + M^{-1} \partial_j (\tilde{\boldsymbol{s}} \cdot \nabla (D^{-1} \partial_j \tilde{\boldsymbol{s}})),\end{aligned} \tag{4-25}$$

$$M(\partial_t \tilde{\boldsymbol{s}} + \operatorname{div}(\boldsymbol{v}\tilde{\boldsymbol{s}})) = \tilde{\boldsymbol{s}} \times \big(\operatorname{div}(D^{-1} \nabla \tilde{\boldsymbol{s}}) + \boldsymbol{B} \big). \tag{4-26}$$

In the special case of $\boldsymbol{\Lambda} = 0$, this agrees with the results of [91] upon changing variables back to $\boldsymbol{s} = \tilde{\boldsymbol{s}}/D$. In more generality, the corresponding circulation theorem for a loop $c(t)$ moving with the fluid velocity $\boldsymbol{v}$ reads

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} \oint_{c(t)} (M\boldsymbol{v} + \hbar \boldsymbol{\Lambda} + \boldsymbol{A}) \cdot \mathrm{d}\boldsymbol{r} &= \frac{\mathrm{d}}{\mathrm{d}t} \oint_{c(t)} \boldsymbol{\mathcal{A}} \cdot \mathrm{d}\boldsymbol{r} \\ &= -\frac{1}{MD} \oint_{c(t)} \big(\nabla \tilde{\boldsymbol{s}} \cdot (\boldsymbol{B} + \operatorname{div}(D^{-1} \nabla \tilde{\boldsymbol{s}})) \big) \cdot \mathrm{d}\boldsymbol{r},\end{aligned} \tag{4-27}$$

which, as in [25], gives an expression for the time evolution of the Berry phase, here governed by the external magnetic field and spin degrees of freedom.

Remark 4.2 (Mermin–Ho relation and Takabayasi vector). In general, the circulation around a fixed loop c_0 (with a surface S_0 such that its boundary defines the loop $\partial S_0 =: c_0$) reads

$$\oint_{c_0} \boldsymbol{v} \cdot \mathrm{d}\boldsymbol{r} = \int_{S_0} \nabla \times \boldsymbol{v} \cdot \mathrm{d}\boldsymbol{S} = M^{-1} \int_{S_0} \left(\frac{\hbar}{2} \boldsymbol{T} - \hbar \nabla \times \boldsymbol{\Lambda} - \boldsymbol{B} \right) \cdot \mathrm{d}\boldsymbol{S}, \tag{4-28}$$

where $\boldsymbol{T} := \epsilon_{ijk} n_i \nabla n_j \times \nabla n_k$ and $\boldsymbol{n} := 2\boldsymbol{s}/\hbar$ is the Bloch vector field. The relation $\nabla \times \boldsymbol{\mathcal{A}} = \hbar \boldsymbol{T}/2$ underlying (4-28) first appeared in Takabayasi's work [91] in 1955, hence later motivating the name *Takabayasi vector* [7], and can more explicitly be written in components as

$$T_c = \epsilon_{ijk} \epsilon_{abc} n_i (\partial_a n_j)(\partial_b n_k) = 2i \epsilon_{abc} \big(\langle \partial_b \psi | \partial_a \psi \rangle - \langle \partial_a \psi | \partial_b \psi \rangle \big) = \frac{2}{\hbar} \mathcal{B}_c, \tag{4-29}$$

relying on the definition $n_i = \langle\phi|\sigma_i\phi\rangle = \phi_a^*(\sigma_i)_{ab}\phi_b$ and the property

$$\epsilon_{ijk}(\sigma_i)_{ab}(\sigma_j)_{cd}(\sigma_k)_{ef} = 2i(\delta_{af}\delta_{cb}\delta_{ed} - \delta_{ad}\delta_{cf}\delta_{eb}).$$

Despite Takabayasi's work, the equality $2\hbar^{-1}\nabla\times\boldsymbol{\mathcal{A}} = \epsilon_{ijk}n_i\nabla n_j\times\nabla n_k$ is more commonly known as the Mermin–Ho relation [69] after its appearance in the context of superfluids two decades later. For applications of the Mermin–Ho relation in the more general context of complex fluids, see also [42].

In [93], Takabayasi pointed out the existence of vortex structures in spin hydrodynamics starting from the analysis of the Pauli equation and his work was later revived in [7], where it was extended to comprise the relativistic Weyl equation. Motivated by these old works and proceeding in analogy with the previous sections, here we shall discuss the Rasetti–Regge dynamics of hydrodynamic vortices upon extending the arguments in Section 2.4. To do so, we write the Rasetti–Regge hydrodynamic Lagrangian

$$\bar{\ell}(\boldsymbol{R}, \partial_t\boldsymbol{R}, \boldsymbol{v}, D, \Xi, \tilde{s}) = \frac{1}{3}\int \partial_t\boldsymbol{R}\cdot\boldsymbol{R}\times\boldsymbol{R}_\sigma\,\mathrm{d}\sigma + \ell(\boldsymbol{v}, \boldsymbol{R}, D, \Xi, \tilde{\boldsymbol{s}}), \tag{4-30}$$

where ℓ is obtained upon replacing (2-35) in (4-23). The resulting vortex equation of motion is $\partial_t\boldsymbol{R} = M(D\boldsymbol{v})_{\boldsymbol{r}=\boldsymbol{R}} + \kappa\boldsymbol{R}_\sigma$ (where as before κ is an arbitrary quantity), complemented by the hydrodynamic form of the Pauli equations (4-24)–(4-26), in which again $\boldsymbol{\Lambda}$ is written in terms of the vortex filament according to (2-35).

Remark 4.3 (Pauli equation with hydrodynamic vortices). Naturally, this construction can also be applied to the full Pauli spinor $\Psi(\boldsymbol{r}, t)$, in which case one writes the Rasetti–Regge Dirac–Frenkel Lagrangian

$$\begin{aligned}L(\boldsymbol{R}, \partial_t\boldsymbol{R}, \Psi, \partial_t\Psi) &= \frac{1}{3}\int \partial_t\boldsymbol{R}\cdot\boldsymbol{R}\times\boldsymbol{R}_\sigma\,\mathrm{d}\sigma \\ &\quad + \mathrm{Re}\int\left(i\hbar\Psi^\dagger\partial_t\Psi - \Psi^\dagger\left[\frac{(-i\hbar\nabla - (\hbar\boldsymbol{\Lambda}+\boldsymbol{A}))^2}{2M} - \frac{\hbar}{2M}\boldsymbol{B}\cdot\hat{\boldsymbol{\sigma}} + V\right]\Psi\right)\mathrm{d}^3r,\end{aligned} \tag{4-31}$$

so that the coupled system reads

$$\partial_t\boldsymbol{R} = \hbar\mathbb{P}\left(\mathrm{Im}(\Psi^\dagger\nabla\Psi) - |\Psi|^2(\boldsymbol{\Lambda} + \hbar^{-1}\boldsymbol{A})\right)\Big|_{\boldsymbol{r}=\boldsymbol{R}} + \kappa\boldsymbol{R}_\sigma, \tag{4-32}$$

$$i\hbar\partial_t\Psi = \frac{1}{2M}(-i\hbar\nabla - (\hbar\boldsymbol{\Lambda}+\boldsymbol{A}))^2\Psi - \frac{\hbar}{2M}\boldsymbol{B}\cdot\hat{\boldsymbol{\sigma}}\,\Psi + V\,\Psi. \tag{4-33}$$

Upon expanding Ψ in terms of the exact factorization and recalling the definition of the velocity (4-22), we see the agreement in the vortex equations. Upon performing a long calculation similar to Appendix A, one can also reconstruct the Pauli equation given here from the hydrodynamic equations (4-24)–(4-26).

5. Nonabelian generalizations

As mentioned in Remark 2.1, the QHD gauge connection $\boldsymbol{\nu}$ from Section 2 was introduced by following an approach that invokes zero curvature, i.e., $\nabla\times\boldsymbol{\nu}=0$, although this relation was later relaxed to comprise a nonzero initial curvature. In this section, motivated by the appearance of the differential of the spin vector $\nabla\boldsymbol{s}$ appearing in the previous sections, we shall include the possibility of nonabelian groups, therefore extending our treatment to a whole class of models employing the general relation $\nabla n=-\gamma n$, where $n\in\mathcal{F}(\mathbb{R}^3, M)$ is an order parameter field and γ is a gauge connection corresponding to an arbitrary gauge group $\mathcal{F}(\mathbb{R}^3, G)$, where G acts on M. Nevertheless, even though the relation $\nabla n=-\gamma n$ again implies zero curvature, the equations resulting from Hamilton's principle still allow for a more general nontrivial connection whose curvature again arises as an initial condition.

To begin, we consider the previous treatment of QHD. We consider a $U(1)$ connection defined by $\nabla\theta=-\boldsymbol{\nu}\theta$, (2-5), and see that this definition immediately implies that the connection has zero curvature. Indeed, one has $0=\nabla\times\nabla\theta=-\nabla\times(\boldsymbol{\nu}\theta)=-(\nabla\times\boldsymbol{\nu})\theta$, so that $\nabla\times\boldsymbol{\nu}=0$.

Now we consider the more general case of an order parameter $n\in\mathcal{F}(\mathbb{R}^3, M)$ (where at this point M is an arbitrary manifold) whose evolution is given by an element g of the Lie group $\mathcal{F}(\mathbb{R}^3, G)$,

$$n(\boldsymbol{x},t)=g(\boldsymbol{x},t)n_0(\boldsymbol{x}). \tag{5-1}$$

Then, one can construct a gauge connection γ from the gradient of n as follows:

$$\begin{aligned}\nabla n&=\nabla g n_0+g\nabla n_0\\ &=\nabla g\, g^{-1}n-g\gamma_0 n_0\\ &=-(-\nabla g\, g^{-1}+g\gamma_0 g^{-1})n=:-\gamma n,\end{aligned}\tag{5-2}$$

and we have $\nabla n=-\gamma n$. Here, we show that such a relation must mean that the connection is trivial, i.e., has zero curvature: $\Omega_{ij}=\partial_i\gamma_j-\partial_j\gamma_i+[\gamma_i,\gamma_j]$. Writing our defining relation in terms of differential forms as $\mathrm{d}n=-\gamma n$, we compute

$$\begin{aligned}0=\mathrm{d}^2 n&=-\mathrm{d}(\gamma_j n\,\mathrm{d}x^j)\\ &=-\big((\partial_{[i}\gamma_{j]})n+\gamma_{[j}(\partial_{i]}n)\big)\,\mathrm{d}x^i\wedge\mathrm{d}x^j\\ &=-(\partial_{[i}\gamma_{j]}-\gamma_{[j}\gamma_{i]})n\,\mathrm{d}x^i\wedge\mathrm{d}x^j\\ &=-\tfrac{1}{2}(\partial_i\gamma_j-\partial_j\gamma_i+\gamma_i\gamma_j-\gamma_j\gamma_i)n\,\mathrm{d}x^i\wedge\mathrm{d}x^j\\ &=-\tfrac{1}{2}\Omega_{ij}n\,\mathrm{d}x^i\wedge\mathrm{d}x^j\\ &=-\Omega n,\end{aligned}\tag{5-3}$$

where the square brackets denote index antisymmetrization. At this point, we observe that since $\gamma := -\nabla g\, g^{-1} + g\gamma_0 g^{-1}$, then

$$\Omega = g\Omega_0 g^{-1}$$

and it follows that $0 = \Omega_0 n_0$. Thus, we end up in a situation in which either $\Omega_0 = 0$ thus rendering $\Omega = \mathrm{d}^\gamma\gamma = 0$ for all time, or n_0 belongs to the kernel of Ω_0, a statement that we cannot impose in general. As a specific example of this relation, reconsider the material involving the spin vector in Section 4. There, the order parameter is the spin vector $\boldsymbol{s} \in \mathcal{F}(\mathbb{R}^3, \mathbb{R}^3)$ which evolves under the action of the rotation group $G = SO(3)$ so that $g = R(\boldsymbol{x}, t)$ and the above formula specialize to

$$\boldsymbol{s}(\boldsymbol{x}, t) = R(\boldsymbol{x}, t)\boldsymbol{s}_0(\boldsymbol{x}), \tag{5-4}$$

$$\nabla\boldsymbol{s} = -\widehat{\gamma}\boldsymbol{s} = -\boldsymbol{\gamma} \times \boldsymbol{s}, \tag{5-5}$$

$$0 = \widehat{\Omega}\boldsymbol{s} = \boldsymbol{\Omega} \times \boldsymbol{s}, \tag{5-6}$$

having used the Lie algebra isomorphism (*hat map*)

$$(\mathfrak{so}(3), [\,\cdot\,,\cdot\,]) \cong (\mathbb{R}^3,\ \cdot \times \cdot\,).$$

Despite this result, we now turn our attention to the particular step in which the gauge connection is introduced in the Lagrangian of a field theory. As an example, consider a Lagrangian of general type

$$\ell = \ell(n, \dot{n}, \nabla n),$$

where $n \in \mathcal{F}(\mathbb{R}^3, M)$. For example, in the case of the Ericksen–Leslie theory of liquid crystal nematodynamics, we have $M = S^2$ [31; 32]. According to the previous discussion one can let n evolve under local rotations $g \in \mathcal{F}(\mathbb{R}^3, G)$, so that $n(t) = g(t)n_0$. This leads to introducing a gauge connection such that $\nabla n = -\gamma n$. In turn, the latter relation can be used to obtain a new Lagrangian of the form $\ell = \ell(n, \xi, \gamma)$, where $\xi := \dot{g}g^{-1}$. Then, the Hamilton's principle associated to this new Lagrangian produces a more general set of equations in which γ is allowed to have a nonzero curvature (constant if the gauge group is abelian), as it appears by taking the covariant differential $\mathrm{d}^\gamma = \mathrm{d} + \gamma$ of the evolution equation $\partial_t\gamma + \mathrm{d}\xi = [\xi, \gamma]$ thereby producing $\partial_t\Omega = [\xi, \Omega]$. Notice that, while one has $(\partial_t - \xi)(\mathrm{d}n + \gamma n) = 0$, allowing for a nontrivial connection enforces the presence of an M-valued one-form $\phi(t) = g(t)\phi_0 \in \Omega^1(\mathbb{R}^3, M)$ such that $\mathrm{d}n(t) + \gamma(t)n(t) = \phi(t) \neq 0$. This observation (basically amounting to $\nabla n_0 \neq -\gamma_0 n_0$) offers a general method for constructing defect theories whose defect topology does not depend on time. This is precisely the approach that we followed in Section 2 and applied in the following sections.

6. Conclusions

This paper has introduced a new method for introducing holonomy in quantum hydrodynamics. Upon focusing on single-valued phase-factors rather than multi-valued phases, we have shown how a constant nonzero curvature can be naturally included to incorporate a nontrivial geometric phase in Madelung's equations. Also, it was shown how this method corresponds to simply applying minimal coupling at the level of Schrödinger's equation. In turn, this new picture led to the possibility of dealing with vortex singularities in the hydrodynamic vorticity. While topological singularities may be captured by the present treatment, our attention focused on vortex filaments of hydrodynamic type. By using the Rasetti–Regge framework, coupled equations were presented for the evolution of a Schrödinger wavefunction interacting with a hydrodynamic vortex filament.

As a first application of our approach, we considered the Born–Oppenheimer approximation in adiabatic molecular dynamics. After reviewing the variational setting of adiabatic dynamics, we presented the standard approach along with a modified approach presented in Appendix B and exploiting Gaussian wavepackets. Remarkably, in the latter approach, conical intersections are filtered by the Gaussian convolution kernel so that the nuclear motion occurs on a smoothed electron energy surface in agreement with the recent proposal by Gross and collaborators [70; 78]. A similar approach was then used on the variational side to incorporate vortex singularities in the Born–Oppenheimer approximation so that nuclei interact with a hydrodynamic vortex incorporating molecular geometric phase effects.

Last, the treatment was extended to the exact factorization of wavefunctions depending on more than one set of coordinates. Recently revived within the chemical physics community, this method has been widely used in the literature on the Pauli equation for a spin particle in an electromagnetic field. After reviewing the theory in both its variational and Hamiltonian variants, we specialized to consider the case of electronic two-level systems thereby studying the dynamics of the spin density vector. Finally, motivated by previous work by Takabayasi, we used this setting to include vortex filament dynamics in the quantum hydrodynamics with spin.

Appendix A. Schrödinger reconstruction calculation

This appendix presents the explicit calculations that reconstruct the Schrödinger equation from the QHD equations in Section 2. We begin with the expansion

$$i\hbar\partial_t\psi = i\hbar(\partial_t R\,\theta + R\,\partial_t\theta)\,.$$

Then, we find $\partial_t R$ from (2-10) as

$$\partial_t R = -\nabla R \cdot \frac{\bar{\boldsymbol{\nu}}}{m} - \frac{R}{2m} \operatorname{div} \bar{\boldsymbol{\nu}} \,.$$

Next, using (2-9) and (2-11), we can also compute $\partial_t \theta$ and obtain

$$\partial_t \theta = -\frac{i}{\hbar} \left(\frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V + V_Q \right) \theta \,.$$

Hence, at this stage the Schrödinger equation reads

$$i\hbar \partial_t \psi = \left[-\frac{i\hbar}{m} \left(\frac{\nabla R}{R} \cdot \bar{\boldsymbol{\nu}} \right) - \frac{i\hbar}{2m} \operatorname{div} \bar{\boldsymbol{\nu}} + \frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V_Q \right] \psi + V\psi \,.$$

Clearly, we must manipulate the kinetic term to get back to ψ. To do so, we recall the relations

$$\frac{\nabla R}{R} = \frac{\operatorname{Re}(\psi^* \nabla \psi)}{|\psi|^2}, \qquad \bar{\boldsymbol{\nu}} = \frac{\hbar \operatorname{Im}(\psi^* \nabla \psi)}{|\psi|^2} - \hbar \boldsymbol{\Lambda} \,,$$
$$V_Q = -\frac{\hbar^2}{2m} \left(\frac{|\nabla R|^2}{R^2} + \operatorname{div} \frac{\nabla R}{R} \right),$$

and compute term by term. Firstly,

$$-\frac{i\hbar}{m} \left(\frac{\nabla R}{R} \cdot \bar{\boldsymbol{\nu}} \right) = -\frac{i\hbar^2}{m} \frac{\operatorname{Re}(\psi^* \nabla \psi) \cdot \operatorname{Im}(\psi^* \nabla \psi)}{|\psi|^2 \, |\psi|^2} + \frac{i\hbar^2}{m} \frac{\operatorname{Re}(\psi^* \nabla \psi)}{|\psi|^2} \cdot \boldsymbol{\Lambda} \,.$$

Secondly,

$$\begin{aligned}
-\frac{i\hbar}{2m} & \operatorname{div} \bar{\boldsymbol{\nu}} \\
&= -\frac{i\hbar^2}{2m} \left(\nabla((\psi^* \psi)^{-1}) \cdot \operatorname{Im}(\psi^* \nabla \psi) + \cancelto{0}{\frac{\operatorname{Im}(\nabla \psi^* \cdot \nabla \psi)}{|\psi|^2}} + \frac{\operatorname{Im}(\psi^* \Delta \psi)}{|\psi|^2} \right) \\
&= -\frac{i\hbar^2}{2m} \left(-(\psi^* \psi)^{-2} (\nabla \psi^* \psi + \psi^* \nabla \psi) \cdot \operatorname{Im}(\psi^* \nabla \psi) + \frac{\operatorname{Im}(\psi^* \Delta \psi)}{|\psi|^2} \right) \\
&= -\frac{i\hbar^2}{2m} \frac{\operatorname{Im}(\psi^* \Delta \psi)}{|\psi|^2} + \frac{i\hbar^2}{m} \frac{\operatorname{Re}(\psi^* \nabla \psi) \cdot \operatorname{Im}(\psi^* \nabla \psi)}{|\psi|^2 \, |\psi|^2},
\end{aligned}$$

where in the second line we have used that $\boldsymbol{\Lambda} = -\nabla \times \boldsymbol{\beta}$ so that its gradient vanishes. Thirdly,

$$\frac{|\bar{\boldsymbol{\nu}}|^2}{2m} = \frac{\hbar^2}{2m} \frac{\operatorname{Im}(\psi^* \nabla \psi) \cdot \operatorname{Im}(\psi^* \nabla \psi)}{|\psi|^2 \, |\psi|^2} - \frac{\hbar^2}{m} \frac{\operatorname{Im}(\psi^* \nabla \psi)}{|\psi|^2} \cdot \boldsymbol{\Lambda} + \frac{\hbar^2}{2m} |\boldsymbol{\Lambda}|^2 \,.$$

Finally, letting $K = \mathrm{Re}(\psi^* \nabla \psi)$ to lighten notation,

$$\begin{aligned} V_Q &= -\frac{\hbar^2}{2m}\left(\frac{K \cdot K}{|\psi|^2|\psi|^2} + \frac{\mathrm{Re}(\nabla\psi^* \cdot \nabla\psi)}{|\psi|^2} + \frac{\mathrm{Re}(\psi^*\Delta\psi)}{|\psi|^2} + \nabla((\psi^*\psi)^{-1}) \cdot K\right) \\ &= -\frac{\hbar^2}{2m}\left(\frac{K \cdot K}{|\psi|^2|\psi|^2} + \frac{|\nabla\psi|^2}{|\psi|^2} + \frac{\mathrm{Re}(\psi^*\Delta\psi)}{|\psi|^2} - 2\frac{K \cdot K}{|\psi|^2|\psi|^2}\right) \\ &= -\frac{\hbar^2}{2m}\left(-\frac{K \cdot K}{|\psi|^2|\psi|^2} + \frac{|\nabla\psi|^2}{|\psi|^2} + \frac{\mathrm{Re}(\psi^*\Delta\psi)}{|\psi|^2}\right). \end{aligned}$$

All together the kinetic term reads

$$\begin{aligned} -\frac{i\hbar}{m}&\left(\frac{\nabla R}{R} \cdot \bar{\boldsymbol{\nu}}\right) - \frac{i\hbar}{2m}\,\mathrm{div}\,\bar{\boldsymbol{\nu}} + \frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V_Q \\ &= -\frac{\hbar^2}{2m}\left(\frac{\mathrm{Re}(\psi^*\Delta\psi)}{|\psi|^2} + \frac{i\,\mathrm{Im}(\psi^*\Delta\psi)}{|\psi|^2}\right) \\ &\quad + \frac{i\hbar^2}{m}\left(\frac{\mathrm{Re}(\psi^*\nabla\psi)}{|\psi|^2} + \frac{i\,\mathrm{Im}(\psi^*\nabla\psi)}{|\psi|^2}\right) \cdot \boldsymbol{\Lambda} + \frac{\hbar^2}{2m}|\boldsymbol{\Lambda}|^2 \\ &\quad + \frac{\hbar^2}{2m}\frac{\mathrm{Re}(\psi^*\nabla\psi) \cdot \mathrm{Re}(\psi^*\nabla\psi)}{|\psi|^2|\psi|^2} \\ &\quad + \frac{\hbar^2}{2m}\frac{\mathrm{Im}(\psi^*\nabla\psi) \cdot \mathrm{Im}(\psi^*\nabla\psi)}{|\psi|^2|\psi|^2} - \frac{\hbar^2}{2m}\frac{|\nabla\psi|^2}{|\psi|^2}, \end{aligned}$$

at which point we rewrite the following terms:

$$\begin{aligned} \frac{\hbar^2}{2m}\frac{\mathrm{Re}(\psi^*\nabla\psi) \cdot \mathrm{Re}(\psi^*\nabla\psi)}{|\psi|^2|\psi|^2} + \frac{\hbar^2}{2m}\frac{\mathrm{Im}(\psi^*\nabla\psi) \cdot \mathrm{Im}(\psi^*\nabla\psi)}{|\psi|^2|\psi|^2} &= \frac{\hbar^2}{2m}\frac{|\psi^*\nabla\psi|^2}{|\psi|^2|\psi|^2} \\ &= \frac{\hbar^2}{2m}\frac{|\nabla\psi|^2}{|\psi|^2}, \end{aligned}$$

and after cancellations one is left with

$$-\frac{i\hbar}{m}\left(\frac{\nabla R}{R} \cdot \bar{\boldsymbol{\nu}}\right) - \frac{i\hbar}{2m}\,\mathrm{div}\,\bar{\boldsymbol{\nu}} + \frac{|\bar{\boldsymbol{\nu}}|^2}{2m} + V_Q = -\frac{\hbar^2}{2m}\frac{\Delta\psi}{\psi} + \frac{i\hbar^2}{m}\frac{\nabla\psi}{\psi} \cdot \boldsymbol{\Lambda} + \frac{\hbar^2}{2m}|\boldsymbol{\Lambda}|^2.$$

Multiplying by ψ and factorizing returns the desired result.

Appendix B. Adiabatic dynamics with Gaussian wavepackets

Whilst the main focus of this paper revolves around employing hydrodynamic descriptions of quantum mechanics, in this appendix we approach the adiabatic problem in quantum chemistry through the use of frozen Gaussian wavepackets at the level of the variational principle.

In line with the adiabatic separation of nuclei and electrons, we model the nuclear wavefunction $\Omega(\boldsymbol{r}, t)$ via a Gaussian wavepacket, which corresponds to the following replacements in the standard Madelung transform $\Omega = \sqrt{D}e^{iS/\hbar}$:

$$D(\boldsymbol{r},t) = D_0(\boldsymbol{r}-\boldsymbol{q}(t)), \qquad S(\boldsymbol{r},t) = \boldsymbol{p}(t)\cdot(\boldsymbol{r}-\boldsymbol{q}(t)/2), \tag{B-1}$$

where D_0 is a Gaussian of constant width (frozen). This implies that $\nabla S = \boldsymbol{p}$ so that the Born–Oppenheimer total energy, corresponding to the Lagrangian (3-5), reads

$$\begin{aligned} h &= \int D_0(\boldsymbol{r}-\boldsymbol{q})\bigg(\frac{|\boldsymbol{p}+\boldsymbol{\mathcal{A}}|^2}{2M} + \frac{\hbar^2}{8M}\frac{|\nabla D_0(\boldsymbol{r}-\boldsymbol{q})|^2}{D_0(\boldsymbol{r}-\boldsymbol{q})^2} + \epsilon(\phi,\nabla\phi)\bigg)\,\mathrm{d}^3r \\ &= \int D_0(\boldsymbol{r}-\boldsymbol{q})\bigg(\frac{|\boldsymbol{p}+\boldsymbol{\mathcal{A}}|^2}{2M} + \epsilon(\phi,\nabla\phi)\bigg)\,\mathrm{d}^3r + \text{const}, \end{aligned} \tag{B-2}$$

where we have noticed that the quantum potential term collapses to an irrelevant constant. At this stage, we invoke the commonly used approximation neglecting the second order coupling $\hbar^2\|\nabla\phi\|^2/(2M)$ in (3-4) so that upon expanding the effective potential the total energy is

$$h = \frac{|\boldsymbol{p}|^2}{2M} + M^{-1}\boldsymbol{p}\cdot\bar{\boldsymbol{\mathcal{A}}} + \bar{E}, \tag{B-3}$$

where we have defined

$$\bar{\boldsymbol{\mathcal{A}}}(\boldsymbol{q}) = \int D_0(\boldsymbol{r}-\boldsymbol{q})\boldsymbol{\mathcal{A}}(\boldsymbol{r})\,\mathrm{d}^3r, \qquad \bar{E}(\boldsymbol{q}) = \int D_0(\boldsymbol{r}-\boldsymbol{q})E(\boldsymbol{r})\,\mathrm{d}^3r.$$

Then, upon performing the Legendre transform $M\dot{\boldsymbol{q}} = \boldsymbol{p}+\bar{\boldsymbol{\mathcal{A}}}(\boldsymbol{q})$, one obtains

$$L(\boldsymbol{q},\dot{\boldsymbol{q}}) = \frac{M}{2}|\dot{\boldsymbol{q}}|^2 - \dot{\boldsymbol{q}}\cdot\bar{\boldsymbol{\mathcal{A}}}(\boldsymbol{q}) - \bar{\epsilon}(\boldsymbol{q}), \tag{B-4}$$

where we have defined

$$\bar{\epsilon}(\boldsymbol{q}) := \bar{E}(\boldsymbol{q}) - \frac{1}{2M}\big|\bar{\boldsymbol{\mathcal{A}}}(\boldsymbol{q})\big|^2.$$

Since both the energy surface and the Berry connection are smoothened by a Gaussian convolution filter, we notice that the resulting equation of motion

$$M\ddot{\boldsymbol{q}} = -\dot{\boldsymbol{q}}\times\nabla_{\boldsymbol{q}}\times\bar{\boldsymbol{\mathcal{A}}}(\boldsymbol{q}) - \nabla_{\boldsymbol{q}}\,\bar{\epsilon}(\boldsymbol{q})$$

is entirely regularized so that conical singularities are smoothened by the Gaussian convolution.

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m.foskett@surrey.ac.uk *University of Surrey, Guildford, GU2 7XH, United Kingdom*

c.tronci@surrey.ac.uk *University of Surrey, Guildford, GU2 7XH, United Kingdom*

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Surfaces of locally minimal flux

ROBERT S. MACKAY

In memory of John Mather (9 June 1942 – 28 January 2017).

For exact area-preserving twist maps, curves were constructed through the gaps of cantori, which were conjectured to have minimal flux subject to passing through the points of the cantorus. It was pointed out by Polterovich (1988) that these curves do *not* have minimal flux if there coexists a rotational invariant circle of a different rotation number, but if hyperbolic they do have *locally* minimal flux even without the constraint of passing through the points of the cantorus. Following the criterion of MacKay (1994) for surfaces of locally minimal flux for 3D volume-preserving flows, I revisit this result and show that in general the analogous curves through the points of rotationally ordered periodic orbits or their heteroclinic orbits do *not* have locally minimal flux. Along the way, various questions are posed. Some results for more degrees of freedom are summarised.

1. Introduction

An *exact area-preserving twist map* is a C^1 map $f:(x, y)\mapsto(x', y')$ of a cylinder $\mathbb{T}\times\mathbb{R}$ (where $\mathbb{T}=\mathbb{R}/\mathbb{Z}$) that preserves the standard area-form $dx\wedge dy$, such that for one or any lift $\tilde{f}$ to $\mathbb{R}\times\mathbb{R}$ the image of each vertical $x=$ constant is a C^1 graph over x' (twist condition), and the nett flux $\int_\gamma y'\,dx'-y\,dx$ for any homotopically nontrivial circle γ is zero. We usually fix a lift and often drop the tilde.

There exists a C^2 function $h:\mathbb{R}\times\mathbb{R}\to\mathbb{R}$, called *generating function*, with $h_{12}<0$ and $h(x+1, x'+1)=h(x, x')$, such that for the lift $\tilde{f}$,

$$\begin{aligned} y &= -h_1(x, x'),\\ y' &= h_2(x, x'), \end{aligned} \tag{1}$$

where subscript i denotes the derivative with respect to the i-th argument. It can be constructed by $h(x, x')=\int_\gamma y'\,dx'-y\,dx$ for any curve γ from a base point (x_0, x_0') to (x, x'), using the functions $y'(x, x')$ and $y(x, x')$ defined by the

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twist condition. It follows that $(x_n, y_n)_{n\in\mathbb{Z}}$ is an orbit of $\tilde{f}$ if and only if for all $M < N \in \mathbb{Z}$, $(x_M, \dots, x_N)$ is a critical point of $W_{MN}(x) = \sum_{n=M}^{N-1} h(x_n, x_{n+1})$ subject to x_M, x_N fixed, and $y_n = -h_1(x_n, x_{n+1})$. An orbit is said to be *minimising* if the sequence $(x_n)_{n\in\mathbb{Z}}$ (globally) minimises $W_{MN}(x)$ for each $M < N$ over variations with fixed endpoints.

For exact area-preserving twist maps f of a cylinder $\mathbb{T} \times \mathbb{R}$ with generating function $h : \mathbb{R}\times\mathbb{R} \to \mathbb{R}$, Aubry–Mather theory (e.g., [10]) establishes the existence for each rational p/q (in lowest terms) of a closed rotationally ordered set $M_{p/q}$ of periodic points (x_n, y_n) of type (p, q) (meaning $x_q = x_0 + p$, $y_q = y_0$ in the cover) that (globally) minimise the action $W_{p,q} = \sum_{n=0}^{q-1} h(x_n, x_{n+1})$. In each gap in $M_{p/q}$, it also establishes the existence of a minimax orbit, which forms a saddle point of the action between the consecutive minima. More precisely, denote the sequences of type (p, q) for the endpoints of a gap g in $M_{p/q}$ by $x^- \ll x^+$ (where $\ll$ means each component on the left is less than the corresponding one on the right), let X_g be the set of sequences x of type (p, q) with $x_n^- \le x_n \le x_n^+$, and let W_g be $W_{p,q}$ on X_g; let H_g be the infimum of $H \in \mathbb{R}$ such that x^- and x^+ lie in the same connected component of $\{x \in X_g : W_g(x) \le H\}$ (note that the endpoints have the same value of W_g). Mather proved there is a critical point x of W_g in the interior of X_g with $W_g(x) = H_g$. The difference $\Delta W_g = H_g - W_g(x^-)$ is known as the Peierls–Nabarro barrier for shifting a type (p, q) sequence between the consecutive pair of minima while maintaining type (p, q).

For any gap (in the rotational order) in the set of minimising periodic orbits of type (p, q), Aubry–Mather theory gives also the existence of heteroclinic orbits from the orbit of the left end of the gap to that of the right end, and vice versa, that are minimising, and associated minimax heteroclinic orbits.

Finally, for each irrational ω, it gives a closed rotationally ordered invariant set with rotation number ω whose orbits minimise the action sum between any pair of its points. Its subset of recurrent points is either a circle or a Cantor set, the latter case being christened "cantorus" by Percival [20]. The gaps of a cantorus come in orbits. We call an orbit of gaps a *hole*. The number of holes in a cantorus is countable (a question is whether it is generically finite). For each hole g in a cantorus, an analogue of ΔW_g is defined and an associated minimax orbit M proved to exist [17], with

$$\Delta W(M, m) := \sum_{n\in\mathbb{Z}} h(M_n, M_{n+1}) - h(m_n, m_{n+1}) \tag{2}$$

equal to ΔW_g, where m is the sequence for either of the minimising orbits bounding the hole. The sum $\Delta W(M, m)$ converges even though the individual sums do not in general. The orbits of the endpoints of a hole converge together in both directions of time and the minimax orbit lies between them, so it is

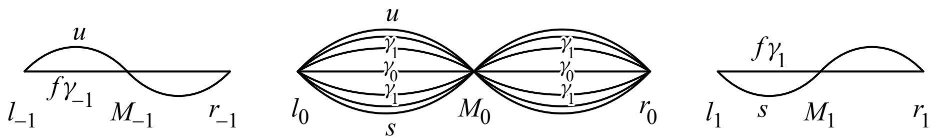

Figure 1. Decomposition of a turnstile.

homoclinic to the cantorus. $\Delta W_g \geq 0$ with equality if and only if there is an arc of minimising orbits connecting the endpoints of the gap (in which case those minimising orbits are all minimax).

For any rotational (i.e., homotopically nontrivial) closed curve γ around the cylinder, the net flux

$$\int_{f(\gamma)} y\,dx - \int_{\gamma} y\,dx$$

is zero, but we define its *flux* to be the area of the set lying in the component below $f(\gamma)$ and not in the component below γ, sometimes called *geometric flux*.

For a rotational invariant circle, the flux is zero. For a cantorus of rotation number ω, one can close its gaps by curves through corresponding minimax orbits, to produce what [15] called a *partial barrier*. For example, if the cantorus is hyperbolic, for each hole one can choose a zeroth gap and close it and its forward images by arcs of stable manifold of the cantorus and its backward images by arcs of unstable manifold.[1] These automatically join the ends of the gaps and pass through the minimax points. This was the choice made in [15], though it was indicated there that there is a wealth of other options. In particular, [15] defined a *turnstile* in the zeroth gap as the structure formed by the arc of stable manifold of the partial barrier and the arc of unstable manifold whose backward images were used to close the backward gaps. In the simplest case when the stable and unstable manifolds in each gap intersect precisely once, thus in the minimax point, the turnstile can be sliced into slivers by disjoint curves γ_n, $n \in \mathbb{Z}$, joining the ends (like the layers of an onion), and the γ_n can be mapped by f^n to the n-th gap to make a curve closing the gaps and having the same flux (see Figure 1).

In this simplest case, the flux of such a curve, whether the original partial barrier or one as constructed by the onion picture, is

$$\widetilde{\Delta W}_\omega = \sum_g \Delta W_g,$$

[1]The stable and unstable manifolds are better called forward-contracting and backward-contracting manifolds but I stick with convention for shorter names.

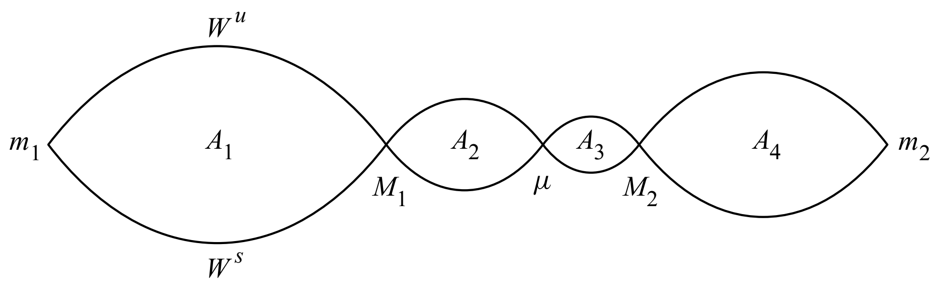

Figure 2. An example of a gap in a cantorus for which the arcs of stable and unstable manifold closing the gap intersect more than once. The endpoints of the gap are m_1, m_2. The areas A_i satisfy $A_2 < A_1$, $A_3 < A_4$, and $A_1 + A_3 = A_2 + A_4$, the common value being the flux of the set of curves formed by iterating the unstable manifold backwards and the stable manifold forwards. If $A_1 > A_4$, as shown here, then the minimax point is M_1, so Mather's $\Delta W = A_1$. The point M_2 is a lower saddle, but to get from the orbit of m_1 to the orbit of m_2 one has to pass at least as high as M_1 in action. The point μ belongs to a local minimum orbit with higher action than m_1 and m_2 (which have the same action).

where the sum ranges over the holes g of the cantorus [15]. Mather defined ΔW_ω for a cantorus to be the maximum of ΔW_g over its holes g [17]. We see here that the *sum* over holes has a valuable interpretation, because it gives the flux for a closed curve through all the points of the cantorus (note that the sum over holes converges even if there are infinitely many, because the gaps are disjoint). Mather was surprisingly (to me) uninterested in replacing the maximum by the sum when I proposed this to him in 1984. I suspect that the continuity properties he proved for the maximum apply equally well to the sum, but it would be good to check this. He was nevertheless interested in the question of motion within a Birkhoff zone of instability, notably proving existence of an orbit whose α-limit set is in the lower boundary and ω-limit set in the upper boundary [18].

More complicated scenarios can occur, however, which might explain Mather's disinterest. One way to construct such examples is to use Aubry's idea of the antiintegrable limit [1]. Firstly, there may be other equilibrium sequences in a hole besides the chosen minimax, as in Figure 2. The stable and unstable manifolds intersect at each of them. If the stable and unstable manifolds are graphs in the gap, or even just if there is a homeomorphism that makes them both graphs, then the flux is the sum of differences of action between alternating successive pairs of equilibrium sequence, which is larger than $\widetilde{\Delta W}_\omega$. A good

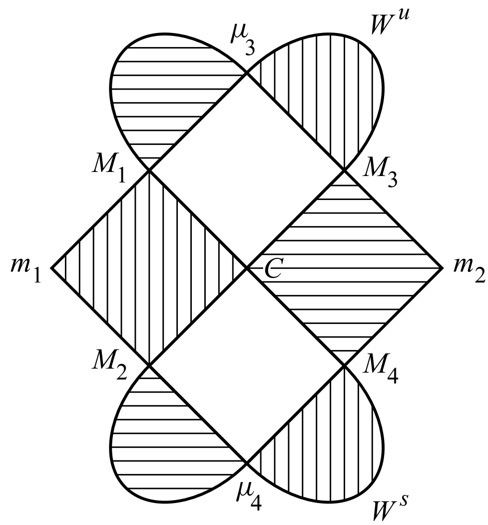

Figure 3. A more complicated scenario for the stable and unstable manifolds of the endpoints m_1, m_2 of a gap in a cantorus. The upward flux of the set of curves formed by iterating the unstable manifold backwards and the stable manifold forwards is the vertically shaded area and the (equal) downward flux is the horizontally shaded area. One of the points M_i is a minimax point, depending which is the lowest saddle permitting to go from m_1 to m_2 without passing to higher action. The points μ_i belong to local minima of the action. The point C belongs to an index-2 critical point of the action.

question, however, is whether there is an alternative way of closing the gaps for which the flux is just $\widetilde{\Delta W}_\omega$.

Secondly, one can make cases where the stable and unstable manifolds in a gap are not simultaneously homeomorphic to graphs, like that of Figure 3. In the case shown, there are seven equilibrium sequences in the hole (plus the two endpoints) and the flux is given by

$$\Delta W(M_2, m) - \Delta W(C, M_1) + \Delta W(M_3, \mu_3) + \Delta W(M_4, \mu_4), \tag{3}$$

where the notation ΔW is extended to arbitrary pairs of equilibrium sequences converging together sufficiently fast to make the sum (2) converge.

It is conjectured in [15] that the curves γ closing the gaps of hyperbolic cantori by arcs of stable or unstable manifold have minimal flux subject to passing through the cantorus (the local minimality or otherwise of the flux of such curves was also addressed by [2]). However, it was proved in [21] that this is false if there coexists a rotational invariant circle (necessarily of a different rotation number), because large deformations of such curves can be made to obtain curves through the cantorus with arbitrarily small flux. Nevertheless, he proved that the curves γ have locally minimal flux, even without the constraint of passing through the points of the cantorus. This makes them valuable for transport theory.

Nevertheless, there are alternative constructions of curves closing the gaps of cantori, and the question arises whether they also have locally minimal flux. We address that here. Secondly, there are related constructions of curves through minimising and minimax periodic orbits and through minimising and minimax heteroclinic orbits to minimising periodic orbits [2; 15; 16], and the question arises whether they have locally minimal flux too. The answer is no: they do not have locally minimal flux, a result that I am not aware has been noted before. Thirdly, the issues arise equally in continuous-time Hamiltonian systems of $1\frac{1}{2}$ degrees of freedom (DoF), and more generally in 3D volume-preserving flows. We address these contexts. Fourthly, we summarise some related results for Hamiltonian systems of more DoF.

2. Other constructions of partial barriers

Various other constructions of curves closing the gaps of cantori can be used. I survey two here. One is Hall's "ridge curves", the other is Dewar's "quadratic flux minimisers".

2.1. ***Ridge curves.*** Ridge curves were proposed by Hall (private communication) and popularised under the name "ghost circles" by Golé [9]. A nice description is via the "invariant ordered circles" (IOC) of [22]. An *ordered circle* is a continuous curve $x : \mathbb{R} \to \mathbb{R}^{\mathbb{Z}}$ that is ordered (for each pair of distinct $t, t' \in \mathbb{R}$ either $x_n(t) < x_n(t')$ for all $n \in \mathbb{Z}$ or vice versa), periodic (invariant under the translation $T_{01}(x)_n = x_n + 1$), and unbounded (there is no $y \in \mathbb{R}^{\mathbb{Z}}$ such that $x(t) \leq y$ for all $t \in \mathbb{R}$, nor x such that $x \leq x(t)$ for all $t \in \mathbb{R}$). It is called *invariant* if it is also invariant under the translation $T_{10}(x)_n = x_{n+1}$ and the gradient flow of the action

$$\dot{x}_n = -h_2(x_{n-1}, x_n) - h_1(x_n, x_{n+1}). \tag{4}$$

Note that the gradient flow, T_{01} and T_{10} commute.

Golé [9] constructs IOCs firstly in the space of sequences of type (p, q) by assuming the action $W_{p,q}$ is a Morse function and using minimax theory iteratively, and then takes limits for the irrational and heteroclinic cases. Qin and Wang [22] construct them by the Schauder fixed point theorem for the time-1 map of the gradient flow, which is more elegant as it does not require the Morse assumption and applies equally well to periodic and irrational cases.

However constructed, they produce curves that close the gaps of cantori and a nice flux formula [9], as follows. If we let

$$y_n^+ = h_2(x_{n-1}, x_n), \tag{5}$$

$$y_n^- = -h_1(x_n, x_{n+1}), \tag{6}$$

then each IOC produces two rotational circles around the cylinder: $\gamma_n^- = (x_n(t), y_n^-(t))$ and $\gamma_n^+(x_n(t), y_n^+(t))$, where t is a parameter along the IOC. Both are graphs over x. Furthermore, $f(\gamma_n^-) = \gamma_{n+1}^+$. We see that γ_n^+ is above γ_n^- at places where $\dot{x}_n < 0$ and below at places where $\dot{x}_n > 0$. The dynamics of the gradient flow (and its time-reverse) are monotone, so if x is an initial condition for which $\dot{x}_n < 0$ for all $n \in \mathbb{Z}$ (we write $\dot{x} \ll 0$) then it remains so for all $t \in \mathbb{R}$. Ridge curves are curves in the space of sequences consisting of gradient curves on which $\dot{x} \gg 0$ or $\dot{x} \ll 0$, joined at equilibria. By the above construction, they produce pairs (γ^-, γ^+) of graphs on the cylinder with $f(\gamma^-) = \gamma^+$ such that for each interval where $\dot{x} \ll 0$ then γ^+ is above γ^- and for each interval where $\dot{x} \gg 0$ then γ^+ is below γ^-. They intersect at orbits corresponding to the equilibrium sequences. Thus the flux of γ^- is produced precisely by its intervals with $\dot{x} \ll 0$. Furthermore the contribution of such an interval to the flux is precisely the difference in action $\Delta W(r, l)$ between the orbits of the equilibrium sequences r, l at its right and left ends. Thus the flux of γ^- is the sum of $\Delta W(r, l)$ over those intervals (l, r) with $\dot{x} \ll 0$, which is Golé's formula.

The construction can be generalised. It is not necessary for the ordered circle to be invariant under the gradient flow. All that we need is for $\dot{x} \geq 0$ or $\dot{x} \leq 0$ in the standard partial order on $\mathbb{R}^{\mathbb{Z}}$ at each point.

2.2. ***Quadratic flux minimisers.*** Dewar didn't like the nonuniqueness of local flux minimisers and proposed an L^2 variational principle instead, to select a preferred L^1 minimiser. He first did this to construct a preferred action variable for a nonintegrable Hamiltonian system. In the context of area-preserving maps, it was worked out with Meiss in [4]. The idea is that the flux of an area-preserving map f across a closed curve γ around the cylinder can be written as

$$\tfrac{1}{2} \int |\Delta y(x)| \, dx$$

if γ and $f(\gamma)$ are both graphs of functions y_0, y_1 of x and $\Delta y(x) = y_1(x) - y_0(x)$. Minimising this is an L^1 variational problem. To overcome the nonuniqueness, they proposed instead to minimise something like $\int |\Delta y(x)|^2 \, dx$, with the hope that there is a local minimiser associated to each rotation number and that the resulting curves γ are disjoint for different rotation numbers.

The approach is somewhat analogous to that for geodesics in a Riemannian manifold. They are defined as curves for which every short enough segment minimises the L^1 functional $\int_{t_0}^{t_1} |\dot{x}(t)|\, dt$ subject to fixed endpoints $x(t_0) = x_0$, $x(t_1) = x_1$. But the minimisers can be reparametrised by any increasing function of t fixing the ends, which does not change the value of the integral. The L^2 variational principle of minimising $\int |\dot{x}|^2\, dt$ selects a preferred parametrisation, namely such that $|\dot{x}(t)|$ is constant. The relation between the two variational principles is nicely summarised in Section 12 of [19].

The variational principle in [4] is slightly more subtle than sketched above. In fact they proposed to locally minimise $\int |\Delta y(x)|^2 x'(\theta)\, d\theta$ over pairs (x, ρ) of increasing diagonally periodic homeomorphisms (i.e., $x(\theta + 1) = x(\theta) + 1$ and the same for ρ), with the functions y_0, y_1 determined by

$$y_0(x(\theta)) = -h_1(x(\theta), x(\rho(\theta))), \tag{7}$$

$$y_1(x(\theta)) = h_2(x(\rho^{-1}(\theta), x(\theta)), \tag{8}$$

so

$$\Delta y(x(\theta)) = h_2(x(\rho^{-1}(\theta), x(\theta)) + h_1(x(\theta), x(\rho(\theta))). \tag{9}$$

The nice result is that the Euler–Lagrange equations for stationarity of the L^2 functional implies that if $\Delta y(x(\theta)) = 0$ for some θ then $\Delta y(x(\rho^n(\theta))) = 0$ for all $n \in \mathbb{Z}$. Thus the L^2 critical points make a curve γ and its image $f(\gamma)$, whose intersections are orbits of f. So the L^2 variational principle constructs preferred curves through selected orbits of f.

Yet many questions remain (at least for me). Does the principle have local minimisers? Is there one for each rotation number? Are the curves γ for different rotation number disjoint? Is there a relation between the L^2 minimisers and the ridge curves? The papers [5; 6; 7] address these questions but I'm not yet clear if they resolve them totally.

An alternative selection procedure among curves of locally minimal flux has been proposed by [8], based on minimising their length.

3. Continuous-time analogues

For many applications, rather than area-preserving maps it is better to consider continuous-time systems, e.g., time-periodic Hamiltonian systems of $1\frac{1}{2}$ DoF:

$$\begin{aligned} \dot{x} &= H_{,p}(x, p, t), \\ \dot{p} &= -H_{,x}(x, p, t), \end{aligned} \tag{10}$$

with $H(x, p, t + 1) = H(x, p, t)$ (where $H_{,p}$ denotes the partial derivative of H with respect to p etc.). They preserve the volume-form $dx \wedge dp \wedge dt$ on the extended state space of (x, p, t). More generally one could consider 3D volume-preserving vector fields, such as a magnetic field B.

Let us take the time-periodic Hamiltonian context, with x an angle variable. The flux-form of the Hamiltonian vector field in extended state space (x, p, t) is $dH \wedge dt + dx \wedge dp$. So the flux across a piece of a C^1 graph $p = P(x, t)$ is

$$\int (H_{,x} + H_{,p}P_{,x} + P_{,t})\, dx \wedge dt. \tag{11}$$

The nett flux across the whole graph is zero, but we define the flux of the surface to be the positive part, so the flux is

$$\tfrac{1}{2} \int |H_{,x} + H_{,p}P_{,x} + P_{,t}|\, dx\, dt.$$

Now we can apply a result from [13], which was derived in the more general context of 3D volume-preserving flows.

Theorem 1. *A surface has locally minimal flux for a* 3*D volume-preserving vector field if and only if it can be decomposed into surfaces of unidirectional flux bounded by trajectories and it has no local recrossings.*

Here, we say an oriented surface S has *local recrossings* if for all $\varepsilon > 0$ there exists an orbit segment $z(t)$, $t_0 \le t \le t_1$, that intersects S in opposite directions at times t_0 and t_1, and for which $0 < d(z(t), S) < \varepsilon$ for all $t \in [t_0, t_1]$, where d denotes distance. There is no requirement for t_0 and t_1 to be close. The idea is close in spirit to Conley's concept of isolating block.

In particular, Aubry–Mather theory extends to time-periodic Hamiltonian systems with x an angle and $H_{,pp} \ge C > 0$. Cantori are now invariant subsets of graphs $p = P(x, t)$ where one or more infinitely long disjoint irrationally winding strips have been removed. They consist of minimisers for the action functional $\int L(x, \dot{x}, t)\, dt$ with $L(x, v, t) = \min_p(pv - H(x, p, t))$. In each strip there is at least one minimax orbit. If the cantorus is hyperbolic the stable and the unstable manifolds of the boundaries of each strip connect the boundaries and the minimax orbits. A surface can be chosen between the invariant manifolds to fill in each strip, passing through the intersection orbits, and having unidirectional flux in between them. One way to do this is to choose the unstable manifold up to $t = 0$ and then switch with a vertical surface to the stable manifold for $t > 0$, but this can be smoothed out if desired. Along the lines of [21], it looks likely that the resulting surface has no local recrossings. It would be good to write out a complete proof. If so, then by the above theorem, hyperbolic cantori can be spanned by surfaces of locally minimal flux.

Note the corollary that every irrational ω is a local minimiser of the function $\widetilde{\Delta W}_{\omega}$. This is because the cantorus of rotation number ω is a limit point of cantori of rotation numbers converging to ω [17].

4. Surfaces through minimising and minimax periodic orbits

We continue the discussion in the time-periodic Hamiltonian context of $1\frac{1}{2}$ DoF with $H_{,pp}$ positive. The set of minimising periodic orbits of type (p,q) is rotationally ordered and closed. For each gap in it there is a minimax periodic orbit. Choose any closed surface that passes through the minimising and minimax orbits in rotational order. Suppose we can choose it so that the parts between neighbouring minimax and minimising orbits have unidirectional flux. Can one choose it so that it has no local recrossings? Not in general, because the vector field rotates around any nondegenerate minimax periodic orbit, so there are arcs of trajectory arbitrarily close that cross the surface in one direction and recross in the other. The flux can be reduced by pushing the surface off the minimax periodic orbit, analogous to [2].

So the conclusion is that (except perhaps for degenerate cases) there are no surfaces of locally minimal flux through minimising and minimax periodic orbits.

5. Surfaces through heteroclinic orbits to minimising periodic orbits

In each gap of the set of minimising periodic orbits of type (p,q) there is a set of minimising advancing heteroclinic orbits and in each gap of the latter there is a minimax heteroclinic orbit. Advancing heteroclinic means that the orbit converges in forwards time to one periodic orbit and in backwards time to another and the forward limit is to the right of the backwards one. The same result holds for retreating heteroclinic orbits (for which the forward limit is to the left of the backward one), but without loss of generality, we will restrict the discussion to the advancing case.

One can construct a surface through the minimising periodic orbits and their minimising advancing heteroclinic orbits, for example by taking the unstable manifold of a minimising periodic orbit up to some minimising heteroclinic orbit and the stable manifold on the other side, for one period of the periodic orbits and then closing by the required part of $t = cst$. The only places where there is flux are the $t = cst$ pieces and it is unidirectional for the pieces between neighbouring pairs of heteroclinic orbits.

But local recrossings occur: see Figure 4. So such surfaces do not have locally minimal flux. This is consistent with numerics (e.g., Figure 11 of [11]) showing that there are cantori of smaller flux with arbitrarily close rotation number and

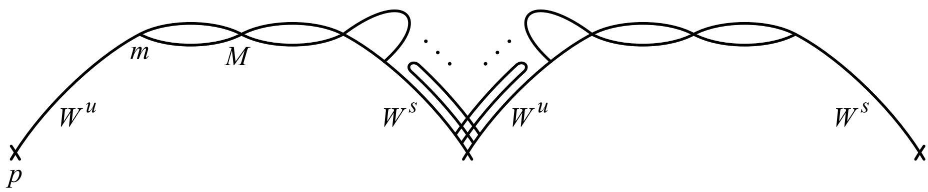

Figure 4. Local recrossings happen for surfaces through hyperbolic minimising advancing heteroclinic orbits formed from stable and unstable manifolds. p is a minimising periodic point, m and minimising advancing heteroclinic point and M a minimax advancing heteroclinic point. The picture is drawn at a Poincaré section $t = cst$.

lying in an arbitrarily small neighbourhood of the minimising periodic orbit. But I am not aware of its having been remarked before.

6. More degrees of freedom

Finally, we summarise some results for Hamiltonian systems of more DoF. An autonomous Hamiltonian system of N DoF is specified by a $2N$-dimensional manifold M, a symplectic form ω on M and a smooth function $H : M \to \mathbb{R}$. The Hamiltonian vector field v is determined by $i_v\omega = dH$.

Let the geometric flux for a codimension-1 closed surface in $H^{-1}(E)$ be the integral of the flux $i_v\sigma$ of energy-surface volume σ (defined so that $dH \wedge \sigma = \omega^N/N!$) across the part where the flux is positive (the net flux = 0). Note that

$$i_v\sigma = \omega^{(N-1)}/(N-1)! \tag{12}$$

A *transition state* (TS) for an autonomous Hamiltonian system is a closed invariant oriented codimension-2 submanifold (not necessarily connected) of an energy level $H^{-1}(E)$ that can be spanned by compact codimension-1 surfaces of unidirectional flux whose union (dividing surface DS) locally separates $H^{-1}(E)$ into two components and has no local recrossings (recall this means there is a neighbourhood of DS that a trajectory has to leave before it can recross) [14].

Theorem 2 [14, Theorem 2.3]. *A codimension-*1 *closed submanifold in* $H^{-1}(E)$ *has locally minimal geometric flux if and only if it is a DS for a TS. If* $\omega = -d\alpha$ *locally then the minimising flux is the action integral of the TS*:

$$\int \alpha \wedge \omega^{(N-2)}/(N-2)!.$$

The result is formulated differently in [14] to motivate the definition of TS later, but it is equivalent to Theorem 2.3 there.

Examples can be constructed, in particular for energies just above an index-1 saddle of the Hamiltonian (these go back a long time in history, but see [14] for a coherent presentation).

A related variational principle for odd-dimensional invariant submanifolds of an autonomous Hamiltonian system, including the case of codimension-2 submanifolds of an energy level, was given in [12], but with no general construction of minimisers.

7. Potential application areas

The theory of surfaces of locally minimal flux has many potential applications. I mention two, to give an idea of the scope. One is chemical reaction dynamics, as discussed in [14]. Another is transport in magnetically confined plasmas, e.g., [3; 23; 24], and the design of divertors. To these one could add interplanetary travel and high energy particle storage rings.

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r.s.mackay@warwick.ac.uk *University of Warwick, Coventry, United Kingdom*

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A symplectic approach to Arnold diffusion problems

JEAN-PIERRE MARCO

The purpose of this text is to present a symplectic approach to Arnold diffusion problems, that is, the existence of orbits of perturbed integrable systems along which the action variables experience a drift whose length is independent of the size of the perturbation. We chose to focus on the construction of orbits drifting along "chains of cylinders", taking for granted the existence of the chains. We however give a rather complete description of these chains, together with some elements on their symplectic features and some main ideas to prove their existence. We adopt the setting introduced by John Mather to prove the Arnold conjecture for perturbations of Tonelli Hamiltonians, which we see as the good one to set out the various (and numerous) problems of the construction, and give some ideas to show how the symplectic approach may enable one to enlarge its scope.

1. Introduction

In this text we denote by $\mathbb{A}^n = T^*\mathbb{T}^n$ the cotangent bundle of the torus $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$, endowed with its angle-action coordinates (θ, r) and its usual exact-symplectic structure.

1. The questions addressed in this paper originate in the famous Boltzmann conjecture, rephrased in the modern mathematical language (following [54]) as:

> For (almost) all proper Hamiltonian function H on a $2n$-dimensional symplectic manifold and (almost) all real value e, the associated Hamiltonian vector field is ergodic on each connected component of $H^{-1}(e)$.

Forgetting about the real scope of this conjecture — certainly limited to m-body problems with very large m — it is well-known that the KAM theorem yields counterexamples to the previous statement as soon as $n \geq 2$. One can see the following weaker *quasiergodic* conjecture by Poincaré and Ehrenfest as an attempt to partially recover its possible dynamical applications:

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> For (almost) all proper Hamiltonian function H on a symplectic manifold and (almost) all real value e, the associated Hamiltonian vector field admits an orbit which is dense in $H^{-1}(e)$.

It turns out that the Poincaré–Ehrenfest conjecture is false too: this is a consequence of the KAM theorem if $n = 2$, while Herman proved (see [54]) that it is false for $n \geq 3$, at least on nonexact symplectic manifolds. He also asked the simpler — but still open — question of the existence of a C^∞ perturbation of $\frac{1}{2}\|r\|^2$ on $\mathbb{A}^n$ with a dense orbit on some energy level.

A possible way to state a correct but even weaker question in the spirit of the previous conjectures comes from [25], where Arnold introduced the first example of an "unstable" family of Hamiltonian systems on $\mathbb{A}^3$, namely:

$$H_\varepsilon(\theta, r) = r_1 + \tfrac{1}{2}(r_2^2 + r_3^2) + \varepsilon(\cos\theta_3 - 1) + \mu(\varepsilon)(\cos\theta_3 - 1)g(\theta), \qquad (1)$$

where g is a suitably chosen trigonometric polynomial, $\varepsilon > 0$ is small enough and $\mu(\varepsilon) \ll \varepsilon$. The main result of Arnold is the existence of $\varepsilon_0 > 0$ such that for $0 < \varepsilon < \varepsilon_0$, the system H_ε admits an "unstable solution" $\gamma_\varepsilon(t) = (\theta(t), r(t))$ such that

$$r_2(0) < 0, \quad r_2(T_\varepsilon) > 1, \qquad (2)$$

for some (large) T_ε. Orbits experiencing this type of behavior are said to be *diffusion orbits*. In view of this result and the associated constructions, Arnold conjectured (see [25]) that for "typical" systems of the form

$$H_\varepsilon(\theta, r) = h(r) + \varepsilon f(\theta, r, \varepsilon) \qquad (3)$$

on $\mathbb{A}^n$, $n \geq 3$, the projection in action of some orbits should visit any element of a prescribed collection of arbitrary open sets intersecting a connected component of a level set of h. One therefore gets an "asymptotic density" of the projection of the orbit onto the action space when the size of the perturbation tends to 0. Taking the variation of the angles into account, one can also produce examples of perturbations of $\frac{1}{2}\|r\|^2$ on the annulus $\mathbb{A}^3$ with orbits dense on subsets of Hausdorff dimension 5 inside an energy level; see [32].

2. The Arnold conjecture is directly related to the existence or nonexistence of particular invariant subsets acting as "barriers" inside an energy level. Assume that X is a complete vector field on a manifold M. Given some open connected subset O and a point x in M, consider the full orbit of O under the flow Φ of X:

$$\mathscr{O} = \Phi(\mathbb{R} \times O).$$

Hence $\mathscr{O}$ is the "accessibility domain" attached to O and its boundary $\partial\mathscr{O} = \operatorname{Adh}\mathscr{O} \setminus \mathscr{O}$ is invariant under the flow Φ. The existence of an orbit connecting O

and x is equivalent to x and O being in the same connected component of the complement of $\partial\mathscr{O}$.

Understanding the structure of the boundaries of the domains of accessibility is in general hopeless. However, in the discrete case of area-preserving twist maps of the annulus $X = \mathbb{T}\times[0, 1]$, Birkhoff's theory gives a satisfactory answer (see Appendix B). Consider a neighborhood $O = \mathbb{T}\times[0, \varepsilon[$ of the lower boundary and assume that $\mathscr{O} \subset \mathbb{T}\times[0, 1[$. Then by the standard trick of "filling the holes" (see [48]), one proves that the boundary $\partial\mathscr{O}$ admits a connected component which disconnects $\mathbb{T}\times\,]0, 1[$ and is the graph of a Lipschitz map $\mathbb{T}\to[0, 1]$. More generally, one proves in the same way the existence of orbits connecting any neighborhoods of the lower and upper essential circles bounding a Birkhoff zone: a first example of diffusion behavior.

In general, an area-preserving twist map of X has essential invariant circles in $\mathbb{T}\times\,]0, 1[$ and do not admit diffusion orbits starting arbitrarily close to $\mathbb{T}\times\{0\}$ and ending arbitrarily close to $\mathbb{T}\times\{1\}$. A crucial idea was introduced by Moeckel [48] and then by Le Calvez [41], who studied the diffusion properties of *bisystems* of maps on the annulus.[1] A bisystem is a pair of maps $(\varphi_0, \varphi_1) : X \circlearrowleft$, and one defines an orbit of (φ_0, φ_1) as a sequence $(x_n)_{n\in\mathbb{N}}$ such that $x_{n+1} = \varphi_i(x_n)$, with $i = 0$ or 1. It turns out that if φ_0 is an area-preserving twist map of $X = \mathbb{T}\times[0, 1]$ and $\varphi_1 : X \to X$ is area-preserving, then a sufficient condition for the bisystem (φ_0, φ_1) to admit an orbit connecting arbitrary neighborhoods of $\mathbb{T}\times\{0\}$ and $\mathbb{T}\times\{1\}$ is that both maps do not admit any essential invariant circle in common, apart from the boundary ones. The underlying idea, close to the setting of control theory, is that the action of φ_1 destroys the boundaries of accessibility of φ_0; see [42] for a study of diffusion bisystems of integrable Hamiltonian systems based on this type of methods.

The previous ideas have been generalized by Koropecki and Nassiri [35; 36] to the dynamics of bisystems of symplectic diffeomorphisms on compact surfaces, which are proved to be generically *transitive*. We will go back to this work in the last section of this text.

Our approach to constructing diffusion orbits for systems (3) on $\mathbb{A}^3$ is based on the embedding of bisystems on subsets of $\mathbb{A}$ into the system generated by H_ε, restricted to some energy level. More precisely, the orbits of our bisystems will only be *pseudoorbits*, which have the additional property to admit genuine shadowing orbits of the Hamiltonian system. Moreover, the bisystems satisfy the previous property of noncoincidence of invariant circles under mild nondegeneracy conditions (which can be made rather explicit), which yields the existence of diffusion pseudoorbits, and thus to diffusion orbits.

[1] Also called IFS.

As an ubiquitous example, setting $\varepsilon = 1$ in (1) yields a class of systems for which the unperturbed part no longer depends on the actions only, but still remains completely integrable (with nondegenerate hyperbolicity). It has been a challenging question to prove the existence of unstable solutions (2) for the slightly more general class of systems

$$G_\mu(\theta, r) = r_1 + \tfrac{1}{2}(r_2^2 + r_3^2) + (\cos\theta_3 - 1) + \mu g(\theta, r), \tag{4}$$

where g belongs to a residual subset of a small enough ball in some appropriate function space (finitely or infinitely differentiable, Gevrey, analytic). This setting (with its natural generalizations) is now called the *a priori* unstable case of Arnold diffusion. In [21] we set out a geometric framework to deal with such systems, using the previous bisystem method; see also [8; 11; 12; 13; 15; 16; 19; 20; 22; 23; 24; 48; 53] amongst others for different approaches. Another different and very promising direction has been introduced in a related context by Nassiri and Pujals [49], where the notion of robust transitivity is used in place of the sole existence of diffusing orbits.

3. To some extent, the *a priori* unstable geometric and dynamical features can be recovered in the so-called *a priori* stable case (3). This problem leads one first to analyze the hyperbolic structure of such systems (under nondegeneracy conditions) in the complement of the set of Lagrangian invariant tori. Due to the many technicalities involved in this geometric part of the study, in this text we will take for granted the existence of a large family of compact 3-dimensional hyperbolic invariant submanifolds (described in the next section), with a rich homoclinic structure, which form “chains” contained in a regular energy level. Given a finite family of open subsets intersecting a connected component of a level $h^{-1}(e)$, there is an ε_0 such that these chains exist for $0 < \varepsilon < \varepsilon_0$ and connect these open sets.

The cylinders could be seen as the counterpart in the Baire category of the Lagrangian tori. The latter form subsets whose complement has relative measure tending to 0 when the size of the perturbation tends to 0, while our invariant cylinders tend to form dense subsets of a given regular level; see [32] for an example.

One main difficulty to recover the *a priori* unstable setting in *a priori* stable perturbations is the essentially singular nature of the problem: no hyperbolicity is present in the unperturbed system, so that the hyperbolicity constants of our 3-dimensional manifolds tend to 0 when $\varepsilon \to 0$, which makes their embedding properties a very delicate matter. We will limit ourselves here to give a description of the cylinders and chains and underline the various difficulties raised by their construction, we refer to [5; 7; 44] for more.

Once the chains are given, one can focus on the construction of diffusion orbits drifting along them. We will describe quite extensively two simple but relevant examples in this paper, which correspond to the two situations encountered in the $n = 3$ setting: the case of doubly resonance cylinders (the so-called *a priori* chaotic case) and the case of simple resonance cylinders (the singular *a priori* unstable case). In both cases, our method is to reduce the problem to the embedding of a bisystem of maps (or correspondences) on an annulus to which one can apply the Moeckel's method under mild nondegeneracy conditions. Then a normally hyperbolic shadowing process using the area preservation and the Poincaré recurrence theorem (as introduced and used in [15; 24]) will provide us with the diffusion orbits connecting the initially given open sets.

4. Let us briefly describe our setting, beginning with the functional spaces. Fix $n \geq 1$. For $2 \leq \kappa < +\infty$ and $f \in C^\kappa(\mathbb{A}^n) := C^\kappa(\mathbb{A}^n, \mathbb{R})$ we let

$$\|f\|_\kappa = \sum_{k \in \mathbb{N}^{2n}, 0 \leq |k| \leq \kappa} \|\partial^k f\|_{C^0(\mathbb{A}^n)} \leq +\infty$$

and we set $C^\kappa_b(\mathbb{A}^n) = \{f \in C^\kappa(\mathbb{A}^n) \mid \|f\|_\kappa < +\infty\}$, so that $C^\kappa_b(\mathbb{A}^n)$ is a Banach space. We consider systems on $\mathbb{A}^3$, of the form

$$H(\theta, r) = h(r) + f(\theta, r), \tag{5}$$

where $h : \mathbb{R}^3 \to \mathbb{R}$ is C^κ and the perturbation $f \in C^\kappa_b(\mathbb{A}^3)$ is small enough.

Even if our point of view here is essentially symplectic, we will adopt the setting introduced by Mather for proving the Arnold conjecture by variational methods. A first restriction in [47] is that the unperturbed part h is a Tonelli Hamiltonian, that is, strictly convex with superlinear growth at infinity ($\lim_{\|r\| \to +\infty} h(r)/\|r\| \to +\infty$). We will limit here to Tonelli Hamiltonians too, since convexity reveals itself to be necessary in our constructions in the neighborhood of double resonance points, in order to get well-defined classical systems as main parts of normal forms. However, the symplectic approach seems to make it possible to relax the convexity assumptions, at least to some extent.

A natural expectation, already illustrated by (1), would be the existence of diffusion orbits for all systems in "segments" in $C^\kappa_b(\mathbb{A}^3)$ originating at h, of the form

$$\{H_\varepsilon(\theta, r) = h(r) + \varepsilon f(\theta, r) \mid \varepsilon \in]0, \varepsilon_0[\} \tag{6}$$

where f is a fixed function, where of course the smallness threshold ε_0 may explicitly depend on f. However, it seems difficult to prove the existence of diffusion over *whole* segments such as (6). To take this observation into account, still following Mather, one uses a more global framework and introduce "anisotropic balls" in which the diffusion phenomenon can be expected to occur

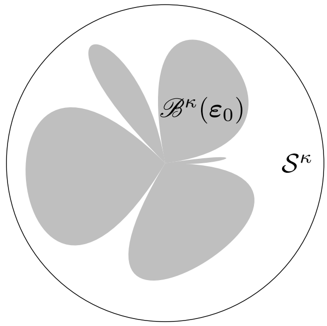


Figure 1. A generalized ball.

generically. Let $\mathcal{S}^\kappa$ be the unit sphere in $C_b^\kappa(\mathbb{A}^3)$. Given $\boldsymbol{\epsilon}_0 : \mathcal{S}^\kappa \to [0, +\infty[$ (a "threshold function"), we define the associated $\boldsymbol{\epsilon}_0$-ball:

$$\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0) := \{\varepsilon \boldsymbol{f} \mid \boldsymbol{f} \in \mathcal{S}^\kappa, \varepsilon \in]0, \boldsymbol{\epsilon}_0(\boldsymbol{f})[\}. \tag{7}$$

Note also that if $\boldsymbol{\epsilon}_0$ is lower-semicontinuous, the associated ball is open in $C_b^\kappa(\mathbb{A}^3)$.

This yields the following version of the diffusion conjecture,[2] to be compared with [25].

Conjecture (diffusion conjecture in the convex setting). *There is an integer $\kappa_0 \geq 2$ such that for $\kappa \geq \kappa_0$, given a C^κ integrable Tonelli Hamiltonian h on $\mathbb{A}^3$, an $\boldsymbol{e} > \operatorname{Min} h$ and a finite family of open sets $O_1, \ldots, O_m$ which intersect $h^{-1}(\boldsymbol{e})$, then there exists a lower semicontinuous function*

$$\boldsymbol{\epsilon}_0 : \mathcal{S}^\kappa \to \mathbb{R}^+$$

with positive values on a dense open subset of $\mathcal{S}^\kappa$ such that for f in a dense open subset of $\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0)$ the system

$$H(\theta, r) = h(r) + f(\theta, r) \tag{8}$$

admits an orbit which intersects each $\mathbb{T}^3 \times O_i$.

The zeros of $\boldsymbol{\epsilon}_0$ correspond to directions along which diffusion cannot occur. Simple examples show that such directions exist in general: for instance if $h(r) = \frac{1}{2}(r_1^2 + r_2^2 + r_3^2)$, the system $H_\varepsilon = h + \varepsilon f$ with $f(\theta) = \sin\theta_3$ is completely integrable and does not admit diffusion orbits connecting open sets which are far from the $\theta_3 = 0$ plane. In view of the shape of $\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0)$, a residual subset in such

[2]Mather's formulation is indeed still more precise and involved.

a ball is said to be *cusp-residual* and a property which holds on a cusp-residual subset is said to be *cusp-generic*.

From our point of view, one main interest (amongst many others) of the Mather setting comes from the possibility of proving first the existence of chains of cylinders for perturbations in a small enough generalized ball, and then prove that a new but arbitrarily small perturbation of any system in that ball yields the existence of diffusion orbits drifting along the chain, so connecting the open sets.

We wish to mention that very important advances has been achieved towards the proof of this conjecture, first by John Mather himself in his unfortunately unpublished notes, and more recently by P. Bernard, C.-Q. Cheng, V. Kaloshin, Ke Zhang and their collaborators; see [5; 7; 10; 33] and the many references therein. The methods in these works are either purely variational, or based on the weak KAM theory developed by A. Fathi; see [18]. Our methods in this text are more geometric and use in a crucial way the symplectic features of the systems.

2. The cusp-generic hyperbolic structure

This section is devoted to the geometric part of our study. We limit ourselves to a description of the main steps and refer to [44] for details and proofs.

2.1. ***Cylinders and chains.*** **1.** Let us briefly describe the various objects involved in our construction. We refer to [21] for precise definitions, which will also be recalled in the next two sections. Let X be a C^1 complete vector field on a smooth manifold M, with flow Φ. Let p be an integer ≥ 1:

- We say that $\mathscr{C} \subset M$ is a C^p *invariant cylinder with boundary* for X if $\mathscr{C}$ is a submanifold of M, C^p-diffeomorphic to $\mathbb{T}^2 \times [0, 1]$, which is invariant under the flow of X: $\Phi^t(\mathscr{C}) = \mathscr{C}$ for all $t \in \mathbb{R}$.

- We denote by $\boldsymbol{Y}$ any realization of the two-sphere S^2 minus three open discs with nonintersecting closures, so that $\partial \boldsymbol{Y}$ is the union of three circles. We say that $\mathscr{C}_\bullet \subset M$ is an *invariant singular cylinder* for X if $\mathscr{C}_\bullet$ is a C^1 submanifold of M, C^1 diffeomorphic to $\mathbb{T} \times \boldsymbol{Y}$ and invariant under Φ. The boundary of a singular cylinder is the disjoint union of three tori.

Throughout this paper we will consider vector fields generated by Hamiltonian functions $H \in C^\kappa(\mathbb{A}^3)$, $\kappa \geq 2$. The cylinders or singular cylinders will be contained in regular levels of H.

2. The notion of normal hyperbolicity for submanifolds with boundary requires some care. We refer to [9] for a general presentation, well-adapted to our setting (see also Appendix A). It suffices here to say that the normally hyperbolic invariant submanifolds we are dealing with here are invariant submanifolds

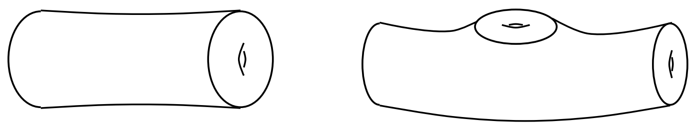


Figure 2. Cylinder and singular cylinder.

with boundary contained in usual normally hyperbolic manifolds of the same dimension (invariant for a new system slightly modified outside the submanifold at hand). In particular, our normally hyperbolic cylinders and singular cylinders admit well-defined 4-dimensional stable and unstable manifolds, contained in their energy level.

3. In addition to the normal hyperbolicity, to reduce the dynamics inside the cylinders to that of twist maps, we require that they admit global Poincaré sections, diffeomorphic to $\mathbb{T} \times [0, 1]$, whose associated Poincaré maps satisfy a twist condition. Analogous (but slightly more involved) notions are required for singular cylinders. The invariant tori contained in the cylinders which intersect these global sections along essential circles will be called *essential tori*. Moreover, in order to reduce the dynamics in the neighborhood of the cylinders to that of a suitable bisystem, we require that they satisfy specific homoclinic conditions, which yields the notion of *admissible cylinders*. Again, we refer to [21] for a complete description of the previous conditions, the necessary ones will be recalled in the following and illustrated by specific examples.

4. Finally, we will introduce various heteroclinic conditions to be satisfied by pairs of cylinders in order for them to admit orbits drifting along both of them. This yields the notion of *admissible chains*, that is, finite ordered families $(\mathscr{C}_k)_{1 \le k \le k_*}$ of admissible cylinders or singular cylinders, in which two consecutive elements satisfy these heteroclinic conditions.

5. Our main statement regarding the existence of chains is the following one, for which we refer to [44].

Statement I (usp-generic existence of admissible chains). *There is an integer $\kappa_0 \ge 2$ such that for $\kappa \ge \kappa_0$, given a C^κ integrable Tonelli Hamiltonian h on $\mathbb{A}^3$, an $\boldsymbol{e} > \operatorname{Min} h$ and a finite family of open sets $O_1, \dots, O_m$ which intersect $h^{-1}(\boldsymbol{e})$, then there exist a $\delta > 0$ and a lower semicontinuous function*

$$\epsilon_0 : \mathcal{S}^\kappa \to \mathbb{R}^+$$

with positive values on a dense open subset of $\mathcal{S}^\kappa$ such that for f in a dense open subset of $\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0)$ the system

$$H(\theta, r) = h(r) + f(\theta, r) \tag{9}$$

admits an admissible chain of cylinders and singular cylinders, such that each open set $\mathbb{T}^3 \times O_k$ contains the δ-neighborhood in $\mathbb{A}^3$ of some essential torus of the chain.

The fact that the statement is true only for f in a dense open subset of $\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0)$ and not for any f in $\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0)$ comes from the transversality conditions on the heteroclinic connections required in the definition of a chain. Less stringent conditions on a chain would be satisfied for all perturbations in $\mathscr{B}^\kappa(\boldsymbol{\epsilon}_0)$.

6. One can be more precise and localize the previous chain. Since h is a Tonelli Hamiltonian, one readily checks that $\omega := \nabla h$ is a diffeomorphism from $\mathbb{R}^3$ onto $\mathbb{R}^3$, and that the level set $h^{-1}(\boldsymbol{e})$ is diffeomorphic to S^2. Given an indivisible vector $k \in \mathbb{Z}^3 \setminus \{0\}$, set

$$\Gamma_k = \omega^{-1}(k^\perp) \cap h^{-1}(\boldsymbol{e}),$$

where $k^\perp$ is the plane orthogonal to k for the Euclidean structure of $\mathbb{R}^3$. Then one checks that Γ_k is diffeomorphic to a circle, and that if $k \neq k'$ then Γ_k and $\Gamma_{k'}$ intersect at exactly two points (such intersection points are said to be *double resonance points*). By projective density, it is possible to choose a family $k_1, \dots, k_{m-1}$ of indivisible and pairwise independent vectors of $\mathbb{Z}^3$ such that

- Γ_{k_i} intersects O_i and O_{i+1} for $1 \le i \le m-1$;
- for $2 \le i \le m-1$, $\Gamma_{k_{i-1}} \cap \Gamma_{k_i}$ contains a point $a_i \in O_i$.

Fix $a_1 \in \Gamma_{k_1} \cap O_1$ and $a_m \in \Gamma_{k_{m-1}} \cap O_m$. Fix an arbitrary orientation on each circle Γ_{k_i} and let $[a_i, a_{i+1}]_{\Gamma_i}$ be the segment of Γ_i bounded by a_i and a_{i+1} according to this orientation. Set finally

$$\boldsymbol{\Gamma} = \bigcup_{1 \le i \le m-1} [a_i, a_{i+1}]_{\Gamma_i}.$$

We will prove that one can choose $\boldsymbol{\epsilon}_0$ in Theorem I so that for $f \in \mathscr{B}(\boldsymbol{\epsilon}_0)$ the projection to $\mathbb{R}^3$ of the admissible chain is located in a $\rho(f)$-tubular neighborhood of $\boldsymbol{\Gamma}$, whose radius $\rho(f)$ tends to 0 when $f \to 0$ in $C^\kappa(\mathbb{A}^3)$.

2.2. *Simple resonance cylinders.* **1.** In this section we assume for simplicity and with no loss of generality that $h(r) = \frac{1}{2}(r_1^2 + r_2^2 + r_3^2)$, so that the frequency vector is just $\omega(r) = r$. We fix an energy $\boldsymbol{e} > 0$ and consider the broken line $\boldsymbol{\Gamma}$ defined in the previous section. We will focus on a single arc $\Gamma = \Gamma_{k_i}$ for which we can assume, up to a linear change, that $k_i = (0, 0, 1)$. Hence Γ is contained

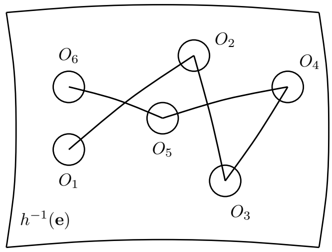


Figure 3. A “broken line” Γ of resonance arcs.

in the great circle intersection of the plane $r_3 = 0$ with the sphere $h^{-1}(\boldsymbol{e})$. The double resonance points $r^0 = (r_1, r_2, 0)$ on Γ are those for which there exists $\hat{k} \in \mathbb{Z}^2 \setminus \{0\}$ such that $\hat{k} \cdot (r_1, r_2) = 0$. The order of r^0 is then the minimal norm of such a vector $\hat{k}$.

The proof of existence of cylinders whose projection in action lies along Γ relies on a suitable averaging of the perturbation, which necessitate to determine the zones where averaging with respect to two fast angles yield a satisfactory normal form. In the complement of these zones, where a single fast angle only is available for averaging, another process is to be used to construct the cylinders. However, the “main part” of the cylinders will come from the former process.

To make this effective, one writes the Fourier expansion of f in the form

$$f(\theta, r) = \sum_{\hat{k} \in \mathbb{Z}^2} \left(\sum_{k_3 \in \mathbb{Z}} [f]_{(\hat{k}, k_3)}(r) e^{2i\pi k_3 \theta_3} \right) e^{2i\pi \hat{k}\hat{\theta}},$$

where $[f]_k$ stands for the Fourier coefficient relative to $k \in \mathbb{Z}^3$. For $K \in \mathbb{N}$, we set

$$f_{>K}(\theta, r) = \sum_{\|\hat{k}\| > K} \left(\sum_{k_3 \in \mathbb{Z}} [f]_{(\hat{k}, k_3)}(r) e^{2i\pi k_3 \theta_3} \right) e^{2i\pi \hat{k}\hat{\theta}}.$$

When $f \in C^\kappa$ with $\kappa \geq 6$ and $p \in \{2, \ldots, \kappa - 4\}$, given a control parameter $\delta > 0$ (which will be one main parameter in the whole construction), one proves the existence of a cutoff K_δ such that

$$\|f_{>K_\delta}\|_{C^p(\mathbb{A}^3)} \leq \delta.$$

Up to a symplectic conjugacy, one can cancel the harmonics of order $< K$ when the homological equation

$$\widehat{\omega}(r) \cdot \partial_{\hat{\theta}} S(\theta, r) = f(\theta, r) - V(\theta_3, r) - f_{>K}(\theta, r).$$

can be solved, where $r \in \Gamma$ and

$$V(\theta_3, r) = \int_{\mathbb{T}^2} f(\hat{\theta}, \theta_3, r) d\hat{\theta}.$$

This yields the definition of a *finite set* $D(\delta) \subset \Gamma$ *of strong double resonance points relative to* δ, namely, those $r \in \Gamma$ for which there exist an integer vector $\hat{k} \in \mathbb{Z}^2 \setminus \{0\}$ with $\|\hat{k}\| \leq K_\delta$ such that

$$\widehat{\omega}(r) \cdot \hat{k} = 0.$$

Far enough from any strong double resonance point, averaging with respect to the angles (θ_1, θ_2) yields a one-degree-of freedom (integrable) normal form + remainder, which makes the geometry of the situation easy to analyze. This becomes irrelevant in the neighborhood of the strong double resonance points, where the main part of the normal form is a classical (nonintegrable) system on $\mathbb{T}^2$.

2. More precisely, in the neighborhood of a (closed) segment $S \subset \Gamma$ located at a distance ρ of $D(\delta)$, averaging with respect to the angles (θ_1, θ_2) yields a close to identity conjugacy Φ_ε such that, setting $\hat{\theta} = (\theta_1, \theta_2)$ and $\hat{r} = (r_1, r_2)$

$$N_\varepsilon(\theta, r) = H_\varepsilon \circ \Phi_\varepsilon(\theta, r) = h(r) + \varepsilon V(\theta_3, \hat{r}) + R(\theta, r, \varepsilon) \tag{10}$$

where R is small (depending on δ, ρ and ε) in some arbitrary C^p topology ($p \in \{2, \ldots, \kappa - 4\}$ has to be chosen large enough, and so also κ, in particular to apply the KAM theorem, see below).[3] The truncated normal form

$$\tfrac{1}{2}(r_1^2 + r_2^2) + \left[\tfrac{1}{2} r_3^2 + \varepsilon V(\theta_3, \hat{r})\right] \tag{11}$$

is the skew-product of the unperturbed Hamiltonian $\frac{1}{2}(r_1^2 + r_2^2)$ with a family of "generalized pendulums", functions of $(\theta_3, r_3) \in \mathbb{A}$ and parametrized by $\hat{r}$. This is indeed a one-parameter family since $(\hat{r}, 0)$ belongs to the curve S.

Assume moreover that for $(\hat{r}, 0) \in S$ the function $V(\cdot, \hat{r})$ admits a single and nondegenerate maximum at some point $\theta_3(\hat{r})$, and, for simplicity, that $V(\theta_3(\hat{r})) = 0$. Then $O_{\hat{r}} = (\theta_3(\hat{r}), 0)$ is a hyperbolic fixed point for the Hamiltonian $\frac{1}{2} r_3^2 + \varepsilon V(\theta_3; \hat{r})$ and one immediately gets a normally hyperbolic cylinder $\mathcal{C}$ at

[3] More precisely

$$N(\theta, r) = H \circ \Phi_\varepsilon(\theta, r) = h(r) + \varepsilon V(\theta_3, r) + \varepsilon W_0(\theta, r) + \varepsilon W_1(\theta, r) + \varepsilon^2 W_2(\theta, r),$$

where the functions $W_0 \in C^p(\mathbb{A}^3)$, $W_1 \in C^{\kappa-1}(\mathscr{W}_{\rho/4})$, $W_2 \in C^\kappa(\mathscr{W}_{\rho/4})$ satisfy

$$\|W_0\|_{C^p(\mathscr{W}_{\rho/4})} \leq \delta, \quad \|W_1\|_{C^2(\mathscr{W}_{\rho/4})} \leq c_1 \rho^{-3} \quad \|W_2\|_{C^2(\mathscr{W}_{\rho/4})} \leq c_2 \rho^{-6},$$

for suitable constants $c_1, c_2 > 0$, where ρ is the distance from the segment S to the closest strong double resonance point.

energy $\boldsymbol{e}$ for N_ε by taking the product of the torus $\mathbb{T}^2$ of the fast angles $\hat{\theta}$ with the curve

$$\{O_{\hat{r}} \mid (\hat{r}, 0) \in S\}.$$

Note that $\mathcal{C}$ is diffeomorphic to $\mathbb{T}^2 \times [0, 1]$ and that its stable and unstable manifolds are the unions for $(\hat{r}, 0) \in S$ of the products of the stable and unstable manifolds $W^{\pm}(O_{\hat{r}})$ with the torus $\mathbb{T}^2$ of fast angles.

3. We have then to choose S far enough from $D(\delta)$ so that the remainder R is small enough for the previous cylinder *together with its boundary* to persist in the system H_ε. This necessitates two steps:

- One first proves the existence of *pseudoinvariant* cylinders (that is, open cylinders which are tangent to the Hamiltonian vector field) which have transverse hyperbolic properties,[4] *but are not necessarily invariant under the flow*.
- One then proves the existence of two dimensional invariant tori inside the previous pseudoinvariant cylinder, so that two of them bound an *invariant* and genuinely normally hyperbolic cylinder.[5]

The main difficulty is to choose S not too far from $D(\delta)$, in such a way that the cylinders one obtains with the previous construction can be compared with those to be constructed below in the neighborhood of double resonance points. The main point is to prove that *pairs of KAM tori* simultaneously belong to the previous cylinders and those close to double resonance, so that one deduces that they bound part of their intersection. This proves that the "double resonance" cylinders continue the "simple resonance" ones.

This process necessitates a smallness condition of the remainder in the C^p topology with $p \leq 2$ for the normally hyperbolic persistence results of Appendix A to apply,[6] and an additional smallness condition in the C^p topology with p large enough to apply the KAM theorem and get invariant boundaries.

As a consequence, one has to make a careful choice of the parameter δ, and to make the distance ρ depend on ε in a proper way; see [44] for these technical details. The main problem is to chose this size so that the boundaries of the cylinders $\mathcal{C}$ constructed above match those which will be proved to exist inside

[4]In this noninvariant setting, the hyperbolic properties can be defined by embedding the manifold in an invariant one, after modification of the vector field. The resulting property depends on this embedding, but we will be concerned only in invariant subsets of those manifolds, limited by KAM tori, which makes our approach legitimate.

[5]This step is indeed one main difference with the other approaches to Arnold diffusion.

[6]I consider the results applied in this study as genuine persistence results, since one starts with a normally hyperbolic manifold for the normal form, which is then perturbed by the remainder -on which nothing but its size is known- and is proved to persist after perturbation.

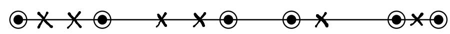


Figure 4. The arc Γ with the low-order double resonance and the bifurcation points.

this neighborhood. Even if one could expect this size to be of the order of $\sqrt{\varepsilon}$ (which would be the optimal one), we find it efficient to use a more flexible scale and work with ε^ν-neighborhoods, with some constant $\nu < \frac{1}{2}$ which will be made precise in the text. The cylinders along the simple resonance segments such as S will be called *s-cylinders*, (where s stands for "pure simple resonance").

This enables us to split Γ into "s-segments" which are bounded by the neighborhoods of consecutive low order double resonance points (denoted by $\odot$ in the following picture where the curved arc is projected onto a plane). Note that one can assume without loss of generality that the extremal points of Γ are double resonance points of low order.

4. The situation is in fact slightly more complicated, due to the possible generic occurrence of *bifurcation points* for the two-phase averaged systems (11). These are the parameters $\hat{r}$ where the potential $V(\,\cdot\,,\hat{r})$ admits *two* nondegenerate global maxima instead of a single one (depicted by a $\times$ in the following figure). In the neighborhood of these points two cylinders coexist, for which we prove the existence of heteroclinic connections. We will not give more details here, since this does not yield serious additional difficulties in the construction (the arguments here are standard in transversality theory).

2.3. ***The generic hyperbolic structure of classical systems on $\mathbb{A}^2$.*** A *classical system on* $\mathbb{A}^2$ is a Hamiltonian of the form

$$C(x,y) = \tfrac{1}{2}T(y) + U(x), \qquad (x,y) \in \mathbb{A}^2 \tag{12}$$

where T is a positive definite quadratic form of $\mathbb{R}^2$ and U a C^κ potential function on $\mathbb{T}^2$, where $\kappa \geq 2$. In the sequel we require the potential U to admit a single maximum at some x^0, which is nondegenerate in the sense that the Hessian of U at x_0 is negative definite. Consequently, the lift of x^0 to the zero section of $\mathbb{A}^2$ is a hyperbolic fixed point which we denote by O. We set $\bar{e} = \operatorname{Max} U$ and we say that $\bar{e}$ is the *critical energy* for C.

Such systems appear, *up to a nonsymplectic rescaling*, in the neighborhood of a double resonance point r^0 of the initial system (8), as the main part of normal forms. The aim of this section is to depict some relevant hyperbolic properties of C, when T *is fixed* and U belongs to a dense open subset of $C^\kappa(\mathbb{T}^2)$, κ large enough.

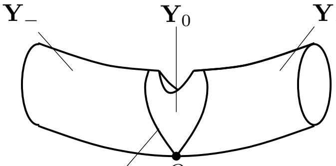


Figure 5. A singular 2-dimensional annulus.

1. Let $\pi : \mathbb{A}^2 \to \mathbb{T}^2$ be the canonical projection.

Definition 1. Let $c \in H_1(\mathbb{T}^2, \mathbb{Z})$. Let $I \subset \mathbb{R}$ be an interval. An *annulus for X^C realizing c and defined over I* is a 2-dimensional submanifold A, contained in $C^{-1}(I) \subset \mathbb{A}^2$, such that for each $e \in I$, $\mathsf{A} \cap C^{-1}(e)$ is the orbit of a periodic solution γ_e of X^C, which is hyperbolic in $C^{-1}(e)$ and such that the projection $\pi \circ \gamma_e$ on $\mathbb{T}^2$ belongs to c. We also require that the period of the orbits decreases with the energy and that for each $e \in I$, the periodic orbit γ_e admits a homoclinic orbit along which $W^{\pm}(\gamma_e)$ intersect transversely in $C^{-1}(e)$. Finally, we require the existence of a finite partition $I = I_1 \cup \cdots \cup I_n$ by consecutive intervals such that the previous homoclinic orbit varies continuously for $e \in I_i$, $1 \leq i \leq n$.

When I is compact, the annulus A is clearly normally hyperbolic in the usual sense (the boundary causes no trouble in this simple setting). The stable and unstable manifolds of A are well-defined, as the unions of those of the periodic solutions γ_e. Moreover, A can be continued to an annulus defined over a slightly larger interval $I' \supset I$.

2. Note that, due to the reversibility of C, the solutions of the vector field X^C occur in "opposite pairs," whose time parametrizations are exchanged by the symmetry $t \mapsto -t$. We introduce now the second definition to be used throughout the whole paper.

Definition 2. Let $c \in H_1(\mathbb{T}^2, \mathbb{Z}) \setminus \{0\}$. A *singular annulus for X^C realizing $\pm c$* is a C^1 compact invariant submanifold $\boldsymbol{Y}$ of $\mathbb{A}^2$, diffeomorphic to the sphere S^2 minus three disjoint open discs with disjoint closures (so that $\partial \boldsymbol{Y}$ is the disjoint union of three circles), such that there exist constants $e_* < \bar{e} < e^*$ which satisfy:

- $\boldsymbol{Y} \cap C^{-1}(\bar{e})$ is the union of the hyperbolic fixed point O and a pair of opposite homoclinic orbits.
- $\boldsymbol{Y} \cap C^{-1}(]\bar{e}, e^*])$ admits two connected components $\boldsymbol{Y}_+$ and $\boldsymbol{Y}_-$, which are annuli defined over the interval $]\bar{e}, e^*]$ and realizing c and $-c$ respectively.
- $\boldsymbol{Y}_0 = \boldsymbol{Y} \cap C^{-1}([e_*, \bar{e}[)$ is an annulus realizing the null class 0.

A singular annulus, endowed with its induced dynamics, is essentially the phase space of a simple pendulum from which an open neighborhood of the elliptic fixed point has been removed.

3. We will finally need the following notion of chains of annuli for C,[7] from which we will deduce the existence and properties of the chains of cylinders near the double resonance points.

Definition 3. Let $c \in H_1(\mathbb{T}^2, \mathbb{Z})$. We say that a family $(I_i)_{1 \le i \le i_*}$ of nontrivial intervals, contained and closed in the energy interval $]\overline{e}, +\infty[$, is *ordered* when $\mathrm{Max}\, I_i = \mathrm{Min}\, I_{i+1}$ for $1 \le i \le i_* - 1$. A *chain of annuli realizing c* is a family $(\mathsf{A}_i)_{1 \le i \le i_*}$ of annuli realizing c, defined over an ordered family $(I_i)_{1 \le i \le i_*}$, with the additional property

$$W^-(\mathsf{A}_i) \cap W^+(\mathsf{A}_{i+1}) \neq \varnothing, \quad W^+(\mathsf{A}_i) \cap W^-(\mathsf{A}_{i+1}) \neq \varnothing,$$

for $1 \le i \le i_* - 1$, both intersections being transverse in their energy levels.

The last condition is equivalent to assuming that the boundary periodic orbits of A_i and A_{i+1} at energy $e = \mathrm{Max}\, I_i = \mathrm{Min}\, I_{i+1}$ admit transverse heteroclinic orbits.[8] Note that, following Definition 1, an annulus can itself be considered as a chain, whose elements are the subannuli along which the homoclinic orbits vary continuously. This slight ambiguity will cause no trouble in the construction.

4. We say that $c \in H_1(\mathbb{T}^2, \mathbb{Z}) \setminus \{0\}$ is *primitive* when the equality $c = \lambda c'$ with $c' \in H_1(\mathbb{T}^2, \mathbb{Z})$ implies $\lambda = \pm 1$. We denote by $\boldsymbol{H}_1(\mathbb{T}^2, \mathbb{Z})$ the set of primitive homology classes, by $\boldsymbol{d}$ be the Hausdorff distance for compact subsets of $\mathbb{R}^2$ and by $\Pi : \mathbb{A}^2 \to \mathbb{R}^2$ the canonical projection.

Statement II (generic hyperbolic properties of classical systems). *Let T be a quadratic form on $\mathbb{R}^2$ and for $\kappa \ge 2$, let $\mathscr{U}_0^\kappa \subset C^\kappa(\mathbb{T}^2)$ be the set of potentials with a single and nondegenerate maximum. Then there is an integer $\kappa_0 \ge 2$ such that if $\kappa \ge \kappa_0$, there exists a dense open subset*

$$\mathscr{U}(T) \subset \mathscr{U}_0^\kappa \tag{13}$$

in $C^\kappa(\mathbb{T}^2)$ such that for $U \in \mathscr{U}(T)$, the associated classical system $C = \frac{1}{2}T + U$ satisfies the following properties:

(1) *For each $c \in \boldsymbol{H}_1(\mathbb{T}^2, \mathbb{Z})$ there exists a chain $\boldsymbol{A}(c) = (\mathsf{A}_0, \dots, \mathsf{A}_m)$ of annuli realizing c, defined over ordered intervals $I_0, \dots, I_m$, with*

$$I_m = [e_P, +\infty[,$$

[7] we keep the same terminology as for the cylinders, with a slightly different sense here.

[8] But the previous formulation is more appropriate when hyperbolic continuations of the annuli are involved.

for a suitable constant e_P which we call the Poincaré energy.

(2) *Given two primitive classes $c \neq c'$, there is a $\sigma \in \{-1, +1\}$ such that the chains $\boldsymbol{A}(c) = (\mathsf{A}_i)_{0\le i\le m}$ and $\boldsymbol{A}(\sigma c') = (\mathsf{A}'_i)_{0\le i\le m'}$ satisfy*

$$W^-(\mathsf{A}_0)\cap W^+(\mathsf{A}'_0)\neq\varnothing \quad \textit{and} \quad W^-(\mathsf{A}'_0)\cap W^+(\mathsf{A}_0)\neq\varnothing,$$

both heteroclinic intersections being transverse in $\mathbb{A}^2$.

(3) *There exists a singular annulus $\boldsymbol{Y}$ which admits transverse heteroclinic connections with the first annulus A_0 of the chain $\boldsymbol{A}(c)$, for all $c \in \boldsymbol{H}_1(\mathbb{T}^2, \mathbb{Z})$.*

(4) *Under the canonical identification of $H_1(\mathbb{T}^2, \mathbb{Z})$ with $\mathbb{Z}^2$ and for $e > 0$, let us set, for a given primitive class $c \sim (c_1, c_2) \in \mathbb{Z}^2$:*

$$Y_c(e) = \frac{\sqrt{2e}c}{\sqrt{c_1^2+c_2^2}} \in \mathbb{R}^2$$

Let $\boldsymbol{A}(c) = (\mathsf{A}_0, \dots, \mathsf{A}_m)$ be the associated chain and set $\boldsymbol{\gamma}_e = \mathsf{A}_m \cap C^{-1}(e)$ for e in $[e_P, +\infty[$. Then

$$\lim_{e\to+\infty} \boldsymbol{d}(\Pi(\boldsymbol{\gamma}_e), \{Y_c(e)\}) = 0.$$

We say that a chain with I_0 and I_m as in 1) is *biasymptotic to $\bar{e} := \operatorname{Max} U$ and to $+\infty$*. We will not only consider chains formed by nonsingular annuli, but also "generalized ones" in which we will allow a single annulus to be singular. With this terminology, one can rephrase the content of 1) and 3) of Statement II in the following concise way: for $U \in \mathscr{U}(T)$ and for each pair of classes $c, c' \in \boldsymbol{H}_1(\mathbb{T}^2, \mathbb{Z})$, there exists a generalized chain:

$$\mathsf{A}_m \leftrightarrow \cdots \leftrightarrow \mathsf{A}_1 \leftrightarrow \boldsymbol{Y} \leftrightarrow \mathsf{A}'_1 \leftrightarrow \cdots \leftrightarrow \mathsf{A}'_{m'}$$

(where $\leftrightarrow$ stands for the heteroclinic connections) which is biasymptotic to $+\infty$, and realize c and c' respectively.

In the x-plane, one therefore gets the following symbolic picture for the projection of 6 generalized chains of annuli, where the annuli are represented by fat segments, the singular annulus by a fat segment with a circle and the various heteroclinic connections are represented by $\leftrightarrow$.

The projections of the annuli on the action space are in fact more complicated than lines, they are rather 2-dimensional submanifolds with boundary, which tend to a line when the energy grows to infinity.

2.4. ***Double resonance cylinders.*** The dynamical structure of Hamiltonian systems at double resonance points has been widely studied, not only in the above mentioned works about Arnold diffusion, but also as an interesting problem *per se*. A complete list of these works would be unrealistic, let us only mention the

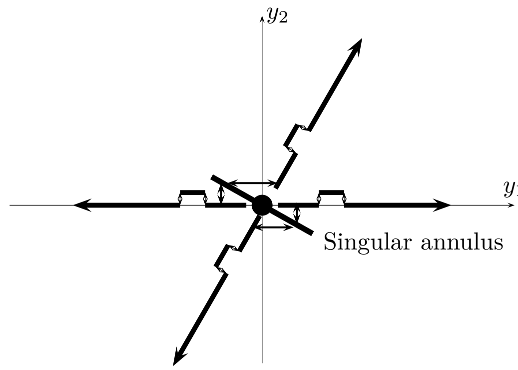


Figure 6. Projections in action of chains of annuli.

ones by G. Haller [27; 28] whose point of view is close to ours in the particular case of the intersection of a strong and a weak resonance.

1. Our point now is to construct cylinders located inside the ε^ν-neighborhoods of the strong double resonance points, and prove that they match the s-cylinders. Fix such a double resonance point r^0 and assume (up to a linear change of variables) that $r^0 = (\sqrt{2\boldsymbol{e}}, 0, 0)$. Hence θ_1 is the only fast angle with respect to which the averaging can be performed. This yields a normal form

$$N_\varepsilon(\theta, r) = h(r) + g_\varepsilon(\bar{\theta}, r) + R_\varepsilon(\theta, r)$$

where

$$\|g_\varepsilon - \varepsilon[f]\|_{C^p(\mathbb{T}^2 \times B(0,\varepsilon^\nu))} \leq \varepsilon^{1+\sigma}, \quad \|R_\varepsilon\|_{C^p(\mathbb{T}^3 \times B(0,\varepsilon^\nu))} \leq \varepsilon^\ell,$$

where $\sigma > 0$ and ℓ arbitrarily large. To derive this normal form in a quite flexible way, we start from Pöschel's normal form for analytic systems and apply an analytic smoothing; see [3].

The dynamical study of this normal form requires some care. To simplify we will assume here that

$$\begin{aligned} N_\varepsilon(\theta, r) &= \tfrac{1}{2} r_1^2 + \left[\tfrac{1}{2}(r_2^2 + r_3^2) + \varepsilon U(\theta_2, \theta_3)\right] + R(\theta, r, \varepsilon), \\ U(\theta_2, \theta_3) &:= \int_{\mathbb{T}} f((\theta_1, (\theta_2, \theta_3)), r^0)\, d\theta_1, \end{aligned} \tag{14}$$

where now the remainder R is extremely small (of order ε^ℓ with large ℓ) in some suitably chosen C^p topology over a neighborhood of r^0 of diameter ε^ν.[9]

[9]The complete study requires a careful analysis of mixed terms which do not appear here and whose size has to be taken into account.

2. The main role in (14) is played by the ε-dependent classical system

$$C_\varepsilon(\bar{\theta}, \bar{r}) = \tfrac{1}{2}(r_2^2 + r_3^2) + \varepsilon U(\theta_2, \theta_3), \quad \bar{\theta} = (\theta_2, \theta_3), \bar{r} = (r_2, r_3).$$

To recover the unperturbed setting of Statement II, we perform the usual linear rescaling $\bar{\mathsf{r}} = \sqrt{\varepsilon}\bar{r}$ of the action variable only, which transforms C_ε into

$$\mathsf{C}(\bar{\theta}, \bar{\mathsf{r}}) = \varepsilon C_\varepsilon(\bar{\theta}, \bar{r}),$$

so that the dynamics is only changed by a time dilatation, *while the geometry is preserved*. We assume that C satisfies the properties of Statement II. Let us fix a finite number of primitive homology classes c_k, $1 \le k \le k_*$, and consider the associated chains $\boldsymbol{A}(c_k)$. Let $e_p(k)$ be the Poincaré energy of $\boldsymbol{A}(c_k)$ and fix $E \ge \max_k e_p(k)$, so that, setting $\boldsymbol{A}(c_k) = (\mathsf{A}_1(c_k), \ldots, \mathsf{A}_{m_k}(c_k))$ the annuli

$$\mathsf{A}_1(c_k), \ldots, \mathsf{A}_{m_k-1}(c_k)$$

are contained in the sublevel $\mathsf{C} \le E$, while the annulus $\mathsf{A}_{m_k}(c_k)$ intersects that level along the compact subannulus

$$\widetilde{\mathsf{A}}_{m_k}(c_k) = \mathsf{A}_{m_k}(c_k) \cap \mathsf{C}^{-1}([e_p(k), E]).$$

The previous coordinate change sends these annuli onto "homothetic" ones (parametrized by ε), contained in the sublevel $C_\varepsilon \le \varepsilon E$. Forgetting about the class c_k, let us denote them by

$$\mathsf{A}_1(\varepsilon), \ldots, \mathsf{A}_{m_k-1}(\varepsilon), \widetilde{\mathsf{A}}_{m_k}(\varepsilon). \tag{15}$$

In addition, the singular annulus $\mathsf{A}^\bullet$ of C is sent onto a singular annulus $\mathsf{A}^\bullet(\varepsilon)$ of C_ε. The "length" of these annuli is of order $\sqrt{\varepsilon}$.

We can now analyze the ε-dependent truncated normal form

$$\overline{N}_\varepsilon(\bar{\theta}, \bar{r}) = \tfrac{1}{2}r_1^2 + \left[\tfrac{1}{2}(r_2^2 + r_3^2) + \varepsilon U(\theta_2, \theta_3)\right] \tag{16}$$

on the energy level $\boldsymbol{e}$. Let $\mathsf{A}(\varepsilon)$ be an element of the family (15). Since r_1 is a first integral of $\overline{N}_\varepsilon$, taking the product of $\mathsf{A}(\varepsilon)$ with the circle $\mathbb{T}$ of the angle θ_1 gives rise to a 3-dimensional (invariant and normally hyperbolic) cylinder $\mathcal{C}(\mathsf{A}(\varepsilon))$ contained in $\overline{N}_\varepsilon^{-1}(\boldsymbol{e})$, the variable r_1 being expressed (for ε small enough) as the function of $(\bar{\theta}, \bar{r})$ deduced from the energy relation

$$r_1 = 2\sqrt{\boldsymbol{e} - e}, \quad e = C_\varepsilon(\bar{\theta}, \bar{r}), \quad (\bar{\theta}, \bar{r}) \in \mathsf{A}(\varepsilon).$$

Similarly, the singular annulus $\mathsf{A}^\bullet(\varepsilon)$ gives rise to a normally hyperbolic invariant singular cylinder $\mathcal{C}(\mathsf{A}_\bullet(\varepsilon))$ at energy $\boldsymbol{e}$ for $\overline{N}_\varepsilon$.

Since $\omega(r^0) = (\sqrt{2\boldsymbol{e}}, 0, 0)$, the tangent space to $h^{-1}(\boldsymbol{e})$ at r^0 is the affine plane $r_1 = \sqrt{2\boldsymbol{e}}$, so that one can see the variables (r_2, r_3) as natural coordinates on $h^{-1}(\boldsymbol{e})$, and the localization of the previous invariant cylinders at energy $\boldsymbol{e}$ is

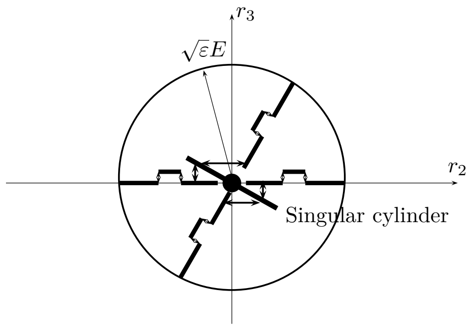


Figure 7. Projections of chains of cylinders for (16).

well-described by their projection on the (r_2, r_3)-plane. As a consequence, the arrangement of cylinders of $\overline{N}_\varepsilon$ in a zone of diameter $\sqrt{\varepsilon}E$ around r^0 is suitably deduced from the arrangement of annuli in the sublevel $C \leq E$, as shown in Figure 7 (in projection on the (r_2, r_3)-plane).

Note finally that the (4-dimensional) stable and unstable manifolds of $\mathcal{C}(\mathsf{A}(\varepsilon))$ and $\mathcal{C}(\mathsf{A}^\bullet(\varepsilon))$ are the products of those of $\mathsf{A}(\varepsilon)$ and $\mathsf{A}^\bullet(\varepsilon)$ with the circle of θ_1. Consequently, the homoclinic and heteroclinic connections are the products of those of the annuli of C with the circle of θ_1. This is a degenerate situation which generically gives rise to transverse intersections when the remainder R is taken into account.

3. Once the invariant cylinders for the truncated normal form are properly determined, it remains to show their persistence in the initial system. In a similar way as for simple resonances, we take advantage of the smallness of R first to use normal hyperbolic persistence and second to show the persistence of the boundaries of the cylinders of $\overline{N}_\varepsilon$. This way we prove the existence in the initial system of a family of invariant 3-dimensional cylinders, with homoclinic and heteroclinic connections, located in an $O(\sqrt{\varepsilon})$ neighborhood of the double resonance point r^0. We call them d-cylinders.

4. So far we have described the global picture in the neighborhood of r^0. We now go back to our initial problem, which is to use (a subset of) the previous family of d-cylinders to form a chain whose extremal elements match the s-cylinders along the simple resonance Γ. To do this, due to the fact that $\Gamma \subset \{r_3 = 0\}$, we only need to consider the d-cylinders located along the r_2-axis in the previous description. Therefore we focus on the chains of annuli of C which realize the homology classes $c = (\pm 1, 0)$, whose projection lies along the r_2-axis. Taking the singular annulus into account and truncating the extremal annuli at the energy E,

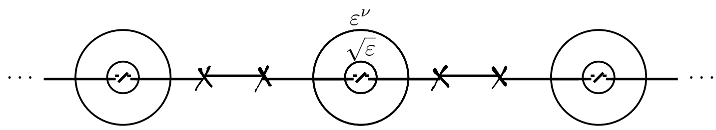


Figure 8. A chain of cylinders along Γ.

we get a generalized chain[10]

$$\widetilde{\mathsf{A}}_m^- \leftrightarrow \cdots \leftrightarrow \mathsf{A}_1^- \leftrightarrow \boldsymbol{Y} \leftrightarrow \mathsf{A}_1^+ \leftrightarrow \cdots \leftrightarrow \widetilde{\mathsf{A}}_m^+,$$

which yields the chain of cylinders

$$\mathcal{C}(\widetilde{\mathsf{A}}_m^-(\varepsilon)) \leftrightarrow \cdots \leftrightarrow \mathcal{C}(\mathsf{A}_1^-(\varepsilon)) \leftrightarrow \mathcal{C}(\boldsymbol{Y}(\varepsilon)) \leftrightarrow \mathcal{C}(\mathsf{A}_1^+(\varepsilon)) \leftrightarrow \cdots \leftrightarrow \mathcal{C}(\widetilde{\mathsf{A}}_m^+(\varepsilon)).$$

Now a crucial observation is that *both extremal cylinders* $\mathcal{C}(\widetilde{\mathsf{A}}_m^{\pm}(\varepsilon))$ *can be continued in a unique way over an* $O(\varepsilon^{\nu})$*-neighborhood of* r^0, giving rise to "longer" cylinders $\widetilde{\mathscr{C}}_m^{\pm}$, still lying along the resonant line Γ. To compare these new cylinders to the s-cylinders $\mathscr{C}^{\pm}$ located on both sides of the double resonance point, we prove that $\widetilde{\mathscr{C}}_m^+$ and $\widetilde{\mathscr{C}}_m^-$ both contain two (essential) KAM tori, which are also contained in the s-cylinders $\mathscr{C}^+$ and $\mathscr{C}^-$ respectively. By normally hyperbolic uniqueness, this proves that the s-cylinders continue $\widetilde{\mathscr{C}}_m^{\pm}$ outside the ε^{ν}-neighborhood and completes the picture: there is a chain of cylinders and singular cylinders *passing through* the double resonance point and connecting together the two s-cylinders $\mathscr{C}^{\pm}$ in the ε^{ν} gluing zone:

$$\mathscr{C}^- \leftrightarrow \cdots \leftrightarrow \mathcal{C}(\mathsf{A}_1^-(\varepsilon)) \leftrightarrow \mathcal{C}(\boldsymbol{Y}(\varepsilon)) \leftrightarrow \mathcal{C}(\mathsf{A}_1^+(\varepsilon)) \leftrightarrow \cdots \leftrightarrow \mathscr{C}^+.$$

Applying this process for all strong double resonance points contained in Γ (and taking the bifurcations points between them into account), we construct a chain $\boldsymbol{C}$ of hyperbolic cylinders and singular cylinders whose projection $\pi(\boldsymbol{C})$ in action satisfies $d_H(\pi(\boldsymbol{C}), \Gamma) \to 0$ when $\varepsilon \to 0$ (where d_H stands for the Hausdorff distance in $\mathbb{A}^3$). This yields the following final picture for the arrangement of cylinders along the arc Γ.

5. This construction applies to each segment Γ_{k_i} of the initial broken line. To get a chain along the full broken line, we have to pass from one resonance arc to another one through the double resonance point at their intersection. For doing this, we use the full structure at this double resonance point and choose two homology classes c_1, c_2 in $\boldsymbol{H}_1(\mathbb{T}^2, \mathbb{Z})$ which correspond to the simple resonances

[10]By symmetry of C, the numbers of annuli realizing $\pm c$ are equal.

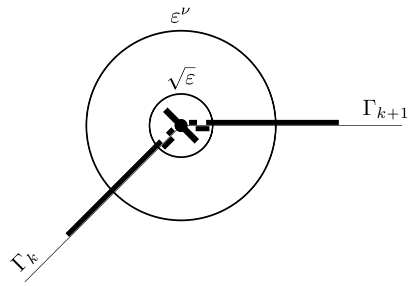


Figure 9. Transition between two arcs at a double resonance point.

arcs crossing at that point. In the same way as above, we get a chain of cylinders (with one singular cylinder) whose projection is located along both resonance arcs in an $O(\sqrt{\varepsilon})$ neighborhood of the double resonance point:

$$\mathcal{C}(\widetilde{\mathsf{A}}^-_{m_1}(c_1,\varepsilon)) \leftrightarrow \cdots \leftrightarrow \mathcal{C}(\mathsf{A}^-_1(c_1,\varepsilon)) \leftrightarrow \mathcal{C}(\boldsymbol{Y}(\varepsilon)) \leftrightarrow \mathcal{C}(\mathsf{A}^+_1(c_2,\varepsilon)) \leftrightarrow \cdots \leftrightarrow \mathcal{C}(\widetilde{\mathsf{A}}^+_{m_2}(c_2,\varepsilon)).$$

Again, we prove that the extremal cylinders $\mathcal{C}(\widetilde{\mathsf{A}}^-_{m_1}(c_1,\varepsilon))$ and $\mathcal{C}(\widetilde{\mathsf{A}}^-_{m_2}(c_2,\varepsilon))$ admit continuations to an ε^ν neighborhood of the double resonance point, and that these continuations match the s-cylinders located on both sides of the neighborhood along the simple resonance arcs.

2.5. ***Thresholds.*** The minimal regularity $\kappa_0 \geq 2$ is assumed to be large enough for our subsequent (finite number of) applications of normally hyperbolic persistence, genericity and KAM theorems to apply for $\kappa \geq \kappa_0$ in the various settings involved in the construction. We fix a Tonelli integrable Hamiltonian $h \in C^\kappa(\mathbb{R}^3)$ with $\kappa \geq \kappa_0$ together with a broken line of simple resonance arcs as in Figure 3. We outline the main steps of a proof of the existence of the lower semicontinuous threshold function $\boldsymbol{\epsilon}_0$ of Statement I. Without loss of generality, we can focus on a single resonant arc Γ and assume that:

- Γ is a graph over the plane $P = \{r_3 = 0\}$, so that its equation reads $r_3 = r_3^*(\hat{r})$ with $\hat{r} := (r_1, r_2)$ in $\widehat{\Gamma} := \pi_P(\Gamma)$.
- The frequency vector along Γ reads $\omega(r) = (\omega_1(r), \omega_2(r), 0)$.

By compactness and convexity, the spectrum of the normal Hessian of h along Γ is bounded from below by a positive constant.

1. *Conditions for the existence of simple resonance cylinders.*

• For $\kappa \geq \kappa_0$, the C^κ one-parameter families of functions on $\mathbb{T}$ with parameter in $\widehat{\Gamma}$ which admit a single and nondegenerate maximum up to a finite number of values of the parameter, for which there are exactly two nondegenerate maxima, form an open and dense subset of $C^\kappa(\mathbb{T}\times\widehat{\Gamma})$. The averaging operator $f \mapsto \langle f\rangle_\Gamma$, where

$$\langle f(\theta_3;\hat{r})\rangle_\Gamma = \int_{\mathbb{T}^2} f(\hat{\theta},\theta^3,\hat{r},r_3^*(\hat{r}))d\hat{\theta}$$

is linear and surjective from $C^\kappa(\mathbb{A}^3,\mathbb{R})$ to $C^\kappa(\mathbb{T}\times\widehat{\Gamma})$, hence is an open mapping. Therefore there is a dense open subset $\mathcal{S}_1 \subset \mathcal{S}^\kappa$ such that for $f \in \mathcal{S}_1^\kappa$ the averaged potential $\langle f(\theta_3;\hat{r})\rangle_\Gamma$ admits a single and nondegenerate maximum $\theta_3^*(\hat{r})$ outside a finite subset of bifurcation points in $\widehat{\Gamma}$, where it admits exactly two nondegenerate maximums.

Consequently, thanks to the remark on the normal Hessian of h along Γ, over closed intervals limited by bifurcation points the hyperbolicity constant of the hyperbolic point $O(\widehat{r}) = (\theta_3^*(\hat{r}), r_3^*(\hat{r}))$ is uniformly bounded from below.[11]

• Using to a suitable $\sqrt{\varepsilon}$ rescaling, one proves (see [5] and early works by Kaloshin) that, given $f \in \mathcal{S}_1^\kappa$, the previous uniform bound yields the existence of a finite number of double resonance points (d_i) in Γ such that one gets (pseudoinvariant) simple resonance cylinders outside the union of ε^ν-neighborhoods of the fibers $\mathbb{T}^3\times\{d_i\}$ in $H_\varepsilon(\boldsymbol{e})$. The choice of κ_0 depends on the required value of $\nu < \frac{1}{2}$ (see [44]) and this statement holds for and $0 < \varepsilon < \boldsymbol{\epsilon}_1(f)$.

• For each $f \in \mathcal{S}_1$, there is an open neighborhood $\mathscr{O}(f)$ of f in $\mathcal{S}_1$ such that the set of double resonance points to be removed from the arc Γ do not depend on the choice of the perturbation $g \in \mathscr{O}$, and moreover the function $\boldsymbol{\epsilon}_1$ can be chosen so as to depend continuously on g in $\mathscr{O}$.

This process provides us with a multivalued locally continuous threshold function $\boldsymbol{\epsilon}_1 : \mathcal{S}_1^\kappa \to \mathbb{R}^{*+}$.

2. *Conditions at a double resonance point.* We fix now an open subset $\mathscr{O} \subset \mathcal{S}_1$ over which the previous two properties (double resonant points and continuity of $\boldsymbol{\epsilon}_1$) are satisfied. It is enough to consider a single double resonance point $r^0 \in \Gamma$, and one can assume its frequency vector to have the form $(\omega_1, 0, 0)$ with $\omega_1 \neq 0$. Set $\bar{\theta} := (\theta_2, \theta_3)$ and for $f \in \mathscr{O}$ let

$$U(\bar{\theta}) := \langle f\rangle_{r^0}(\bar{\theta}) = \int_{\mathbb{T}} f(\theta_1,\bar{\theta},r^0)d\theta_1$$

[11] This point is uniquely defined by continuity at the boundaries of the interval.

be the averaged potential at r^0. The ($\sqrt{\varepsilon}$-rescaled) main part of the averaged system at r^0 reads

$$C(\bar{\theta}, \bar{r}) = \tfrac{1}{2} Q(\bar{r}) + U(\bar{\theta}), \tag{17}$$

where Q is a *fixed* quadratic form deduced from the Hessian of h at r^0. We fix a finite number of homology classes in $\boldsymbol{H}_1(\mathbb{T}^2)$ (one class in the case of a double resonant point in $\operatorname{Int}\Gamma$ and two classes in the case of a boundary point, according to the fact that one wants to construct chains following Γ in the first case and passing to another resonance arc in the second):

- Since the averaging operator $\langle\ \rangle_{r^0}$ is an open mapping $C^\kappa(\mathbb{A}^3) \to C^\kappa(\mathbb{T}^2)$, provided that κ_0 is large enough, there is a dense open subset $\mathscr{O}' \subset \mathscr{O}$ such that the classical system (17) satisfies the properties quoted in Statement II relative to the previous homology classes. In particular, there is a chain of annuli (with a single singular annulus) attached to the previous homology class (in the case of an inner double resonance point) and to the pair of classes (in the case of a boundary point).
- By (singular) normally hyperbolic persistence of the annuli, there is a multivalued locally continuous function $\boldsymbol{\epsilon}_2 : \mathscr{O}_2 \to \mathbb{R}^{*+}$ such that for $0 < \varepsilon < \boldsymbol{\epsilon}_2(g) < \boldsymbol{\epsilon}_1(g)$ there exist chains of (pseudoinvariant) cylinders (with a single singular cylinder) obtained by suspension relative to the fast angle, and then perturbation, of the chains of annuli in the averaged system
$$C_\varepsilon(\bar{\theta}, \bar{r}) = \tfrac{1}{2} Q(\bar{r}) + \varepsilon \langle g \rangle_{r^0}(\bar{\theta}).$$
- The Poincaré pseudoinvariant cylinders in these chains extend to an ε^ν-distance away from the double resonance.

This step (applied to each double resonance point in Γ) provides us with a cover $(\mathscr{O}_j)$ of $\mathcal{S}_1$ by open sets over which the function $\boldsymbol{\epsilon}_2$ is continuous and is a threshold for the existence of pseudoinvariant cylinders along Γ, and along two other resonant arcs in a small neighborhood of the boundary double resonance points.

3. *Conditions for the existence of KAM tori and invariant cylinders.* We fix now f in some $\mathscr{O}_j$. For $0 < \varepsilon < \boldsymbol{\epsilon}_2(f)$, the existence of a sufficiently large set of 2-dimensional unperturbed tori inside the pseudoinvariant cylinders (neglecting the remainders of the various normal forms) is guaranteed by usual considerations from Diophantine theory; see for instance [15]. After reducing the system (in normal form) inside the pseudoinvariant cylinders to a two dimensional discrete setting, one can apply a version of KAM theorem with vanishing torsion (which reflects the singular nature of the perturbation), deduced from Herman's work (see [29; 30]), to show the existence of 2-dimensional invariant tori close to the "boundaries" of the pseudoinvariant cylinders. These tori therefore bound genuinely invariant and normally hyperbolic tori. In the same way, one proves the existence of invariant tori inside the matching zone at an ε^{ν} distance of the double resonance points, proving that the simple resonance cylinders and the (suitably chosen) double resonance Poincaré cylinders continue one another. This provides us with a new open cover of $\mathscr{O}$ and a multivalued threshold function $0 < \boldsymbol{\epsilon}_3 < \boldsymbol{\epsilon}_2$ which is continuous on each open set of the cover and is a threshold for the existence of a family of compact invariant normally hyperbolic cylinders and singular cylinders along the arc Γ.

4. *The lower-semicontinuous threshold* $\boldsymbol{\epsilon}_0$. At this point the initial open dense set $\mathcal{S}_1$ is endowed with an open cover $(\mathscr{U}_i)_{i\in I}$ together with a threshold function $\boldsymbol{\epsilon}_3$ which is positive and continuous on each $\mathscr{U}_i$. For each i, we continue the function $(\boldsymbol{\epsilon}_3)_{|\mathscr{O}_i}$ to $\mathcal{S}^{\kappa}$ by 0 on the closed set $\mathcal{S}^{\kappa} \setminus \mathscr{U}_i$. The resulting continuation $\bar{\boldsymbol{\epsilon}}_3^{(i)}$ is therefore lower-semicontinuous on $\mathcal{S}^{\kappa}$. Applying the previous process to each arc in the initial broken line, one gets a final threshold

$$\boldsymbol{\epsilon}_0 = \mathrm{Sup}_{i\in I}\, \bar{\boldsymbol{\epsilon}}_3^{(i)},$$

which is lower-semicontinuous, positive on the dense open set $\mathcal{S}_1$ and such that *each element* in the generalized ball $\mathscr{B}^{\kappa}(\boldsymbol{\epsilon}_0)$ admits a family of compact normally hyperbolic invariant cylinders along the broken line.

5. *Connections.* We will not address in detail here the question of homoclinic and heteroclinic connections. New conditions to ensure the existence of transverse heteroclinic connections between distinct consecutive cylinders come from usual arguments from transversality theory, while the (topologically transverse) homoclinic connections require more subtle arguments (see Section 5 and [44]) from dimension theory, which finally yield the *admissible* chains along which the diffusion orbits can be proved to exist. Both type of connections require adding arbitrarily small perturbations to the elements of the generalized ball $\mathscr{B}(\boldsymbol{\epsilon}_0)$ (which is legitimized by the fact that $\mathscr{B}(\varepsilon_0)$ is open), which explains that our admissible chains exist only for a dense open set of perturbations in $\mathscr{B}(\varepsilon_0)$ in our Statement I (openness being trivial by continuity).

2.6. ***Conclusion.*** To conclude this geometric description, we want to emphasize that, while the geometric analysis is more complicated near double resonances than along simple resonance arcs, the dynamical analysis along d-cylinders is by far simpler than that along s-cylinders. Indeed, due to the existence of a global transverse intersection of the stable and unstable manifolds of a 2-dimensional annulus in the averaged classical system on $\mathbb{T}^2$, the stable and unstable manifolds of the corresponding perturbed cylinder in the initial system at fixed energy intersect transversely along a two-dimensional homoclinic annulus. After a two-dimensional reduction of the dynamics on a Poincaré section inside the cylinder (see Section 5), this yields a bisystem of *globally defined* maps (the inner and the homoclinic one) for which the existence of drifting orbits is easy to prove (see the next section for a simplified model). By contrast, the stable and unstable manifolds of an s-cylinder do coincide if the remainder of the normal form is neglected. This makes the construction of homoclinic orbits more difficult: after taking the remainder into account, they essentially come from the homoclinic intersections of invariant tori contained inside the cylinder, which yields only a locally defined homoclinic correspondence. In this case usual transversality arguments do not apply, due to the uncountable number of objects to control. Sections 4 and 5 below are devoted to this difficulty, in the general discrete case in Section 4, which is then applied in a simplified model in Section 5.

3. Diffusion orbits in the *a priori* chaotic discrete setting

The purpose of this section is to exhibit a class of symplectic diffeomorphisms of $\mathbb{A}^2 = T^*\mathbb{T}^2$, for which diffusion properties can be detected with minimal technicalities, which in addition are good models for the dynamics along double resonance cylinders.

Our framework is a discrete version of the so-called "*a priori* chaotic" setting developed in relation to Mather's work on unbounded growth of energy for nonautonomous perturbations of geodesic flows. This problem was investigated by Bolotin and Treschev [8] and Delshams, De la Llave, Seara [16]; more recently Gelfreich and Turaev systematically revisited this question in the analytic category [19]. However some significant features of our systems are rather different and make our approach both simpler and more general to some extent, since they are *far from any integrable ones*.

The main feature of our diffeomorphisms $g : \mathbb{A}^2 \circlearrowleft$ is the existence of a normally hyperbolic annulus $\mathscr{A}$ (diffeomorphic to $\mathbb{A}$) that admits a homoclinic intersection *which is itself diffeomorphic to an annulus*. This yields the existence of a natural bisystem on $\mathscr{A}$, formed by the restriction of g to $\mathscr{A}$ together with a homoclinic map defined everywhere on $\mathscr{A}$. It is then easy to show that an arbitrarily small perturbation of g puts this bisystem in a general position and allows one to apply Moeckel's theorem [48]. This yields the existence of drifting pseudoorbits, which are in turn shadowed by genuine orbits, due to normally hyperbolic shadowing properties.

3.1. ***The setting.*** We fix once and for all a closed interval $I \subset [-1, 2]$ of $\mathbb{R}$ which contains [0, 1] in its interior. We work in the space $\mathscr{D}^\kappa$ of C^κ symplectic diffeomorphisms of $\mathbb{A}^2$ with support contained in $\mathbb{T}^2 \times I^2$, endowed with the natural uniform C^κ metric d_κ. The space $(\mathscr{D}^\kappa, d_\kappa)$ is complete.

We first introduce a diffusion property for diffeomorphisms in $\mathscr{D}^\kappa$ together with a specific class $\mathscr{F}^\kappa \subset \mathscr{D}^\kappa$ (uncoupled products), whose elements do not satisfy this property and which we consider as "unperturbed systems". Our main result then proves the existence of a large subset of suitable C^κ perturbations of f which admit the diffusion property.

1. Let us now give precise definitions, beginning with that of diffusion orbits.

Definition 4. Fix $\delta > 0$ and set

$$\mathscr{U}^0(\delta) = \{(\theta, r) \in \mathbb{A}^2 \mid |r_1|\} < \delta\}, \quad \mathscr{U}^1(\delta) = \{(\theta, r) \in \mathbb{A}^2 \mid |r_1 - 1| < \delta\}. \tag{18}$$

Given a diffeomorphism $g \in \mathscr{D}^\kappa$, we say that a finite orbit $x_0, \dots, x_N$ of g is a δ-*diffusion orbit* when $x_0 \in \mathscr{U}^0$ and $x_N \in \mathscr{U}^1$.

2. The elements $f \in \mathscr{F}^\kappa$ are C^κ symplectic diffeomorphisms of $\mathbb{A}^2$ and admit the product form

$$f(\theta, r) = (f_1(\theta_1, r_1), f_2(\theta_2, r_2)), \quad (\theta, r) \in \mathbb{A}^2, \tag{19}$$

where the diffeomorphisms $f_i : \mathbb{A} \circlearrowleft$ satisfy some additional conditions:

• *Conditions on* f_1. We denote by $\mathrm{DD}(\tau)$ the set of real numbers which are Diophantine of exponent $\tau > 1$. Given $\kappa \geq 1$, we introduce the set $\mathscr{F}_1^\kappa$ of C^κ symplectic diffeomorphisms $f_1 : \mathbb{A} \circlearrowleft$ which satisfy the following conditions:

(C_1) Supp $f_1 \subset \mathbb{T} \times I$.

(C_2) *The circles* $\Gamma^0 = \mathbb{T} \times \{0\}$ *and* $\Gamma^1 = \mathbb{T} \times \{1\}$ *are invariant under* f_1, *and their rotation numbers* ρ^0, ρ^1 *are in* $\mathrm{DD}(\tau)$ *for some* $\tau > 1$.

To introduce the third condition we use the coordinate chart (θ_1, r_1) of $\mathbb{A}$ and write

$$f_1(\theta_1, r_1) = (\Theta_1(\theta_1, r_1), R_1(\theta_1, r_1)). \tag{20}$$

(C_3) *The restriction of* f_1 *to the annulus* $\mathbb{T} \times [0, 1]$ *uniformly tilts the vertical to the right*, *that is*, *there is a* $c > 0$ *such that*

$$\frac{\partial \Theta_1}{\partial r_1}(\theta_1, r_1) \geq c, \quad \forall (\theta_1, r_1) \in \mathbb{T} \times [0, 1]. \tag{21}$$

Note that, due to (C_1) and (C_2), the annulus $\mathbb{T} \times [0, 1]$ is invariant under f_1. The condition that the rotation numbers of the circles Γ^i are in $\mathrm{DD}(\tau)$ will ensure their persistence under perturbation.

• *Conditions on* f_2. We introduce the set $\mathscr{F}_2^\kappa$ of C^κ symplectic diffeomorphisms $f_2 : \mathbb{A} \circlearrowleft$ which satisfy the following conditions:

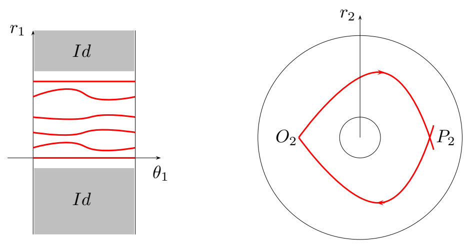


Figure 10. An unperturbed diffeomorphism.

(C_4) Supp $f_2 \subset \mathbb{T} \times I$.

(C_5) *The diffeomorphism* f_2 *possesses a hyperbolic fixed point* O_2.

(C_6) *The point* O_2 *admits a transverse homoclinic point* P_2.

We will denote by

$$\lambda(O_2) > 1 \tag{22}$$

the maximal eigenvalue of the derivative $D_{O_2} f_2$. Note that O_2 and P_2 are contained in the support of f_2.

3. We now define our set of "unperturbed" diffeomorphisms in order to guarantee additional stability properties under perturbations.

Definition 5. We define $\mathscr{F}^\kappa$ as the set of (symplectic) diffeomorphisms on $\mathbb{A}^2$ of the form (19), where $f_1 \in \mathscr{F}_1^\kappa$ and $f_2 \in \mathscr{F}_2^\kappa$ with

$$(\mathrm{Max}_{x\in\mathbb{A}} \|T_x f_1\|)^\kappa < \lambda(O_2). \tag{23}$$

where $\|\cdot\|$ stands for the operator norm.

The domination condition (23) ensures that the invariant annulus $\mathbb{A} \times \{O_2\}$ is uniformly normally hyperbolic for f, with persistence properties in the C^κ topology and additional specific symplectic features.[12]

4. Given $\tau > 1$, when κ is large enough, for any $f \in \mathscr{F}^\kappa$ there exists an arbitrarily small $\delta > 0$ such that f does not possess any δ-diffusion orbit: classical KAM theorems in the finitely differentiable setting prove the existence of an essential invariant circle Γ for f_1 located in the zone $r_1 > 0$ (one indeed gets an infinite family of such circles), and the claim comes from the product structure of f. However, we will prove that under generic and small enough perturbations, *any* element of $\mathscr{F}^\kappa$ gives rise to a diffeomorphism which admits diffusion orbits. More precisely, our main result is the following.

[12] A weaker condition could be required, at the cost of a smoothing argument which would obscure the description.

Theorem 6. *There is a κ_0 such that, given $f \in \mathscr{F}^\kappa$ and $\delta > 0$, then there is an $\varepsilon(f) > 0$ such that the subset of all diffeomorphisms g in $B^\kappa(f, \varepsilon(f))$ which admit a δ-diffusion orbit is open in the C^0 topology and dense in $B^{\kappa-1}(f, \varepsilon(f))$.*

The existence of δ-diffusion orbits being clearly an open property in the C^0 topology, we will therefore focus on the "density". The loss of 1 derivative could be avoided using a smoothing argument that we will not describe here.

5. As already mentioned in the introduction, the proof of Theorem 6 is based on a method introduced by Moeckel in [48] to prove the existence of drifting orbits for bisystems of maps τ_0, τ_1 on the annulus. If $\Gamma_\bullet$ and $\Gamma^\bullet$ are two disjoint graphs of C^1 functions $\mathbb{T} \to \mathbb{R}$, we denote by $\boldsymbol{A}[\Gamma_\bullet, \Gamma^\bullet] \subset \mathbb{A}$ the subannulus bounded by their union.

Theorem A [48]. *Let $\tau_0, \tau_1 : \mathbb{A} \circlearrowleft$ be C^1 diffeomorphisms with compact support in $\mathbb{T} \times I$, where τ_0 is area-preserving and τ_1 is exact symplectic. Assume that there exist two disjoint τ_0-invariant C^1 graphs $\Gamma_\bullet, \Gamma^\bullet$ in $\mathbb{T} \times I$ and that τ_0 is a twist map in restriction to the annulus $\boldsymbol{A} := \boldsymbol{A}[\Gamma_\bullet, \Gamma^\bullet]$. Let $\mathrm{Ess}_{\boldsymbol{A}}(\tau_i)$ be the set of essential τ_i-invariant circles contained in $\boldsymbol{A}$. Assume that*

$$\mathrm{Ess}_{\boldsymbol{A}}(\tau_0) \cap \mathrm{Ess}(\tau_1) = \varnothing. \tag{24}$$

Then for any connected neighborhoods $U_\bullet$ and $U^\bullet$ of $\Gamma_\bullet$ and $\Gamma^\bullet$ in $\mathbb{A}$, with $\tau_1(\Gamma_\bullet) \subset U_\bullet$ and $\tau_1(\Gamma^\bullet) \subset U^\bullet$ the bisystem (τ_0, τ_1) admits an orbit with first point in $U_\bullet$ and last point in $U^\bullet$.

This in fact is a slight generalization of the theorem of [48], since the boundaries $\Gamma_\bullet$ and $\Gamma^\bullet$ are not assumed to be invariant under τ_1.

The next result, based on the study of the Minkowski dimension of the sets $\mathrm{Ess}_{\boldsymbol{A}}(\tau_0)$ and $\mathrm{Ess}(\tau_1)$, will provide us with the necessary tool for proving the density statement in Theorem 6.

Theorem B [48]. *Fix an integer $p \geq 1$. Let $\tau_0, \tau_1 : \mathbb{A} \circlearrowleft$ be C^p area-preserving diffeomorphisms with compact support in $\mathbb{T} \times I$. Assume that there exist two disjoint τ_0-invariant C^1 graphs $\Gamma_\bullet, \Gamma^\bullet$ in $\mathbb{T} \times I$, and that τ_0 is a twist map in restriction to $\boldsymbol{A} := \boldsymbol{A}[\Gamma_\bullet, \Gamma^\bullet]$. Assume moreover that $(\tau_0)_{|\boldsymbol{A}}$ has no essential invariant circle with rational rotation number. Then there exists a C^∞ Hamiltonian $h : \mathbb{A} \to \mathbb{R}$ with support in $\mathbb{T} \times I$, arbitrarily small in the C^∞ topology, such that*

$$\mathrm{Ess}_{\boldsymbol{A}}(\tau_0) \cap \mathrm{Ess}(\Phi^h \circ \tau_1 \circ \Phi^{-h}) = \varnothing, \tag{25}$$

where Φ^h stands for the time-one map of the Hamiltonian flow generated by h.

Note that assuming that the τ_i are area-preserving is equivalent to assuming that they are exact-symplectic a property directly related to the constructions of our bisystems in the following. The proof of Theorem B is exactly the same as in [48].

3.2. ***Proof of Theorem 6.*** Let us first informally describe the proof. The first ingredient is the choice of ε small enough so that any g in $B^\kappa(f, \varepsilon(f))$ exhibits some of the main dynamical features of f. In particular, we require that g admits a normally hyperbolic invariant annulus $\mathscr{A}_g$ close to $\mathbb{A} \times \{O_2\}$ and a homoclinic annulus $\mathscr{H}_g$ close to $\mathbb{A} \times \{P_2\}$. We then consider two diffeomorphisms of $\mathscr{A}_g$.

• The first one, φ_g, is nothing but the restriction of g to $\mathscr{A}_g$. Thanks to the domination condition (23) normally hyperbolic persistence proves that φ_g is C^κ close to f_1 (in suitable coordinates). In particular, the initial invariant circles Γ^i of f_1 will persist and give rise to essential invariant circles Γ^i_g for φ_g, which bound a compact annulus $\mathsf{A}_g \subset \mathscr{A}_g$.

• The definition of the second diffeomorphism — the *homoclinic map* ψ_g — is based on the existence of a (full) homoclinic annulus $\mathscr{H}_g$. The diffeomorphism ψ_g encodes the asymptotic properties of the associated homoclinic orbits of $\mathscr{A}_g$. More precisely, if x, y in $\mathscr{A}_g$ satisfy $y = \psi_g(x)$, then there exists an orbit $z_{-M}, \dots, z_N$ of g, located in $\mathbb{A}^2 \setminus \mathscr{A}_g$, with z_{-M} arbitrarily close to $g^{-M}(x) = \varphi_g^{-M}(x)$ and z_N arbitrarily close to $g^N(y) = \varphi_g^N(y)$, where the integers N and M can be chosen arbitrarily large.

A key observation (introduced in [24]) is that the Poincaré recurrence theorem applies to φ_g on the compact annulus $\mathscr{A}_g$ and allows one to choose M and N so that $\varphi_g^{-M}(x)$ and $\varphi_g^N(y)$ are arbitrarily close to the initial points x and y respectively.

Using Moeckel's results, we prove that *after a small perturbation of g* the bisystem (φ_g, ψ_g) admits "drifting orbits", whose initial and final points are arbitrarily close to the boundary circles of A_g.

Finally, in view of the definition of φ_g and the asymptotic properties of ψ_g, one expects that the connecting orbits of the bisystem can be uniformly approximated by genuine orbits of g. Here, for completeness, we prove that this is the case by means of a normally hyperbolic shadowing lemma, whose idea is reminiscent of [8; 17]. Our proof closely follows the (more general) one in [23].

3.2.1. *The symplectic geometry of perturbed products.* **1.** Let us first examine the dynamical features of a diffeomorphism $f \in \mathscr{F}^\kappa(\tau)$, which are immediately deduced from the product form (19):

• The annulus $\mathscr{A} = \mathbb{A} \times \{O_2\}$ is invariant under f and diffeomorphic to $\mathbb{A}$. It is moreover κ-normally hyperbolic, due to condition (23). The stable and unstable manifolds of $\mathscr{A}$ inherit the product structure of f:

$$W^{\pm}(\mathscr{A}) = \mathbb{A} \times W^{\pm}(O_2). \tag{26}$$

These are hypersurfaces of $\mathbb{A}^2$ of class C^κ (since $W^{\pm}(O_2)$ are C^κ), and so are coisotropic in $\mathbb{A}^2$. Their characteristic leaves are the 1-dimensional submanifolds

$$\{x\} \times W^{\pm}(O_2), \quad x \in \mathbb{A}. \tag{27}$$

which coincide with the stable and unstable manifolds of the points of $\mathscr{A}$ respectively (this fact is general, see Appendix A). Let $\Pi^{\pm} : W^{\pm}(\mathscr{A}) \to \mathscr{A}$ stand for the characteristic projections, so that if $(x, w) \in W^{\pm}(x)$, then $\Pi^{\pm}(x, w) = (x, O_2)$.

• The manifolds $W^{\pm}(\mathscr{A})$ intersect transversely in $\mathbb{A}^2$ along both $\mathscr{A}$ and the homoclinic annulus

$$\mathscr{H} = \mathbb{A} \times \{P_2\}. \tag{28}$$

Moreover, for each $(x, O_2) \in \mathscr{A}$, the leaf $W^{-}((x, O_2))$ transversely intersect the manifold $W^{+}(\mathscr{A})$ at a unique point of $\mathscr{H}$, namely

$$W^{-}((x, O_2)) \cap \mathscr{H} = \{(x, P_2)\}. \tag{29}$$

One has a similar observation for the stable leaves. We denote by $\pi^{\pm}$ the restrictions of $\Pi^{\pm}$ to the annulus $\mathscr{H}$, so that

$$\pi^{\pm} : \mathscr{H} \to \mathscr{A}, \quad \pi^{\pm}(x, P_2) = (x, O_2), \quad x \in \mathbb{A}. \tag{30}$$

• Clearly $\mathscr{A}$ and $\mathscr{H}$ are symplectic submanifolds of $\mathbb{A}^2$ and $\pi^{\pm}$ are symplectic diffeomorphisms.

• There exists a pair of natural f-induced symplectic diffeomorphisms of $\mathscr{A}$. The first one is just the restriction $\varphi = f_{|\mathscr{A}}$, which here admits a natural identification with f_1. The second one is the map

$$\psi = \pi^{+} \circ (\pi^{-})^{-1}$$

which describes the homoclinic excursion of the orbits, we call it the *homoclinic map*. Clearly $\psi = \mathrm{Id}$ here.

The manifolds $W^{\pm}(\mathscr{A})$ do indeed admit a much larger intersection than $\mathscr{A} \cup \mathscr{H}$, but we neglect the other components which play no role in our construction.

The homoclinic map has been introduced in [14] and carefully studied in [17] and subsequent papers by the same authors, under the name of scattering map. We use this new terminology here to make a distinction between the homoclinic maps (or correspondences) and the heteroclinic ones, which necessarily appear when chains of cylinders are considered. While the ideas are very close, one slight difference in our (complete) work is that we perform a systematic reduction of the homo-heteroclinic map to a two-dimensional object (in order to obtain a two-dimensional bisystem), while the scattering map is usually used in a more global higher dimensional setting.

2. The symplectic features of small enough perturbations of f are immediately deduced from the symplectic normally hyperbolic persistence theorem (see Appendix A). Note in particular that even if the unperturbed annulus is noncompact, the existence and uniqueness of the perturbed one is not difficult, thanks to the compact-supported character of the perturbation.

Lemma 7. *Let $f = (f_1, f_2) \in \mathscr{F}^\kappa(\tau)$ be fixed. Then there exists $\bar\varepsilon(f) > 0$ such that for each g in $B^\kappa(f, \bar\varepsilon(f))$:*

- *There exists a (uniquely defined) symplectic normally hyperbolic g-invariant annulus $\mathscr{A}_g$ of the form*

$$\mathscr{A}_g = \{(x, a_g(x)) \mid x \in \mathbb{A}\}, \tag{31}$$

where a_g is a C^κ function $\mathbb{A} \to B^2(O_2, \alpha) \subset \mathbb{A}$ such that $\|a_g - O_2\|_{C^\kappa(\mathbb{A})} \to 0$ when $d_\kappa(g, f) \to 0$ (where $\alpha > 0$ is a suitable constant).

- *The manifolds $W^\pm(\mathscr{A}_g)$ are coisotropic with characteristic foliations*

$$(W^\pm(z))_{z \in \mathscr{A}_g},$$

and the characteristic projections $\Pi_g^\pm : W^\pm(\mathscr{A}_g) \to \mathscr{A}_g$ are $C^{\kappa-1}$.

- *There exists a (uniquely defined) symplectic homoclinic annulus*

$$\mathscr{H}_g \subset W^+(\mathscr{A}_g) \cap W^-(\mathscr{A}_g),$$

of the form

$$\mathscr{H}_g = \{(x, h_g(x)) \mid x \in \mathbb{A}\}, \tag{32}$$

where h_g is a C^κ function $\mathbb{A} \to B^2(P_2, \alpha) \subset \mathbb{A}$ such that $\|h_g - P_2\|_{C^\kappa(\mathbb{A})} \to 0$ when $d_\kappa(g, f) \to 0$.

- *The restrictions*

$$\pi_g^\pm := (\Pi_g^\pm)_{|\mathscr{H}_g} : \mathscr{H}_g \to \mathscr{A}_g \tag{33}$$

are $C^{\kappa-1}$ symplectic diffeomorphisms.

- *For each $z \in \mathscr{A}_g$, the unstable manifold $W^-(z)$ intersects $\mathscr{H}_g$ at $(\pi_g^-)^{-1}(z)$ transversely in $\mathbb{A}^2$, with an analogous property for the stable manifold.*

3.2.2. *The bisystem.* We can now introduce our bisystem on $\mathscr{A}_g$, assuming that $g \in B^\kappa(f, \bar{\varepsilon}(f))$. We first consider the restriction

$$\varphi_g : \mathscr{A}_g \circlearrowleft, \quad \varphi_g = g_{|\mathscr{A}_g}, \tag{34}$$

which is a C^κ symplectic diffeomorphism for the induced structure on $\mathscr{A}_g$. As for our second map, we set

$$\psi_g : \mathscr{A}_g \circlearrowleft, \quad \psi_g = \pi_g^+ \circ (\pi_g^-)^{-1}. \tag{35}$$

Therefore ψ_g is a $C^{\kappa-1}$ symplectic map. The next lemma (which is an application of Moser's isotopy argument) enables us to identify φ_g (and ψ_g) with a diffeomorphism of the standard annulus $\mathbb{A}$ in a proper way.

Lemma 8. *If $\bar{\varepsilon}(f)$ is small enough and $g \in B^\kappa(f, \bar{\varepsilon}(f))$, there exists a $C^{\kappa-1}$ symplectic embedding Φ_g of $\mathbb{A}$, equipped with the standard form, into $\mathbb{A}^2$ such that*:

- $\Phi_g(\mathbb{A}) = \mathscr{A}_g$.
- *The diffeomorphism $\widehat{\varphi}_g = \Phi_g^{-1} \circ \varphi_g \circ \Phi_g : \mathbb{A} \circlearrowleft$ has support in $\mathbb{T} \times I$ and tends to f_1 in the $C^{\kappa-1}$ uniform topology when $d_\kappa(g, f) \to 0$.*
- *The diffeomorphism $\widehat{\psi}_g = \Phi_g^{-1} \circ \psi_g \circ \Phi_g : \mathbb{A} \circlearrowleft$ has support in $\mathbb{T} \times I$ and tends to* Id *in the $C^{\kappa-1}$ uniform topology when $d_\kappa(g, f) \to 0$.*

The following corollary is an immediate application of the previous lemma and finitely differentiable KAM theory.

Corollary 9. *There is an $\varepsilon(f) \in]0, \bar{\varepsilon}(f)]$ such that for each diffeomorphism $g \in B^\kappa(f, \varepsilon(f))$ there exists a $C^{\kappa-1}$ symplectic embedding Φ_g of $\mathbb{A}$ into $\mathscr{A}_g$ such that the map $\widehat{\varphi}_g = \Phi^{-1} \circ \varphi_g \circ \Phi$ admits two* (*disjoint*) *essential invariant circles $\Gamma_\bullet$ and $\Gamma^\bullet$ with rotation numbers ρ^0 and ρ^1 respectively* (*see* (C_2)), *such that $\Gamma_\bullet \to \Gamma^0$ and $\Gamma^\bullet \to \Gamma^1$ in the C^0 topology when $d_\kappa(g, f) \to 0$. Moreover, the map $\widehat{\varphi}_g$ uniformly tilts the vertical over the annulus $\boldsymbol{A}_g$ bounded by $\Gamma_\bullet$ and $\Gamma^\bullet$.*

3.2.3. *The perturbative step.* We fix now a diffeomorphism $g \in B^\kappa(f, \varepsilon(f))$, where $\varepsilon(f)$ is defined in Corollary 9, and get rid of the $\hat{}$ in the previous corollary. We want to prove the existence of a perturbed diffeomorphism $\tilde{g} \in B^\kappa(f, \varepsilon(f))$, arbitrarily close to g in the $C^{\kappa-1}$ topology, for which the associated bisystem $(\varphi_{\tilde{g}}, \psi_{\tilde{g}})$ satisfies condition (24). We proceed in two steps: we first perturb g so that φ_g has no rational essential circle, and we then perturb the resulting diffeomorphism again (without perturbing φ_g) to ensure condition (24). We write ε instead of $\varepsilon(f)$ in the following.

1. *First perturbation of g: making φ_g admissible* Let J be a closed interval of $\mathbb{R}$ containing $[0, 1]$ in its interior and contained in the interior of I. Taking into account that $\mathscr{A}_g$ is of class C^κ and invariant under g, by usual perturbation techniques (see [50; 51]), there exists a C^κ diffeomorphism $g^* \in B^\kappa(f,\varepsilon)$, arbitrarily close to g in the uniform C^κ topology, which satisfies:

- The invariant annulus $\mathscr{A}_{g^*}$ coincides with $\mathscr{A}_g$.
- All periodic points of $\varphi_{g^*} = g^*_{|\mathscr{A}_{g^*}}$ in $\mathbb{T}^2 \times J^2$ are either hyperbolic or elliptic with nondegenerate Birkhoff invariant.
- The stable and unstable manifolds of the periodic orbits intersect transversely.

As a consequence, if κ is large enough to ensure the existence of invariant curves surrounding each elliptic point, one easily proves that φ_{g^*} cannot admit an essential invariant circle with rational rotation number in the compact annulus $\boldsymbol{A}_{g^*}$ defined in Corollary 9.

2. *Second perturbation of* g: *making* ψ_g *admissible* In view of the last section, replacing g with g^*, we can assume that g has no invariant circle in $\boldsymbol{A}_g$ with rational rotation number. We want now to perturb g into a new diffeomorphism $\tilde g$ such that

$$\mathscr{A}_{\tilde g} = \mathscr{A}_g, \quad \mathscr{H}_{\tilde g} = \mathscr{H}_g, \quad \varphi_{\tilde g} = \varphi_g, \quad \mathrm{Ess}_{\boldsymbol{A}_g}(\varphi_g) \cap \mathrm{Ess}(\psi_{\tilde g}) = \varnothing. \tag{36}$$

We first analyze the composition of g with a diffeomorphism with support localized in a small enough neighborhood of the annulus $\mathscr{H}_g$.

Lemma 10. *Let* $W_0^\pm$ *be the submanifolds* (*diffeomorphic to* $[0,1] \times \mathbb{A}$) *of* $W^\pm(\mathscr{A}_g)$ *bounded by* $\mathscr{A}_g$ *and* $\mathscr{H}_g$. *Let* $\mathscr{N}$ *be a neighborhood of* $\mathscr{H}_g$ *such that*

$$\mathrm{dist}(\mathscr{A}_g, \mathscr{N}) > 0, \quad g(W_0^+) \cap \mathscr{N} = \varnothing, \quad g^{-1}(W_0^-) \cap \mathscr{N} = \varnothing. \tag{37}$$

Assume that $\boldsymbol{\chi}$ *is a diffeomorphism of* $\mathbb{A}^2$ *with support in* $\mathscr{N}$, *which leaves the annulus* $\mathscr{H}_g$ *invariant, and set* $\tilde g = \boldsymbol{\chi} \circ g$. *Then* $\mathscr{A}_{\tilde g} = \mathscr{A}_g$, $\mathscr{H}_{\tilde g} = \mathscr{H}_g$ *and*

$$\varphi_{\tilde g} = \varphi_g, \quad \psi_{\tilde g} = \psi_g \circ (\pi_g^- \circ \boldsymbol{\chi} \circ (\pi_g^-)^{-1}). \tag{38}$$

See [45] for a proof. We can now use Moeckel's Theorem B in order to produce our perturbation $\tilde g$.

Lemma 11. *There exists a diffeomorphism* $\tilde g \in \mathscr{D}^{\kappa-1}$, *arbitrarily close to* g *in the* $C^{\kappa-1}$ *topology such that* $\mathscr{A}_{\tilde g} = \mathscr{A}_g$, $\varphi_{\tilde g} = \varphi_g$ *and the maps* $\tau_0 = \varphi_g$ *and* $\tau_1 = \psi_{\tilde g}$ *satisfy condition* (24) *of Theorem A.*

Proof. By Theorem B there exists a C^∞ Hamiltonian $h : \mathbb{A} \to \mathbb{R}$ arbitrarily close to 0 such that φ_g and the modified diffeomorphism

$$\Phi^h \circ \psi_g \circ \Phi^{-h} \tag{39}$$

satisfy (24). In view of Lemma 10, (38), let us introduce the perturbed diffeomorphism

$$\psi_{\text{pert}} = \psi_g \circ [\pi_g^- \circ \chi \circ (\pi_g^-)^{-1}] : \mathbb{A} \circlearrowleft, \tag{40}$$

where $\chi : \mathscr{H}_g \circlearrowleft$ is a diffeomorphism we want to determine (and which we then have to continue to a diffeomorphism $\boldsymbol{\chi}$ defined in a neighborhood of $\mathscr{H}_g$). We want to choose χ in order to solve the equation

$$\psi_{\text{pert}} = \Phi^h \circ \psi_g \circ \Phi^{-h}. \tag{41}$$

Straightforward computation yields

$$\chi = (\pi_g^-)^{-1} \circ \psi_g^{-1} \circ \Phi^h \circ \psi_g \circ \Phi^{-h} \circ \pi_g^-. \tag{42}$$

Therefore χ is a $C^{\kappa-1}$ Hamiltonian diffeomorphism of the annulus $\mathscr{H}_g$, with compact support, which tends to Id in the $C^{\kappa-1}$ topology when $d_\kappa(g, f) \to 0$. As a consequence, there is a C^κ function $\xi : \mathbb{R} \times \mathscr{H}_g \to \mathbb{R}$, with support in $]0, 1[\times \mathscr{H}_g$ such that

$$\chi = \Phi^\xi : \mathscr{H}_g \circlearrowleft, \tag{43}$$

where Φ^ξ is the time-one map starting at 0 generated by ξ. Using the Moser isotopy argument, one proves the existence of a $C^{\kappa-1}$ symplectic diffeomorphism

$$T : \mathbb{A} \times B^2(0, \alpha) \to \mathscr{N}, \quad T(\mathbb{A} \times 0\}) = \mathscr{H}_g, \tag{44}$$

where $\mathscr{N}$ is a neighborhood of $\mathscr{H}_g$ in $\mathbb{A}^2$, α is a positive constant and the first factor is endowed with the usual symplectic structure. Fix a C^∞ bump function $\eta : B^2(0, \alpha) \to \mathbb{R}$ equal to 1 in a neighborhood of 0 and define a function $H : \mathbb{R} \times \mathbb{A} \times B^2(0, \alpha) \to \mathbb{R}$ by

$$H(t, x_1, x_2) = \eta(x_2)\xi(t, T(x_1, 0)). \tag{45}$$

Then clearly the time-one map $\boldsymbol{\chi} = T \circ \Phi^H$ leaves $\mathscr{H}_g$ invariant, with $\boldsymbol{\chi}_{|\mathscr{H}_g} = \chi$ and the support of $\boldsymbol{\chi}$ is contained in $\mathscr{N}$. Moreover, $\boldsymbol{\chi}$ tends to the identity in the $C^{\kappa-1}$ topology when h tends to 0 in the C^κ topology. Setting $\tilde{g} = \boldsymbol{\chi} \circ g$ provides us with the perturbed diffeomorphism we were looking for. □

3.2.4. *Conclusion of the proof of Theorem 6.* Fix $f \in \mathscr{F}^\kappa$ and $\delta > 0$. We assume that κ is large enough so that all the conclusions and identifications of the last sections hold. Set

$$\begin{aligned}
U_\bullet &= \{(\theta_1, r_1) \in \mathbb{A} \mid r_1 \in \,]{-\delta/4}, \delta/4[\},\\
U^\bullet &= \{(\theta_1, r_1) \in \mathbb{A} \mid r_1 \in \,]1 - \delta/4, 1 + \delta/4[\},\\
\mathscr{U}_\bullet &= \{(\theta, r) \in \mathbb{A}^2 \mid r_1 \in \,]{-\delta/2}, \delta/2[\},\\
\mathscr{U}^\bullet &= \{(\theta, r) \in \mathbb{A}^2 \mid r_1 \in \,]1 - \delta/2, 1 + \delta/2[\}.
\end{aligned} \tag{46}$$

By Lemma 8 and Corollary 9, one can choose $\varepsilon \in\,]0, \varepsilon(f)[$ small enough so that for any diffeomorphism $g \in B(f, \varepsilon)$, with the notation of Lemma 8, the invariant circles $\Gamma_\bullet$ and $\Gamma^\bullet$ of φ_g satisfy

$$\Gamma_\bullet \subset U_\bullet, \quad \psi(\Gamma_\bullet) \subset U_\bullet, \quad \Gamma^\bullet \subset U^\bullet, \quad \psi(\Gamma^\bullet) \subset U^\bullet, \tag{47}$$

and are such that moreover

$$\Phi_g(U_\bullet \times \{0\}) \subset \mathscr{U}_\bullet, \quad \Phi_g(U^\bullet \times \{0\}) \subset \mathscr{U}^\bullet. \tag{48}$$

We then proved the existence of a $C^{\kappa-1}$ diffeomorphism $\tilde{g} \in B(f, \varepsilon(f))$ arbitrarily close to g in the $C^{\kappa-1}$ topology, such that the bisystem $(\varphi_{\tilde{g}}, \psi_{\tilde{g}})$ associated with $\tilde{g}$ satisfies (24). In particular, $(\varphi_{\tilde{g}}, \psi_{\tilde{g}})$ admits an orbit with first point in $\mathscr{U}_\bullet$ and last point in $\mathscr{U}^\bullet$.

The last step is to apply the normally hyperbolic shadowing lemma (see Theorem 40 in Appendix C) (with $\delta/2$ instead of δ) to the bisystem $(\varphi_{\tilde{g}}, \psi_{\tilde{g}})$. The previous orbit produces an orbit of $\tilde{g}$ with first point in $\mathscr{U}^0$ and last point in $\mathscr{U}^1$ (see Definition 4). This concludes the proof. $\square$

4. The discrete setting for simple resonance annuli

Our objective now is to generalize the previous result to a (still discrete) case which well-adapted to the diffusion properties of the dynamics along simple resonance cylinders. The main difference with the previous model is that we have to replace the globally defined homoclinic map by a correspondence formed by a family of locally defined maps. We therefore have to introduce a local version of the Moeckel noncoincidence condition and prove that it yields the existence of drifting orbits for this type of bisystem: we require that each essential invariant circle of g admits a *splitting arc*, that is, a C^0 arc located below the invariant circle and which is sent into the invariant circle by some locally defined maps of the previous family. The question of the generic existence of such arcs for relevant examples will necessitate specific symplectic ingredients and will be examined in the next section — together with the definition of these examples. This section is extracted from the joint work [21].

4.1. ***Special twist maps and splitting arcs.*** Given $a < b$, we set $\boldsymbol{A} = \mathbb{T} \times [a, b]$ and for each $c \in [a, b]$, we write $\Gamma(c)$ for $\mathbb{T} \times \{c\}$. Given a map $f : \boldsymbol{A} \circlearrowleft$, we denote by $\mathrm{Ess}(f)$ its set of invariant essential circles.

1. We begin with the following definition for twist maps.

Definition 12. Here we say that an area-preserving twist map φ of $\boldsymbol{A}$ is *special* if φ does not admit any essential invariant circle with rational rotation number.[13]

[13] Our definition in [21] is more stringent but we will not need it in the present setting.

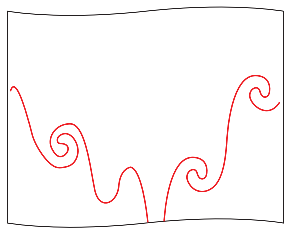


Figure 11. Positively and negatively tilted arcs.

Given an essential circle $\Gamma\subset\mathbb{T}\times]a,b[$, Γ^- (resp. Γ^+) stands for the connected component of $\boldsymbol{A}\setminus\Gamma$ located below Γ (resp. above Γ) in $\boldsymbol{A}$. In the following we will crucially use the following result.

Lemma 13. *Let φ be a special area-preserving twist map φ of $\boldsymbol{A}$. Then any two distinct elements of* $\mathrm{Ess}(\varphi)$ *are disjoint. Moreover, given an invariant essential circle $\Gamma\subset(\boldsymbol{A}\setminus\Gamma(a))$, then either Γ is the upper boundary of a Birkhoff zone of φ, or it is accumulated by a sequence of elements of* $\mathrm{Ess}(\varphi)$ *located in Γ^-.*

See Appendix B for a proof.

2. We now list the necessary definitions and results for arcs. Given $(u,v)\in\mathbb{R}^2$, let $\angle(u,v)$ be the oriented angle of (u,v) in $[0,2\pi[$. Let $f:\boldsymbol{A}\circlearrowleft$ be an area-preserving twist map. Fix a circle $\Gamma\in\mathrm{Ess}(f)$. An *arc based on* Γ is a C^0 function $\gamma:[0,1]\to\boldsymbol{A}$ such that $\gamma(0)\in\Gamma$ and $\gamma(]0,1])\in\Gamma^+$. We usually denote by $\tilde{\gamma}$ the image $\gamma([0,1])$.

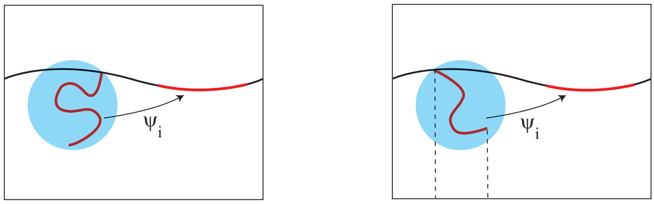
A C^1 arc based on Γ with $\gamma'(s)\neq 0$ for $s\in[0,1]$ is said to be *positively tilted* (resp. *negatively tilted*) when $\angle((0,1),\gamma'(0))\in]0,\pi[$ (resp. $\angle((0,1),\gamma'(0))\in]-\pi,0[$) and when the continuous lift to $\mathbb{R}$ of $s\mapsto\angle((0,1),\gamma'(s))$ is positive (resp. negative) over $[0,1]$.

Definition 14. Let $\varphi:\boldsymbol{A}\circlearrowleft$ be a twist map and let $\psi=(\psi_i)_{i\in I}$ be a correspondence on $\boldsymbol{A}$, where each $\psi_i:\mathrm{Dom}\,\psi_i\to\mathrm{Im}\,\psi_i$ is a local homeomorphism of $\boldsymbol{A}$. Fix $\Gamma\in\mathrm{Ess}(\varphi)$, $\Gamma\subset\boldsymbol{A}\setminus\Gamma(a)$:

- A *splitting arc* based at α for these data is an arc ζ of $\boldsymbol{A}$ whose projection on $\Gamma(a)$ has length $<\frac{1}{2}$, for which

$$\zeta(0)=\alpha,\quad \zeta(]0,1])\subset\Gamma^-;\quad \exists i\in I,\ \zeta(]0,1])\subset\mathrm{Dom}\,\psi_i,\quad \psi_i(\zeta(]0,1]))\subset\Gamma.$$

- A *right splitting arc* based at $\alpha=(\theta,r)$ is a splitting arc ζ based at α, which admits a derivative $\zeta'(0)=(u,v)$ with $u>0$, and such that $\pi(\tilde{\zeta})=[\theta,\theta+\tau]$ with $0<\tau<\frac{1}{2}$.
- A *left splitting arc* based at $\alpha=(\theta,r)$ is a splitting arc ζ based at α, which admits a derivative $\zeta'(0)=(u,v)$ with $u<0$, and such that $\pi(\tilde{\zeta})=[\theta-\tau,\theta]$ with $0<\tau<\frac{1}{2}$.



A splitting arc

A right splitting arc

Figure 12. Splitting arcs.

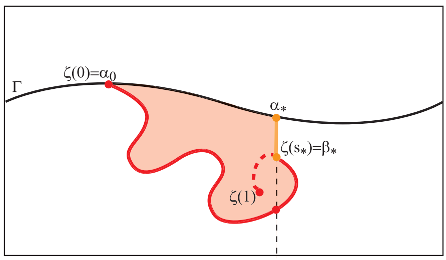


Figure 13. Domain associated to a right splitting arc.

The length $< \frac{1}{2}$ condition on an arc is there just to ensure the existence of a natural order between the projections of points located in the neighborhood of it. We will implicitly use this order in the following. One easy remark is that if ζ is a right (resp. left) splitting arc, then (up to reparametrization) the restriction $\zeta_{|[0,s]}$ with $0 < s \leq 1$ is also a right (resp. left) splitting arc, so that the previous condition is not restrictive.

Given a point $\alpha = (\theta_0, r_0)$ in $\boldsymbol{A}$, we denote by

$$V^-(\alpha) = \{(\theta_0, r) \mid r \in [a, r_0]\}$$

the vertical below α in $\boldsymbol{A}$.

Definition 15. Let $\Gamma \in \mathrm{Ess}(\varphi)$, $\Gamma \subset \boldsymbol{A} \setminus \Gamma(a)$, be the graph of the continuous function $\gamma : \mathbb{T} \to [a, b]$ and $\alpha_0 \in \Gamma$. Let ζ be a right splitting arc based on Γ at $\alpha_0 = \zeta(0)$, let α_* be a point in Γ such that

$$\pi(\alpha_0) < \pi(\alpha_*) < \mathrm{Max}_{s \in [0,1]} \pi(\zeta(s)),$$

and let $\beta_* = \zeta(s_*)$ be the point in $V^-(\alpha_*) \cap \tilde{\zeta}$ with maximal r-coordinate. Let C be the Jordan curve formed by the concatenation of the arcs $\zeta([0, s_*])$, $[\beta_*, \alpha_*]$, and $[\alpha_*, \alpha_0] \subseteq \Gamma$. We denote by $D(\zeta_{|[0,s_*]})$ the connected component of the complement of C contained in Γ^-. We say that $D(\zeta_{|[0,s_*]})$ is a *domain associated with* ζ. We define a domain associated with a left splitting arc similarly.

The first obvious property of the domains defined above is the obvious following remark.

Lemma 16. *For any $x \in D(\zeta)$, the vertical $V^-(x)$ below x intersects $\zeta(]0,1[)$.*

The crucial property is the following.

Lemma 17. *Consider an essential circle $\Gamma \in \mathrm{Ess}(\widehat{\varphi})$ contained in $\boldsymbol{A} \setminus \Gamma(a)$, and a right (resp. left) splitting arc ζ based on Γ. Consider an essential circle $\Gamma_\bullet \subset \boldsymbol{A}$ such that $\tilde{\zeta}$ is contained in the domain $\Gamma_\bullet^+$ above $\Gamma_\bullet$. Let D be a domain associated to ζ. Let η be a negatively (resp. positively) tilted arc with $\eta(0) \in \Gamma_\bullet$, $\eta(]0,1]) \subset \Gamma_\bullet^+ \cap \Gamma^-$, and $\eta(1) \in D$. Then $\eta(]0,1[) \cap \zeta(]0,1]) \neq \varnothing$.*

The proof is an immediate consequence of Lemmas 34 and 38.

4.2. ***Existence of pseudoorbits for bisystems of correspondences.*** We can now state and prove a generalization of Moeckel's theorem to bisystems of correspondences on a two-dimensional annulus, which has to be seen as a Poincaré section of a compact hyperbolic invariant cylinder. We prove the existence of pseudoorbits "drifting from the bottom to the top of the annulus". We do not present here the more complete formalism of [21] which is adapted to the case of pseudoorbits drifting along chains of heteroclinically connected annuli.

1. We first need to make the definition of an orbit of a polysystem more precise. Let A be some set and consider a set $f = \{f_i \mid i \in I\}$ of locally defined maps $f_i : \mathrm{Dom}\, f_i \to A$. We say that a finite sequence $(x_n)_{0 \le n \le n_*-1}$ of points of A is a *finite orbit of f, of length $n_* \ge 1$*, when there exists a sequence $\omega = (i_n)_{0 \le n \le n_*-1} \in I^{n_*}$ such that, for $0 \le n \le n_* - 1$,

$$x_{n+1} = f_{i_n}(x_n),$$

and we write

$$x_{n_*} = f^\omega(x_0).$$

We formally consider the point x_0 as being the 0-length orbit of x_0.

Given a subset $B \subset A$, we set

$$f^\omega(B) = \bigcup_{x \in B_\omega} f^\omega(x)$$

where B_ω is the subset of B formed by the points x such that $f^\omega(x)$ is well-defined.

The *full orbit of $B \subset A$* under f is the subset of A formed by the union of all $f^\omega(B)$ for all sequences (of any length) ω (so that in particular B is contained in its full orbit under f).

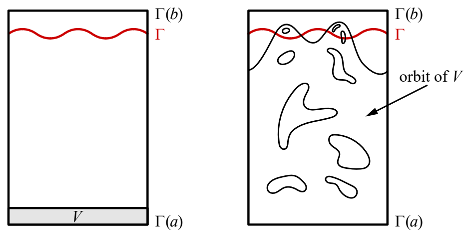


Figure 14. The setting of Theorem 19.

2. To deal with the notions of right and left splitting arcs in a similar way, we will need the following result of symmetrization of a polysystem; see [21] for a proof.

Lemma 18. *Let A be a metric space endowed with a finite Borel measure, positive on the nonempty open subsets of A. Let φ be a measure-preserving homeomorphism of A and let $(\psi_i)_{i\in I}$ be a polysystem on A, where* $\operatorname{Dom}\psi_i$ *is open and the map* $\psi_i : \operatorname{Dom}\psi_i \to \operatorname{Im}\psi_i$ *is a homeomorphism, for all $i \in I$. Fix a nonempty open subset $V \subset A$. Let U_f and U_g be the full orbit of V under the polysystems*

$$f = (\varphi, \psi = (\psi_i)_{i\in I}) \quad \textit{and} \quad g = (\varphi, \varphi^{-1}, \psi = (\psi_i)_{i\in I})$$

respectively. Then U_f is contained and dense in U_g.

3. The main result of this section is the following.

Theorem 19. *Let $\varphi : \boldsymbol{A} \circlearrowleft$ be a special twist map and let $\psi = (\psi_i)_{i\in I}$ be a correspondence on $\boldsymbol{A}$. Assume that for each element $\Gamma \in \operatorname{Ess}(\varphi)$ there is a right or left splitting arc based on Γ. Fix $\Gamma \in \operatorname{Ess}(\varphi) \setminus \{\Gamma(a), \Gamma(b)\}$ together with a neighborhood V of $\Gamma(a)$ in $\boldsymbol{A}$. Then given $\delta > 0$, the full orbit of V under the polysystem $f = (\varphi, \psi = (\psi_i)_{i\in I})$ intersects $\Gamma(b-\delta)^+$.*

Given $\nu > 0$, we define a *ν-ball* of $\mathbb{T} \times \mathbb{R}$ as a subset $B = B_\theta \times B_r$ where B_θ and B_r are intervals of $\mathbb{T}$ and $\mathbb{R}$ respectively, such that

$$\operatorname{length} B_r > \nu \operatorname{length} B_\theta. \tag{49}$$

The *center of B* is (a_θ, a_r), where a_θ, a_r are the mid-points of B_θ and B_r. Given a topological space E and $A \subset B \subset E$ with A connected, $\mathrm{CC}(B, A)$ stands for the connected component of B containing A.

Proof. We assume for example that φ tilts the vertical to the right, the other case being exactly similar:

• We assume without loss of generality that V is open in $\boldsymbol{A}$, and connected. Let U be the full orbit of the open set V under the symmetrized polysystem

$g = (\varphi, \varphi^{-1}, \psi = (\psi_i)_{i\in I})$ on $\boldsymbol{A}$. Note that $\varphi(U) = U$ and $\psi_i(U) \subset U$. Set $U_c = \mathrm{CC}(U, \Gamma(a))$. Then U_c is open and contains V, so $\varphi(U_c) = U_c$. Thanks to Lemma 18, it is enough to prove that U_c intersects $\Gamma(b-\delta)^+$.

Let us assume by contradiction that U_c is contained in $\Gamma(b-\delta)^-$.

• Set $O = \boldsymbol{A} \setminus \overline{U_c}$, so that O is open, contains $\Gamma(b)$, and $O \cap V = \varnothing$. Moreover, since $\varphi(\overline{U_c}) = \overline{U_c}$,

$$\varphi(O) = \boldsymbol{A} \setminus \varphi(\overline{U_c}) = \boldsymbol{A} \setminus \overline{U_c} = O.$$

Then $\varphi(\mathrm{CC}(O, \Gamma(b))) = \mathrm{CC}(O, \Gamma(b))$ and so $\varphi(\overline{\mathrm{CC}(O, \Gamma(b))}) = \overline{\mathrm{CC}(O, \Gamma(b))}$. Let

$$U = \boldsymbol{A} \setminus \overline{\mathrm{CC}(O, \Gamma(b))},$$

so that U is open and $\varphi(U) = U$, and set finally

$$\mathcal{U} = \mathrm{CC}(U, \Gamma(a)), \tag{50}$$

hence $\mathcal{U}$ is open, connected and $\varphi(\mathcal{U}) = \mathcal{U}$. Moreover clearly

$$\bar{\mathcal{U}} \subset \boldsymbol{A} \setminus \mathrm{CC}(O, \Gamma(b)), \tag{51}$$

and

$$U_c \subset \mathcal{U}, \tag{52}$$

since $\overline{O} = \boldsymbol{A} \setminus \mathrm{Int}(\overline{U_c}) \subset \boldsymbol{A} \setminus U_c$, so $\overline{\mathrm{CC}(O, \Gamma(b))} \subset \boldsymbol{A} \setminus U_c$ and $U_c \subset \boldsymbol{A} \setminus \overline{\mathrm{CC}(O, \Gamma(b))} = U$, which proves our claim since $\Gamma(a) \subset U_c$.

• Let us prove that $\Gamma := \mathrm{Fr}\,\mathcal{U}$ is a Lipschitz graph over $\mathbb{T}$, invariant under φ, by the Birkhoff theorem (see Appendix B). By local connectedness of $\boldsymbol{A}$, one readily proves that $\mathrm{Int}\,\bar{\mathcal{U}} = \mathcal{U}$, since $\mathcal{U}$ is a connected component of the complement of the closure of an open set. Moreover $\varphi(\mathcal{U}) = \mathcal{U}$. Let now $\boldsymbol{S}$ be the quotient of $\boldsymbol{A}$ by the identification of each boundary circle to one point, so that $\boldsymbol{S}$ is homeomorphic to S^2. Up to this quotient, $\mathcal{U}$ is a connected component of the complement in $\boldsymbol{S}$ of a compact connected subset, so is homeomorphic to a disk. Going back to the initial space $\boldsymbol{A}$ proves that $\mathcal{U}$ is homeomorphic to $\mathbb{T} \times [0, 1[$. So by the Birkhoff theorem, $\Gamma = \partial\mathcal{U}$ is a Lipschitz graph over $\mathbb{T}$, invariant under φ; see [48] for more details.

• We now prove that $\Gamma \subset \overline{U_c}$, and so $\Gamma \subseteq \mathrm{Fr}(U_c) = \mathrm{cl}(U_c) \setminus U_c$. Assume that $x \in \Gamma$ is not in $\overline{U_c}$, so that there exists a small ball $B(x, \varepsilon)$ with $B(x, \varepsilon) \cap \overline{U}_c = \varnothing$. Let z be some point on the vertical through x, located under Γ and inside $B(x, \varepsilon)$. Let us show that the semivertical σ over z in $\boldsymbol{A}$ is disjoint from $\overline{U_c}$. First $\Gamma \cap \sigma = \{x\}$, since Γ is a graph, so that $\sigma = [z, x] \cup [x, \xi]$, with $\xi \in \Gamma(b)$. Clearly $[z, x] \subset B(x, \varepsilon)$ so $[z, x] \cap \overline{U_c} = \varnothing$, and $]x, \xi] \cap \bar{\mathcal{U}} = \varnothing$ since $\Gamma = \partial\mathcal{U}$ is a graph. Since $U_c \subset \mathcal{U}$, this proves that $\sigma \cap \overline{U}_c = \varnothing$.

As a consequence $\sigma \cup \Gamma(b)$ is a connected set which satisfies $(\sigma \cup \Gamma(b)) \cap \overline{U_c} = \varnothing$. Therefore

$$(\sigma \cup \Gamma(b)) \subset \mathrm{CC}(O, \Gamma(b))$$

and thus $(\sigma \cup \Gamma(b)) \cap \bar{\mathcal{U}} = \varnothing$ by (51). This is a contradiction since $x \in \Gamma \subset \bar{\mathcal{U}}$. Therefore $\Gamma \subset \overline{U_c}$.

- Since Γ is an invariant essential circle for the special twist map φ, there are only two possibilities:
  - Γ is the upper boundary of a Birkhoff zone.
  - Γ is accumulated from below by essential invariant circles in the Hausdorff topology.

We will prove that both possibilities yield a contradiction with the initial assumption that $U_c \cap \Gamma(b) = \varnothing$.

- Assume first that Γ is the upper boundary of a Birkhoff zone $\mathscr{Z}$ and let Γ_* be the lower boundary of $\mathscr{Z}$. Let ν be the Lipschitz constant of Γ_*. Since Γ_* is a graph and U_c is open, connected, contains V and $\overline{U_c} \cap \Gamma \neq \varnothing$, then $U_c \cap \Gamma_* \neq \varnothing$. So there exists a ν-ball $\boldsymbol{B} \subset U_c$ centered on Γ_*.

We assumed that there exists a right or left splitting arc ζ based at some point α of Γ. Let D be its associated domain. By restricting ζ if necessary, one can moreover assume without loss of generality that $D \subset \mathscr{Z}$. We introduce the closed connected set $X = \Gamma \cup \tilde{\zeta}$, where $\tilde{\zeta} = \zeta([0, 1])$, which disconnects the annulus $\boldsymbol{A}$ since it contains Γ.

Assume first that ζ is a right splitting arc. By Proposition 39, there exist $z_0 \in \boldsymbol{B}$ and $n \in \mathbb{N}$ such that $z_n := \varphi^n(z_0) \in D$. Then, by Lemma 17 there exists a *positively* tilted arc based on Γ_* and ending at z_n which does not intersect X.

By Lemma 35 there exists a *negatively* tilted arc γ with image in $\boldsymbol{B}$ based on Γ_* and ending at z_0. Therefore, by Lemma 37, $\gamma_n := f^n \circ \gamma$ is a *negatively* tilted arc based on Γ_* and ending at z_n.

Assume that the image $\widetilde{\gamma}_n$ does not intersect X, then by Lemma 38 the vertical $V^-(z_n)$ does not intersect X, which contradicts Lemma 16. Therefore $\widetilde{\gamma}_n \cap X \neq \varnothing$, thus $\widetilde{\gamma}_n \cap \tilde{\zeta} \neq \varnothing$.

If now ζ is a left splitting arc, we use φ^{-1} instead of φ. This first yields a $z_0 \in \boldsymbol{B}$ such that $z_{-n} := \varphi^{-n}(z_0) \in D$, then a negatively tilted arc based on Γ_* and ending at z_{-n} which does not intersect X, and a positively tilted arc, still denoted by γ_n, based on Γ_* and ending at z_{-n}. As above, this proves that $\widetilde{\gamma}_n \cap \tilde{\zeta} \neq \varnothing$.

As a consequence, $U_c \cap \tilde{\zeta} \neq \varnothing$ since $\widetilde{\gamma}_n \subset U_c$, and therefore there is a small open ball $B \subset U_c$ centered on $\zeta(]0, 1])$ and, by definition, an index $i \in I$ such that $B \subset \mathrm{Dom}\, \psi_i$. Thus $\psi_i(B)$ is an open set which intersects Γ, and therefore also U_c since $\Gamma \subset \overline{U_c}$. This proves that $\psi_i(B) \subset U_c$ by connectedness, so that

U_c contains points strictly above the circle Γ. This is a contradiction with the construction of $\Gamma = \mathrm{Fr}\,\mathcal{U}$ and the inclusion $U_c \subset \mathcal{U}$, which ensures that all points of U_c are located below Γ.

• Assume now that Γ is accumulated from below by an increasing sequence $(\Gamma_m)_{m\geq 1}$ of essential invariant circles for φ. Let ζ be a splitting arc based on Γ. Let S_m be the closed strip limited by Γ_m and Γ_{m+1}. For m large enough, $S_m \cap \tilde{\zeta}$ contains a C^0 curve ℓ which intersects both Γ_m and Γ_{m+1}. Now $\Gamma \subset \overline{U_c}$, so that $U_c \cap S_m$ contains a C^0 curve ℓ' which also intersects both Γ_m and Γ_{m+1}. Therefore, by Lemma 36, there exists an integer n such that $\varphi^n(U_c) \cap \ell \neq \varnothing$, and so by invariance of U_c under φ, $U_c \cap \ell \neq \varnothing$. Since $\ell \subset \tilde{\zeta} \subset \mathrm{Dom}\,\psi_i$ for some $i \in I$, there exists a ball $B \subset U_c$ centered on $\ell \subset \tilde{\zeta}$ and contained in $\mathrm{Dom}\,\psi_i$. This yields the same contradiction as in the previous paragraph. $\square$

Slightly more involved assumptions and arguments show that the full orbit of V intersects each pair of disjoint essential circles located in $\mathbb{T}\times]a,b[$, which enables us in [21] to prove the existence of orbits drifting along chains of heteroclinically connected annuli (and cylinders). We show in the next section how the present result can be implemented in a model of a single s-resonance cylinder.

5. Diffusion orbits along simple resonance cylinders

In this section we introduce an example of *a priori* unstable perturbation of an integrable Hamiltonian on the annulus $\mathbb{A}^3$, which admits a normally hyperbolic 3-dimensional cylinders with coinciding stable and unstable manifolds. To deal with this degenerate situation, symplectic geometry reveals itself to be crucial at two levels.

First, to prove the existence of homoclinic solutions for the essential invariant tori located inside the cylinders. Then, to reduce the problem to a two-dimensional setting and use the result of the previous section, we introduce a Poincaré section (diffeomorphic to $\mathbb{A}$) of the flow in the cylinder and we assume that the unperturbed system induces a twist return map — not necessarily close to any integrable one. The homoclinic intersections then enable us to construct a homoclinic correspondence (a family of locally defined diffeomorphisms) on the annulus, which breaks each essential invariant circle of the twist map (due to the existence of a splitting arc).

The second crucial resort to symplectic geometry is to prove the genericity of the existence of these splitting arcs. Our approach consist proving a general result on the existence of homoclinic intersections, which would be violated if some invariant circle would not admit a splitting arc.

The results of this section give an account of a work joint work in progress with L. Lazzarini, devoted to the complete description of a simple example illustrating the methods of [43].

5.1. ***Setting and main result.*** We write $\theta = (\theta_0, \theta_1, \theta_2)$ and $r = (r_0, r_1, r_2)$ for the angle and action variables in $\mathbb{A}^3$. We set $\hat{\theta} = (\theta_0, \theta_1)$, $\hat{r} = (r_0, r_1)$.

1. Given an integer $\kappa \geq 2$, we denote by $\mathscr{G}^\kappa$ the affine subspace of Hamiltonians on $\mathbb{A}^3$ of the form

$$G(\theta, r) = r_0 + g(\theta_0, \theta_1, \theta_2, r_1, r_2), \quad (\theta, r) \in \mathbb{A}^3, \tag{53}$$

where g is of class C^κ and satisfies

$$\|g\|_\kappa := \sum_{k=0}^{\kappa} \mathrm{Sup}_{x \in \mathbb{A}^3} \|D^k g(x)\| < +\infty. \tag{54}$$

We endow $\mathscr{G}^\kappa$ with the uniform distance induced by the previous norm and we denote by $B^\kappa(G, r)$ the associated open ball centered at $G \in \mathscr{G}^\kappa$, with radius r.

2. We introduce a subset of $\mathscr{G}^\kappa$ formed by the "unperturbed" Hamiltonians of the form

$$\begin{aligned} F(\theta, r) &= F_1(\theta_0, \theta_1, r_0, r_1) + F_2(\theta_2, r_2), \\ F_1(\theta_0, \theta_1, r_0, r_1) &= r_0 + f_1(\theta_0, \theta_1, r_1), \end{aligned} \tag{55}$$

where the Hamiltonians F_i satisfy a set of additional conditions:

• **Conditions on F_1.** The level $F_1^{-1}(0)$ is a cylinder which admits the global coordinates $(\theta_0, \theta_1, r_1)$. To set out our first conditions we focus on the dynamics generated by F_1 on $F_1^{-1}(0)$ only. For each $\theta_0^* \in \mathbb{T}$, the surface

$$\Sigma^{\theta_0^*} = \{\theta_0 = \theta_0^*\} \cap F_1^{-1}(0) \subset \mathbb{A}^2$$

is a global section for the restriction of X_{F_1} to $F_1^{-1}(0)$, since $\dot{\theta}_0 = 1$. Moreover, the standard Liouville form $\boldsymbol{\lambda}$ on $\mathbb{A}^3$ induces on $\Sigma^{\theta_0^*}$ the form $r_1 d\theta_1$, so that (θ_1, r_1) are global exact-symplectic coordinates on $\Sigma^{\theta_0^*}$. We denote by $\varphi^{\theta_0^*}$ the (exact-symplectic) Poincaré map induced on $\Sigma^{\theta_0^*}$ by the flow Φ_{F_1}. In the coordinates chart (θ_1, r_1) we write

$$\varphi^{\theta_0^*}(\theta_1, r_1) = (\Theta_1^{\theta_0^*}(\theta_1, r_1), R_1^{\theta_0^*}(\theta_1, r_1)). \tag{56}$$

The maps $\varphi^{\theta_0^*}$ are clearly pairwise conjugated. We now list the conditions to be satisfied by the Hamiltonians F_1:

(C_1) For each $\theta_0^* \in \mathbb{T}$, the circles $\Gamma(0) = \mathbb{T} \times \{0\}$ and $\Gamma(1) = \mathbb{T} \times \{1\}$ in $\Sigma^{\theta_0^*}$ (relative the coordinates (θ_1, r_1)) are invariant under $\varphi^{\theta_0^*}$, and their rotation numbers ν_0 and ν_1 are Diophantine.[14]

(C_2) There is a constant $\mu > 0$ such that for all $\theta_0^* \in \mathbb{T}$,

$$\frac{\partial \Theta_1^{\theta_0^*}}{\partial r_1}(\theta_1, r_1) \geqslant \mu$$

for all $(\theta_1, r_1) \in \mathbb{T} \times [0, 1]$.

By (C_1), the 2-dimensional tori $T(i) = \mathbb{T}^2 \times \{r_1 = i\} \subset F_1^{-1}(0)$ are invariant, and they bound a compact invariant cylinder $\boldsymbol{C} \subset F_1^{-1}(0)$. Moreover, by (C_2), the map $\varphi^{\theta_0^*}$ induces is a twist map of $\Sigma^{\theta_0^*} \cap \boldsymbol{C} = \mathbb{T} \times [0, 1]$, with twist constant μ independent of θ_0^*.

• **Conditions on F_2.** On the last factor $\mathbb{A}$, endowed with the coordinates (θ_2, r_2), we introduce the following conditions to be satisfied by the Hamiltonians F_2.

(C_3) The vector field X_{F_2} possesses a hyperbolic fixed point O_2, with $F_2(O_2) = 0$.

(C_4) The fixed point O_2 admits a homoclinic orbit $\boldsymbol{\zeta}$ for X_{F_2} and there exists an open interval $I \subset \mathbb{R}$ such that $\boldsymbol{\zeta}$ transversely intersects $\boldsymbol{\sigma} = \left\{\frac{1}{2}\right\} \times I$ at exactly one point, that we denote by P_2. Moreover the map $r_2 \mapsto F_2\left(\frac{1}{2}, r_2\right)$ is a diffeomorphism from I_2 onto its image.

(C_5) Let λ_{O_2} stand for the positive eigenvalue of $T_{O_2} X_{F_2}$. Then there is a $p > 0$ such that

$$\lambda_{O_2} > p[\mathrm{Max}_{\hat{x} \in \mathbb{A}^2} \| T_{\hat{x}} X_{\boldsymbol{F}_1} \|]. \tag{57}$$

In the sequel, we denote by $\mathscr{F}^\kappa(p)$, or $\mathscr{F}^\kappa$ for short, the set of Hamiltonians F of the form (55) *which satisfy conditions* (C_1)–(C_5).[15]

Note in particular that when $\varepsilon = 0$, the Arnold Hamiltonian is in $\mathscr{F}^\omega$, so that our study extends Arnold's one.

3. As in Section 3, it is not difficult to prove that given $F \in \mathscr{F}^\kappa(p)$ with p large enough for the normally hyperbolic persistence to hold and $\kappa \geq \kappa_0$ large enough for the KAM theorem to apply,[16] there is a $\delta_0 \in]0, 1[$ such that no orbit of X_F can intersect both zones $\{r_1 < \delta_0\}$ and $\{r_1 > 1 - \delta_0\}$. This motivates the following definition.

Definition 20. Fix $\delta > 0$. Given a Hamiltonian $G \in \mathscr{G}^\kappa$, we say that a solution $\gamma(t) = (\theta(t), r(t))$ of the system generated by G on $\mathbb{A}^3$ is a δ-*diffusion solution*

[14] These rotation numbers are independent of θ_0^*.

[15] The choice of μ is quite innocuous.

[16] Both values being dependent.

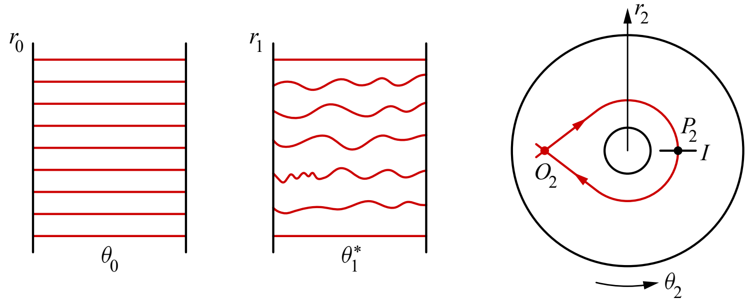


Figure 15. An unperturbed system.

when it is defined on some interval $[0, T]$ and satisfies

$$r_1(0) < \delta, \quad r_1(T) > 1 - \delta. \tag{58}$$

The main result of this section is the following.

Theorem 21. *There exist $p > 0$ and $\kappa_0 \geq p$ such that for $\kappa \geq \kappa_0$ and $F \in \mathscr{F}^\kappa(p)$, then for any $\delta \in]0, 1[$ there is an $\varepsilon > 0$ such that the set of Hamiltonians in the ball $B^\kappa(F, \varepsilon) \subset \mathscr{G}^\kappa$ which admit a δ-diffusion solution is dense for the induced C^κ topology and open for the C^2 topology.*

The existence of δ-diffusion solutions is clearly an open condition in the C^1 topology for Hamiltonians of $\mathscr{G}^\kappa$. So the main task to prove Theorem 21 is to ensure that the conditions introduced in [21], which yield the existence of diffusion solutions and are encoded in the notion of "good cylinders" below (see Theorem 31), are satisfied for a dense subset of $B^\kappa(F, \varepsilon)$ in the C^κ topology.

5.2. ***Geometry and dynamics of the perturbed systems.*** The proof of the following lemma is a simple application of the normally hyperbolic persistence theorem, the normally hyperbolic symplectic theorem of Appendix A and the KAM theorem in the version of Herman [29].

Lemma 22. *Fix $\kappa \geq \kappa_0 \geq p$ (large enough) and $F \in \mathscr{F}^\kappa(p)$. Let $\boldsymbol{R} = \boldsymbol{I}_0 \times \boldsymbol{I}_1$ be a fixed rectangle (with $I_1 \subset \mathrm{Int}\, \boldsymbol{I}_1$) in and fix $\rho > 0$. Then there is an $\varepsilon_0(F) > 0$ such that for any Hamiltonian $G \in B^\kappa(F, \varepsilon_0(F))$ the following properties are satisfied*:

(1) *There exists a normally hyperbolic symplectic invariant annulus for X_G, of the form*

$$\mathcal{A}_G = \{(\theta, r) \in \mathbb{A}^3 \mid (\theta_2, r_2) = a_G(\hat{\theta}, \hat{r})\} \tag{59}$$

where $a_G : \mathbb{A}^2 \to \mathbb{A}$ is a C^4 function whose image is contained in a small ball centered at O_2, which satisfies

$$\|a_G - O_2\|_{C^p(\mathbb{T}^2 \times \boldsymbol{R})} \to 0 \quad \textit{when} \quad \|G - F\|_{C^\kappa(\mathbb{A}^3)} \to 0. \tag{60}$$

Moreover, $\mathcal{A}_G$ admits $(\hat{\theta}, \hat{r}) \in \mathbb{T}^2 \times \mathbb{R}^2$ as global coordinates (nonsymplectic in general).

(2) *The level $G^{-1}(0)$ intersects $\mathcal{A}_G \cap (\mathbb{T}^2 \times \boldsymbol{R})$ transversely in $\mathbb{A}^3$ and*

$$\mathcal{C}_G := \mathcal{A}_G \cap (\mathbb{T}^2 \times \boldsymbol{R}) \cap G^{-1}(0) \tag{61}$$

is a 3-dimensional submanifold of $\mathbb{A}^3$, diffeomorphic to $\mathbb{T}^2 \times \mathbb{R}$, with coordinates $(\theta_0, \theta_1, r_1)$. There is an open interval $I_1 \subset \boldsymbol{I}_1$ containing $[0, 1]$ such that the domain $(\theta_0, \theta_1, r_1) \in \mathbb{T}^2 \times I_1$ is well-defined in $\mathcal{C}_G$.

(3) *For any $\theta_0^* \in \mathbb{T}^2$, the surface*

$$\Sigma_G^{\theta_0^*} = \mathcal{C}_G \cap \{\theta_0 = \theta_0^*\} \tag{62}$$

is a global symplectic section of the Hamiltonian flow Φ_G restricted to $\mathcal{C}_G$, with coordinates (θ_1, r_1) (nonsymplectic in general). The domain $(\theta_1, r_1) \in \mathbb{T} \times I_1$ is well-defined in $\Sigma_G^{\theta_0^*}$, for any $\theta_0^* \in \mathbb{T}$.

(4) *For any θ_0^*, in the coordinates (θ_1, r_1), the Poincaré return map $\varphi_G^{\theta_0^*}$ associated with $\Sigma_G^{\theta_0^*}$ converges to the map $\varphi_F^{\theta_0^*}$ in the compact-open C^p topology when $\|G - F\|_{C^\kappa} \to 0$.*

(5) *For any θ_0^*, the map $\varphi_G^{\theta_0^*}$ leaves invariant two (uniquely defined) essential circles $\Gamma_G^{\theta_0^*}(0)$ and $\Gamma_G^{\theta_0^*}(1)$ in Σ_G, with rotation numbers ν_0 and ν_1 (see (C_1)), which moreover satisfy*

$$\Gamma_G^{\theta_0^*}(0) \subset \{|r_1| < \rho\}, \quad \Gamma_G^{\theta_0^*}(1) \subset \{|1 - r_1| < \rho\}. \tag{63}$$

(6) *For any θ_0^*, let $\boldsymbol{A}_G^{\theta_0^*}$ be the compact annulus bounded by $\Gamma_G^{\theta_0^*}(0)$ and $\Gamma_G^{\theta_0^*}(1)$ inside $\Sigma_G^{\theta_0^*}$. Then the restriction of $\varphi_G^{\theta_0^*}$ to $\boldsymbol{A}_G^{\theta_0^*}$ is a twist map, with twist constant $\geq \mu/2$. We denote by $\mathrm{Ess}(\varphi_G^{\theta_0^*})$ the set of essential invariant circles of this restriction. Each element of $\mathrm{Ess}(\varphi_G^{\theta_0^*})$ is a $2/\mu$-Lipschitz-continuous graph relative to the coordinates (θ_1, r_1).*

(7) *Set $\varphi_G := \varphi_G^0$. For each $\Gamma \in \mathrm{Ess}(\varphi_G)$ we set $T(\Gamma) = \Phi_G(\mathbb{R} \times \Gamma)$, so that $T(\Gamma)$ is a 2-dimensional invariant torus. We set*

$$\mathrm{Tess}(G) = \{T(\Gamma) \mid \Gamma \in \mathrm{Ess}(\varphi_G)\}.$$

(8) *For $x \in \mathcal{A}_G$, let $W^{\pm}(x)$ be the local invariant manifolds attached to x. Let $W^{\pm}(\mathcal{C}_G)$ and $W^{\pm}(\mathcal{A}_G)$ be those attached to $\mathcal{C}_G$ and $\mathcal{A}_G$ (defined as the unions of the previous ones). Then $W^{\pm}(\mathcal{A}_G)$ are coisotropic and their characteristic foliations coincide with their foliations $\{W^{\pm}(x) \mid x \in\}$.*

(9) *For $x \in \mathcal{A}_G$, $W^{\pm}(x)$ intersect transversely $\boldsymbol{\Lambda} = \left\{\theta_2 = \frac{1}{2}\right\}$ in $\mathbb{A}^3$ and for $x \in \mathcal{C}_G$, $W^{\pm}(x)$ intersect transversely $\boldsymbol{\Delta}_G$ in $G^{-1}(0)$. Both intersections are singletons.*

We set

$$\mathcal{A}_G^\pm := W^\pm(\mathcal{A}_G) \cap \mathbf{\Lambda}, \quad \mathcal{C}_G^\pm := W^\pm(\mathcal{C}_G) \cap \mathbf{\Delta}_G,$$

The first intersection is transverse in $\mathbb{A}^3$, *while the second one is transverse in* $G^{-1}(0)$.

(10) *The annuli* $\mathcal{A}_G$ *admits* $(\hat\theta, \hat r)$ *as coordinates, while the cylinders* $\mathcal{C}_G$) *admit* $(\hat\theta, r_1)$ *as coordinates. Due to the particular choice of the section* $\mathbf{\Lambda}$, *the induced Liouville form on* $\mathscr{A}_G^\pm$ *reads*

$$r_0 d\theta_0 + r_1 d\theta_1,$$

so that $(\hat\theta, \hat r)$ *are exact-symplectic coordinates.*[17]

(11) *We denote by* $\Pi_G^\pm : W^\pm(\mathcal{A}_G) \to \mathcal{A}_G$ *the characteristic projections, by* $\pi_G^\pm : \mathcal{A}_G^\pm \to \mathcal{A}_G$ *the restrictions of* $\Pi_G^\pm$ *to* $\mathcal{A}_G^\pm$ *and by* $j_G^\pm := (\pi_G^\pm)^{-1} : \mathcal{A}_G \to \mathcal{A}_G^\pm$. *The maps* $\pi_G^\pm$ *and* $j_G^\pm$ *are exact-symplectic and converge to* $\pi_F^\pm$ *and* $j_F^\pm$ *in the compact-open* C^{p-1} *topology when* $\|G - F\|_\kappa \to 0$. *As a consequence,* $\pi_G^\pm \circ j_G^\pm$ *converge to* Id *in the compact-open* C^{p-1} *topology.*

We denote by $\boldsymbol{C}_G$ the compact cylinder bounded in $\mathcal{C}_G$ by $T(\Gamma_G(0))$ and $T(\Gamma_G(1))$, so that

$$\boldsymbol{C}_G = \Phi_G(\mathbb{R} \times \boldsymbol{A}_G). \tag{64}$$

In the following we will implicitly assume that κ_0 and p are large enough for the previous conclusions to hold true.

5.3. *Homoclinic intersections.* This section is devoted to the existence of homoclinic intersections for tori in $\mathrm{Tess}(G)$, where G is a small enough perturbation of an element of $\mathscr{F}^\kappa$.

Proposition 23. *Fix* $F \in \mathscr{F}^\kappa$, $\kappa \geq \kappa_0$. *Then there is a positive* $\varepsilon_1(F) < \varepsilon_0(F)$ (*where* $\varepsilon_0(F)$ *was defined in Lemma 22*) *such that for any* $G \in B^\kappa(F, \varepsilon_1(F))$, *and for any torus* $T \in \mathrm{Tess}(G)$

$$\#(W^-(T) \cap W^+(T) \cap \mathbf{\Delta}_G) \geq 3.$$

Under specific convexity assumptions on G, this could easily be deduced from Fathi's weak KAM theory, but we deal here with more general Hamiltonians and we want a purely symplectic proof based on Lagrangian intersection arguments. The main difficulty here is that the tori of $\mathrm{Tess}(G)$ are not smooth, so that we need to generalize the standard notion of Lagrangian manifold. There are several ways for doing this, see [1], here we adopt Herman's one since our tori are Lipschitz-continuous graphs. The Lagrangian character of such a graph amounts to saying that the induced Liouville form is closed in the sense of distributions.

[17] This property will be crucial in the following.

We will take advantage of the Lipschitzian character of the tori of at each step, and since the proof is not completely standard, we will give all details for the sake of completeness.

Here we only give a sketch of proof in the regular case. Assume that T is smooth (at least C^2) and, with the notation of Lemma 22, set

$$T^{\pm} := j_G^{\pm}(T) \subset \mathcal{A}_G^{\pm} \cap \mathbf{\Delta}_G.$$

• We identify $\mathbf{\Delta}_G$ with $\mathbb{A}^2$ by using the global symplectic chart $(\widehat{\theta}, \widehat{r}) \in \mathbb{A}^2$ of $\mathbf{\Delta}_G$. A simple application of the usual implicit function theorem proves that for G close enough to F in $\mathscr{G}^\kappa$, the tori $T^{\pm}$ are graphs over the base $\mathbb{T}^2$.

• The torus T is clearly Lagrangian in $\mathcal{A}_G$ (transport of an isotropic curve by the Hamiltonian flow) and, since the maps $j_G^{\pm}$ are exact-symplectic for the induced structures on $\mathcal{A}_G$ and $\mathcal{A}_G^{\pm}$, the tori $T^{\pm}$ are Lagrangian in $\mathcal{A}_G^{\pm}$. They are therefore isotropic and contained in $\mathbf{\Delta}_G$, so $T^{\pm}$ are Lagrangian in $\mathbf{\Delta}_G$. As a consequence,

$$T^{\pm} = \alpha^{\pm}(\mathbb{T}^2),$$

where $\alpha^{\pm} : \mathbb{T}^2 \to \mathbb{A}^2$ are closed 1-form on $\mathbb{T}^2$.

• By compactness, $T^+ \cap T^-$ is nonempty if the form $\alpha = \alpha^+ - \alpha^-$ is exact. Thus all we need is to check that the class $[\alpha] \in H^1(\mathbb{T}^2, \mathbb{Z})$ vanishes on $H_1(\mathbb{T}^2, \mathbb{Z})$. This can be done by comparing the integrals of $\alpha^{\pm}$ along two closed curves c_1 and c_2 in $\mathbb{T}^2$ generating $H_1(\mathbb{T}^2, \mathbb{Z})$. But since the induced Liouville form $\iota^*\boldsymbol{\lambda}$ satisfies $(\alpha^{\pm})^*(\iota^*\boldsymbol{\lambda}) = \alpha^{\pm}$, where ι is the inclusion $\mathbf{\Delta}_G \subset \mathbb{A}^3$, we may equivalently compare the integrals of the ambient Liouville form $\boldsymbol{\lambda}$ along $c_i^{\pm} = (\iota \circ \alpha^{\pm})(c_i)$, for $i = 1, 2$.

• The key observation is that the cycles $c_i^{\pm}$ belong to $\mathcal{A}_G^{\pm}$, and these two annuli are exchanged by the exact symplectic map $j_G^+ \circ (j_G^-)^{-1}$. This yields the equalities:

$$\int_{c_i^-} \boldsymbol{\lambda} = \int_{(j_G^+ \circ (j_G^-)^{-1})(c_i^-)} \boldsymbol{\lambda} = \int_{c_i^+} \boldsymbol{\lambda},$$

where the first one comes from the exactness of $j_G^+ \circ (j_G^-)^{-1}$ and the second one from the fact that j_G^+ and $(j_G^-)^{-1}$ are close to the identity relative to the charts $(\widehat{\theta}, \widehat{r})$ in their respective domains, so that $(j_G^+ \circ (j_G^-)^{-1})(c_i^-)$ is homotopic to c_i^+ in T^+.

• As a consequence $[\alpha]$ vanishes on $H_1(\mathbb{T}^2, \mathbb{Z})$ and α is exact. This ends the sketch of proof in the regular case.

5.4. ***Generic properties of $\boldsymbol{C}_G$ and $\boldsymbol{W}^{\pm}(\boldsymbol{C}_G)$.*** **1.** The following statement is the continuous version of the one in Section 3.2.3. It is now based of the global flow-box theorem (Appendix D), together with the methods introduced by Robinson in [50; 51]; see also [29].

Proposition 24. *For $\kappa \geq \kappa_0$, the subset of all Hamiltonians G in $B^\kappa(F, \varepsilon_1(F))$ such that no circle in* $\mathrm{Ess}(\varphi_G)$ *has rational rotation number is a residual subset of $B^\kappa(F, \varepsilon_1(F))$.*

2. The following result is also an application of the global flow-box theorem, it is also a continuous version of the perturbative result used in the discrete setting. Given $G \in B^\kappa(F, \varepsilon_1(F))$, we examine the perturbations of the asymptotic manifolds of $\boldsymbol{C}_G$ and their characteristic foliations that come from the perturbation of G.

Proposition 25. *Fix $G \in B^\kappa(F, \varepsilon_1(F))$. Then there exists a compact neighborhood K of $\boldsymbol{C}_G^- \cup \boldsymbol{C}_G^+$ in $\boldsymbol{\Delta}_G$, which satisfies*

$$\Phi_G([-2, 2] \times K) \cap \boldsymbol{C}_G = \varnothing, \tag{65}$$

such that for any pair of C^∞ Hamiltonian diffeomorphisms $\phi^- : \boldsymbol{\Delta}_G \circlearrowleft$ and $\phi^+ : \boldsymbol{\Delta}_G \circlearrowleft$ with support in $\mathrm{Int}\, K$, *there exists a C^κ Hamiltonian $\widetilde{G} \in B^\kappa(F, \varepsilon_1(F))$ which coincides with G outside a compact subset of $\Phi_G(]-1, 0[\times K) \cup \Phi_G(]0, 1[\times K)$, so that $\boldsymbol{C}_{\widetilde{G}} = \boldsymbol{C}_G$, which satisfies*

$$\begin{aligned} \phi^-(\boldsymbol{C}_G^-) &= \boldsymbol{C}_{\widetilde{G}}^-, \quad j_{\widetilde{G}}^- = \phi^- \circ j_G^-, \\ \phi^+(\boldsymbol{C}_G^+) &= \boldsymbol{C}_{\widetilde{G}}^+, \quad j_{\widetilde{G}}^+ = \phi^+ \circ j_G^+. \end{aligned} \tag{66}$$

Moreover one can choose $\widetilde{G}$ so that $\|\widetilde{G} - G\|_\kappa \to 0$ when $\phi^\pm$ are generated by Hamiltonians which tend to 0 *in the C^∞ topology.*

3. Our first application of the previous result ensures the generic transversality of the intersection $\mathcal{C}_G^+ \cap \mathcal{C}_G^-$, it is based only on standard transversality arguments.

Proposition 26. *The set $\mathscr{G}_0$ of hamiltonians $G \in B^\kappa(F, \varepsilon_1(F))$ such that the intersection $\mathcal{C}_G^+ \cap \mathcal{C}_G^-$ is transverse in $\boldsymbol{\Delta}_G$ in the neighborhood of $\boldsymbol{C}_G^+ \cap \boldsymbol{C}_G^-$ is open and dense in $B^\kappa(F, \varepsilon_1(F))$.*

The existence of homoclinic intersections hence immediately yields the following.

Corollary 27. *There is a neighborhood $\mathscr{O}$ of $\boldsymbol{C}_G^- \cap \boldsymbol{C}_G^+$ in $\boldsymbol{\Delta}_G$ such that $\mathscr{I}_G \cap \mathscr{O}$ is a* 2*-dimensional submanifold of $\boldsymbol{\Delta}_G$.*

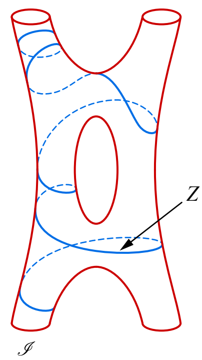


Figure 16. Intersection and singular curve.

5.5. ***Reduction to the 2-dimensional setting.*** The last corollary gives us now the possibility to recover the two-dimensional discrete setting introduced in Section 4.

1. The submanifold $\mathscr{I}_G$ is an interesting example of intersection of two transverse coisotropic submanifolds of a symplectic manifold. We were unable to find a systematic study of the generic singularities of such intersections, so let us quote here one remarkable genericity property. We first introduce the vector fields along $\mathcal{C}_G^\pm$ defined by

$$X_G^\pm = X_G - (j_G^\pm)_\star X_G \tag{67}$$

One easily proves that they are tangent to the leaves of the characteristic foliations of $W^\pm(\mathcal{C}_G)$.

We introduce the following sets:

- $Z_G = \{x \in \mathscr{I}_G \mid T_x W^-(\mathcal{C}_G) \cap T_x W^+(\mathcal{C}_G) \text{ is Lagrangian}\}$.
- $Z_G^+ = \{x \in \mathscr{I}_G \mid X_G^+(x) \in T_x W^-(\mathcal{C}_G)\}$.
- $Z_G^- = \{x \in \mathscr{I}_G \mid X_G^-(x) \in T_x W^+(\mathcal{C}_G)\}$.

Note that Z_G is precisely the complement of the symplectic locus inside $\mathscr{I}_G$. The striking fact is the following remark.

Lemma 28. *The sets $Z_G^\pm$ and Z_G coincide, and the set $\mathscr{G}_1$ of Hamiltonians $G \in \mathscr{G}_0$ such that Z_G is a 1-dimensional submanifold of $\mathscr{I}_G$ in the neighborhood of $\mathbf{C}_G^- \cap \mathbf{C}_G^+$ is open and dense in $B^\kappa(F, \varepsilon_1(F))$.*

The points of the singular locus Z_G are precisely those where the characteristic projections $\Pi_G^\pm$ restricted to the intersection $W^+(\mathcal{C}_G) \cap W^-(\mathcal{C}_G)$ are not local diffeomorphisms (by definitions of $Z_G^\pm$). These points necessitate special care in our construction, and we will forget about them in the following.

2. Recall that

$$\Sigma_G = \mathcal{C}_G \cap \{\theta_0 = 0\}$$

is a two dimensional annulus, which contains two disjoint invariant circles $\Gamma_0(G)$ and $\Gamma_1(G)$ bounding a compact invariant annulus $\boldsymbol{A}_G$. We therefore have a first global return (twist) map φ_G at our disposal and we need to construct a homoclinic correspondence to get the bisystem of Section 4. This correspondence would ideally be obtained by transport of small pieces of the intersection $\mathscr{I}_G$ on $\mathscr{C}_G$ by the characteristic projections, and then on Σ_G by the Hamiltonian flow inside $\mathcal{C}_G$, which is not possible in the neighborhood of points of Z_G. Let us introduce the subset

$$\Xi \subset \mathscr{I}$$

of all homoclinic points corresponding to the essential invariant tori contained in $\boldsymbol{C}_G$, and, for simplicity, assume that

$$\Xi \cap Z_G = \varnothing.$$

By compactness, one can find a cover $(D_\alpha)_{\alpha\in A}$ of Ξ by small discs contained in $\mathscr{I} \setminus Z_G$, such that moreover, setting $D^\pm = \pi^\pm(D) \subset \boldsymbol{C}_G$:

- There are C^1 functions $\boldsymbol{\tau}^\pm : D^\pm \to \mathbb{R}$ such that $\Phi_G^{\boldsymbol{\tau}^\pm}(D^\pm) \subset \Sigma_G$ and $\Phi_G^{\boldsymbol{\tau}^\pm}$ are C^1 diffeomorphisms onto their images.

Definition 29 (homoclinic diffeomorphisms and correspondences). Given a small disc D satisfying the previous constraint, we define the *homoclinic diffeomorphism* ψ_D attached to D by

$$\begin{aligned} \psi_D : \operatorname{Dom}\psi_D &\to \operatorname{Im}\psi_D \\ x &\mapsto \Phi_G^{\boldsymbol{\tau}^+} \circ \Pi^- \circ (\Pi^+_{|D})^{-1} \circ (\Phi_G^{\boldsymbol{\tau}^-})^{-1}(x). \end{aligned} \tag{68}$$

where

$$\operatorname{Dom}\psi_D := \Phi_G^{\boldsymbol{\tau}^-}(D^-) \subset \Sigma_G, \quad \operatorname{Im}\psi_D := \Phi_G^{\boldsymbol{\tau}^-}(D^+) \subset \Sigma_G.$$

We define a *homoclinic correspondence* for Σ_G as a family of homoclinic diffeomorphisms $\psi = (\psi_\alpha := \psi_{D_\alpha})_{\alpha\in A}$ attached to a cover $(D_\alpha)_{\alpha\in A}$ of Ξ by small discs in $\mathscr{I} \setminus Z_G$.

Note that we do not require the supports of the homoclinic diffeomorphisms in a homoclinic correspondence to be pairwise disjoint. Given a homoclinic correspondence $\psi = (\psi_\alpha)_{\alpha\in A}$, we define the associated set $\mathscr{X}^-$ of (negative) transported homoclinic points as

$$\mathscr{X}^- = \bigcup_{\alpha\in A} \psi_\alpha(\Xi \cap D_\alpha).$$

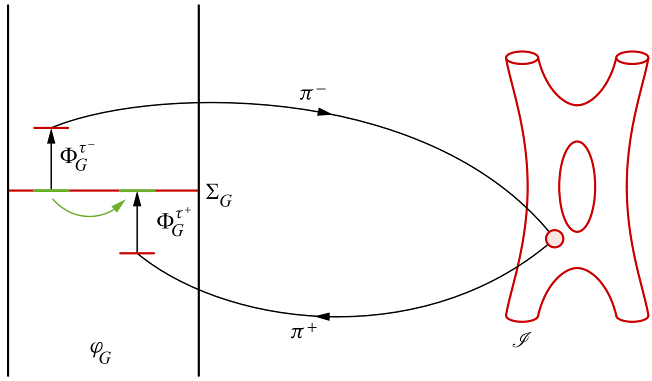


Figure 17. A homoclinic diffeomorphism.

3. *Good cylinders.* We now come to our main definition and result; see [21].

Definition 30. We say that the compact invariant cylinder $\boldsymbol{C}_G$ defined in (64) is a *good cylinder* when the return map φ_G attached to the section $\boldsymbol{A}_G$ is a simple twist map, and when there exists a homoclinic correspondence $\psi_G = (\psi_\alpha)_{\alpha\in A}$ of $\mathcal{C}_G$ such that for any $\Gamma \in \mathrm{Ess}(\varphi_G)$ there exists a (right or left) splitting arc based on Γ for the correspondence ψ_G.

Theorem 31. *Fix $F \in \mathscr{F}^\kappa$, $\kappa \geq \kappa_0$. Then there is an $\boldsymbol{\epsilon}(F) \in]0, \varepsilon_1(F)]$ such that the set of Hamiltonians G in the ball $B^\kappa(F, \boldsymbol{\epsilon}(F))$ for which $\boldsymbol{C}_G$ is a good cylinder is dense in $B^\kappa(F, \varepsilon)$.*

The results of Section 4 (Theorem 19) immediately enables us to deduce Theorem 21 from Theorem 31.

4. *Idea of the proof of Theorem 31.* The genericity results of Section 5.4 are taken for granted. It therefore remains to show the following proposition, where, given $G, \widetilde{G}$ in $\mathscr{G}^\kappa$, we say that $\widetilde{G}$ is G-admissible when $\widetilde{G}$ coincides with G outside a neighborhood of $\mathscr{A}_G$.

Proposition 32. *Fix $F \in \mathscr{F}^\kappa$ with $\kappa \geq \kappa_0$ and $G \in \mathscr{G}_1(F)$. Then for any $\alpha > 0$, there exists an admissible Hamiltonian $\widetilde{G} \in \mathscr{G}_1(F)$ with*

$$\|\widetilde{G} - G\|_\kappa < \alpha \tag{69}$$

such that $\boldsymbol{C}_{\widetilde{G}} = \boldsymbol{C}_G$ is a good cylinder for $\widetilde{G}$.

We require the admissibility condition to ensure that the inner map $\varphi_{\widetilde{G}}$ and φ_G coincide, and therefore admit the same set of essential invariant circles. To prove Proposition 32, we have to find an arbitrarily small perturbation $\widetilde{G}$ of G such that each invariant circle of $\mathrm{Ess}(\varphi_G)$ admits a (right or left) splitting arc.

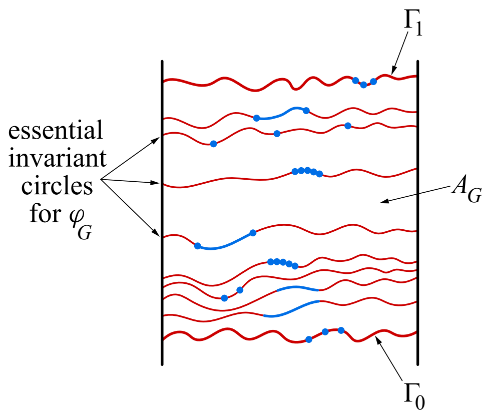


Figure 18. Essential circles and homoclinic points for φ_G.

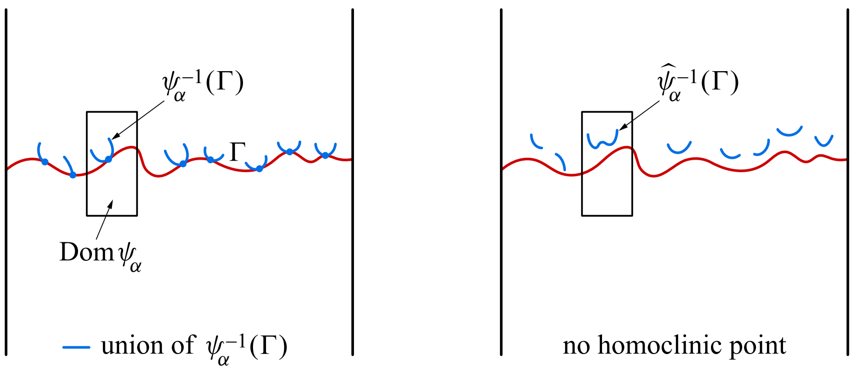


Figure 19. Disjunction of the arcs.

The idea is essentially symplectic and is based on the existence of (transported) homoclinic points on each invariant circle of $\varphi_{\widehat{G}}$ for each $\widehat{G}$ in $\mathscr{G}_1(F)$ (by construction and Proposition 23).

We argue by contradiction. The main ingredient is the possibility to construct an arbitrarily small and admissible perturbation $\widehat{G} \in \mathscr{G}_1(F)$ of G whose set of transported homoclinic points is *totally disconnected.*[18] We then prove that if $\varphi_{\widehat{G}}$ admits an invariant circle Γ with no splitting arc, then it is possible to perturb $\widehat{G}$ another time — still inside $\mathscr{G}_1(F)$ — to ensure that the new homoclinic correspondence satisfies

$$\psi_\alpha^{-1}(\Gamma) \cap \Gamma = \varnothing, \quad \forall \alpha \in A.$$

[18]This is done by local arguments of Minkowski dimension and a convergent sequence of Hamiltonian perturbations of the homoclinic correspondence, of the same type as Moeckel's ones.

Consequently the circle Γ do not posses (transported) homoclinic points, which contradicts Proposition 23. The disconnectedness of the set of homoclinic points is used to produce local perturbations of the homoclinic correspondence by composition with local Hamiltonian diffeomorphisms which increase the action r in a very small neighborhood of each homoclinic point, and decrease the action where the arcs a far from the circle Γ. The proof will full details will appear in the joint work with L. Lazzarini.

6. Broadening the scope

The previous presentation has to be seen as a first introduction to the geometric approach to Arnold diffusion, whose methods, results and scope can be improved on by using recent developments in symplectic topology, two-dimensional dynamics and control theory. We briefly discuss the first two points in this section.

6.1. ***Symplectic topology.*** We refer to [2] for a survey of the origins of the questions in symplectic topology and to Gromov's seminal paper [26], and Laudenbach and Sikorav [38] for seminal results in Lagrangian intersection problems. Here we will a similar result, in its most basic form proved by Lalonde and Sikorav [37].

One main difficulty in the application of the methods presented in Section 5 to the *a priori* stable case comes from the essentially singular perturbations involved in this setting. The absence of hyperbolicity in the unperturbed system makes the embedding of the cylinders very delicate, in the sense that they are graphs of function whose C^1 norm tends to infinity when the size of the perturbation tends to 0. This makes in turn very difficult the detection of the graph properties of the essential circles contained in these cylinders.[19] This difficulty can be overcome by a very careful analysis of the location of these objects (as in [33]) or by cutting the cylinders into smaller and smaller pieces (as in [44]). However a way to get rid of the graph constraint in the proof of existence of Lagrangian intersection would be much more satisfactory, and this is precisely the content of another famous Arnold conjecture — which could perhaps have been inspired by the present problem.

Let us recall one first result in the direction of the Arnold intersection conjecture. Let M and L be compact manifolds of the same dimension. Endow T^*M with its usual Liouville form $\boldsymbol{\lambda}$ and set $\boldsymbol{\Omega} = d\boldsymbol{\lambda}$. Recall that an embedding $j : L \to T^*M$ is said to be exact when $j^*\lambda$ is an exact form. An embedded submanifold of T^*M is said to be exact when it is the image of an exact embedding.

[19] As is the also case for the usual invariant objects from weak KAM theory.

Theorem [37]. *Let L and L' be two exact submanifolds of $T^*\mathbb{T}^n$. Then $L \cap L'$ is nonempty.*

This enables us to some extent to relax the graph assumption for the essential circles in the previous section. Indeed, given an essential smooth torus T contained in the hyperbolic cylinder $\boldsymbol{C}_G$, without any torsion assumption on return map, one can introduce a Weinstein tubular neighborhood $N \sim T^*(j^-(T))$ of the image $j_G^-(T) \subset \boldsymbol{\Delta}_G$. Then, since $j_{\widetilde{G}}^{\pm}$ are exact-symplectic for the induced Liouville form on $\mathscr{A}_{\widetilde{G}}^{\pm}$, one can prove that $j^+(T)$ is an exact submanifolds of N (for the usual exact structure), hence the previous theorem proves that the intersection $j^-(T) \cap j^+(T)$ is nonempty (where $j^-(T)$ is identified with the zero section of N).

To conclude in the case of Lipschitz tori, it suffices to prove the existence of two sequences $(T_n^{\pm})_{n\in\mathbb{N}}$ of tori of Δ with $T_n^+ \cap T_n^- \neq \varnothing$ which converge to $j_{\widetilde{G}}^{\pm}(T)$ in the C^0 topology. To see this, one can first perform a smoothing of the initial torus $T = \Phi_{\widetilde{G}}(\mathbb{R} \times \Gamma)$ by symplectic plumbing of the transport of a smoothed invariant circle Γ, and then to perform a smoothing of $j_{\widetilde{G}}^{\pm}$ by means of their generating Hamiltonians. We expect this strong result to enable us to give simpler proofs of the existence of homoclinic orbits in the *a priori* stable case, as well as to deal with a larger set of perturbations of the completely integrable Hamiltonian h.

6.2. ***Two-dimensional dynamics without convexity.*** One can also expect new results for diffusion without the convexity assumption on h, using the generic transitivity result of [35; 36]. Let us give an example which mimics the *a priori* chaotic setting of Section 3, *without any twist condition*. Let $\mathscr{D}^\kappa$ be the group of C^κ symplectic diffeomorphisms of the product $S = S_1 \times S_2$, where (S_i, ω_i) are compact symplectic smooth surfaces, equipped with the symplectic form $\omega = \omega_1 \oplus \omega_2$. Let $\mathscr{F}^\kappa \subset \mathscr{D}^\kappa$ be the subset formed by the product diffeomorphisms of the form

$$f(x_1, x_2) = (f_1(x_1), f_2(x_2)), \quad x_i \in S_i, \tag{70}$$

satisfying the following conditions:

(C1) Both f_1, f_2 are symplectic.

(C2) f_2 admits a hyperbolic fixed point O_2.

(C3) The Lyapunov exponents of f_2 at O_2 dominate the Lyapunov exponents of f_1 on S_1.

(C4) f_2 has a transverse homoclinic point P_2 for O_2 in S_2.

Then the following result (from a current joint work with M. Gidea) holds true: there is a κ_0 such that for $\kappa \geq \kappa_0$, for every $f \in \mathscr{F}^\kappa$ there exists an $\varepsilon_0 > 0$

(depending on f) such that for every diffeomorphism g in a residual subset $R^\kappa(f, \varepsilon_0)$ of the ball $B^\kappa(f, \varepsilon_0)$, there exists an orbit $(x_1^n, x_2^n)_{n\in\mathbb{N}}$ of g such that the projected sequence $(x_1^n)_{n\in\mathbb{N}}$ is dense in S_1.

An extension to this result to the discrete setting for *a priori* unstable systems as in section IV is a very challenging question which has deep consequences for diffusion for perturbations of nonconvex completely integrable Hamiltonians.

Appendix A. Normal hyperbolicity and symplectic geometry

We refer to [4; 9; 31] for general definitions an results on normal hyperbolicity. Here we limit ourselves to a very simple class of systems which admit a normally hyperbolic invariant (noncompact) submanifold, which serves us as a model from which all other definitions and properties will be deduced.

1. The following statement is a simple version of the persistence theorem for normally hyperbolic manifolds well-adapted to our setting, whose germ can be found in [6]. We limit ourselves to the case of 1-dimensional stable and unstable directions, which is the only one we have to deal with in this paper. We fix an integer $m \geq 1$ and endow $\mathbb{R}^{m+2}$ with the coordinates (x, u, s), with $x \in \mathbb{R}^m$, $(u, s) \in \mathbb{R}^2$.

Theorem (the normally hyperbolic persistence theorem). *Fix $m \geq 1$ and consider a vector field of class C^1 V_0 on $\mathbb{R}^{m+2}$ of the form*

$$V_0(x, u, s) = (X(x, u, s), \lambda_u(x)u, -\lambda_s(x)s), \quad (x, u, s) \in \mathbb{R}^{m+2}. \tag{71}$$

Assume moreover that there exists $\lambda > 0$ such that for $x \in \mathbb{R}^m$:

$$\lambda_u(x) \geq \lambda, \quad \lambda_s(x) \geq \lambda. \tag{72}$$

Fix a constant $R > 0$ and set $O_R = \{(x, u, s) \in \mathbb{R}^{m+2} \mid \|(u, s)\| < R\}$ and assume that

$$\|\partial_x X\|_{C^0(O_R)} < \lambda. \tag{73}$$

Then there exist constants $\delta_* > 0$, $c_* > 0$, $C > 0$, such that if V_r is a C^1 vector field on $\mathbb{R}^{m+2}$ such that

$$\|V_r\|_{C^1(\mathbb{R}^{m+2})} \leq \delta_*, \tag{74}$$

setting $V = V_0 + V_r$, the following assertions hold:

• *The maximal invariant set for V contained in O_R is an m-dimensional manifold $\mathcal{A}(V)$ which admits the graph representation*:

$$\mathcal{A}(V) = \{(x, u = U(x), s = S(x)) \mid x \in \mathbb{R}^m\},$$

where U and S are C^1 maps $\mathbb{R}^m \to \mathbb{R}$ such that

$$\|(U, S)\|_{C^0(\mathbb{R}^m)} \le c_* \|V_r\|_{C^0}. \tag{75}$$

• *The maximal positively invariant set for V contained in O_R is an $(m+1)$-dimensional manifold $W^+(\mathcal{A}(V))$ which admits the graph representation*:

$$W^+(\mathcal{A}(V)) = \{(x, u = U^+(x, s), s) \mid x \in \mathbb{R}^m, s \in \,]-R, R[\},$$

where $U^+ : \mathbb{R}^m \times \,]-R, R[\,\to \mathbb{R}$ is a C^1 map such that

$$\|U^+\|_{C^0(\mathbb{R}^m)} \le c_* \|V_r\|_{C^0}. \tag{76}$$

• *The maximal negatively invariant set for V contained in O_R is an $(m+1)$-dimensional manifold $W^-(\mathcal{A}(V))$ which admits the graph representation*:

$$W^-(\mathcal{A}(V)) = \{(x, u, s = S^-(x, u)) \mid x \in \mathbb{R}^m, u \in \,]-R, R[\},$$

where $S^- : \mathbb{R}^m \times \,]-R, R[\,\to \mathbb{R}$ is a C^1 map such that

$$\|S^-\|_{C^0(\mathbb{R}^m)} \le c_* \|V_r\|_{C^0}. \tag{77}$$

• *The manifolds $W^\pm(\mathcal{A}(V))$ admit C^0 foliations $(W^\pm(x))_{x \in \mathcal{A}(V)}$ such that for $w \in W^\pm(x)$*

$$\mathrm{dist}(\Phi^t(w), \Phi^t(x)) \le C \exp(\pm\lambda t), \quad t \ge 0. \tag{78}$$

• *If moreover V_0 and V_r are assumed to be of class C^p, $p \ge 1$, and if*

$$p\|\partial_x X\|_{C^0(O_R)} < \lambda \tag{79}$$

then the functions U, S, U^+, S^- are of class C^p and there is a constant C_p, depending only on V_0, such that U, S U^+, S^+ tend to 0 in the C^p compact-open topology when V_r tends to 0 in the C^p topology.

• *Assume moreover that the vector fields V_0, V_r are $\boldsymbol{L}$-periodic in x, where $\boldsymbol{L}$ is a lattice in $\mathbb{R}^m$. Then their flows and the manifolds $\mathcal{A}(V)$ and $W^\pm(\mathcal{A}(V))$ pass to the quotient $(\mathbb{R}^m/\boldsymbol{L}) \times \mathbb{R}^2$*

The last statement will be applied in the case where $m = 2\ell$ and $\boldsymbol{L} = \mathbb{Z}^\ell \times \{0\}$, so that the quotient $\mathcal{A}(V)$ is diffeomorphic to the annulus $\mathbb{A}^\ell$.

2. The following result describes the symplectic geometry of our system in the case where V is a Hamiltonian vector field. We keep the notation of the previous theorem.

Theorem (the symplectic normally hyperbolic theorem). *Endow $\mathbb{R}^{2m+2}$ with a symplectic form Ω such that there exists a constant $C > 0$ such that for all $z \in O_R$*

$$|\Omega(v, w)| \le C\|v\|\|w\|, \quad \forall v, w \in T_z M. \tag{80}$$

Let H_0 be a C^2 Hamiltonian on $\mathbb{R}^{2m+2}$ whose Hamiltonian vector field V_0 satisfies (71) *and* (72), *and consider a Hamiltonian $H = H_0 + P$. Then if the vector field V generated by H satisfies* (73) *and* (74) *the following properties hold*:

- *The manifold $\mathcal{A}(V)$ is Ω-symplectic.*
- *The manifolds $W^{\pm}(\mathcal{A}(V))$ are coisotropic and the* 1*-dimensional stable and unstable foliations $(W^{\pm}(x))_{x\in\mathcal{A}(V)}$ coincide with the characteristic foliations of $W^{\pm}(\mathcal{A}(V))$.*
- *If H is C^{p+1} and condition* (79) *is satisfied, then the manifolds $\mathcal{A}(V)$, $W^{\pm}(\mathcal{A}(V))$ are of class C^p and the foliations $(W^{\pm}(x))_{x\in\mathcal{A}(V)}$ are of class C^{p-1}.*

Appendix B. A reminder on twist maps

We refer to the appendix of [29] and [40; 41] for more details and proofs about the Birkhoff theory of twist maps. Let $a < b$ be fixed. We set

$$\boldsymbol{A} = \mathbb{T} \times [a, b], \quad \Gamma(a) = \mathbb{T} \times \{a\}, \quad \Gamma(b) = \mathbb{T} \times \{b\}.$$

The closure of a subset $E \subset \boldsymbol{A}$ will be indifferently denoted by $\operatorname{cl} E$ or $\bar{E}$, and its interior will be denoted by $\operatorname{Int} E$. The set $\operatorname{Fr} E = \operatorname{cl} E \setminus \operatorname{Int} E$ is the frontier of E. A disk is an open connected and simply connected subset of $\boldsymbol{A}$.

Here we say that $f : \boldsymbol{A} \to \boldsymbol{A}$ is a *twist map* when it is a C^1 diffeomorphism, preserves $\Gamma(a)$ and $\Gamma(b)$ and tilts the vertical, that is, $f(\theta, r) = (\Theta, R)$ with

$$\partial_r\Theta(\theta, r) > 0 \quad \text{or} \quad \partial_r\Theta(\theta, r) < 0, \quad \forall(\theta, r) \in \boldsymbol{A}.$$

Then f tilts the vertical *to the right* in the former case and *to the left* in the latter one. A continuous map $f : \boldsymbol{A} \to \boldsymbol{A}$ is said to be *area-preserving* when it leaves invariant a Radon measure which is positive on the open subsets of $\boldsymbol{A}$. An essential circle in $\boldsymbol{A}$ is a C^0 curve which is homotopic to $\Gamma(a)$.

Theorem (Birkhoff). *Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be an area-preserving twist map. Then there exists $\nu > 0$ such that any essential circle invariant under f is the graph of some ν-Lipschitz function $\ell : \mathbb{T} \to [a, b]$.*

The second result from Birkhoff's theory we need is the following.

Theorem (Birkhoff). *Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be an area-preserving twist map. Assume that U is an open subset of $\boldsymbol{A}$ homeomorphic to $\mathbb{T} \times [0, 1[$, with $\Gamma(a) \subset U$, such that $f(U) \subset U$ and such that U is the interior of its closure. Then the frontier* $\operatorname{Fr} U$ *is an invariant essential circle.*

One easily deduces from the first Birkhoff theorem that the set $\operatorname{Ess}(f)$ of essential invariant circles of f, endowed with the Hausdorff topology, is compact.

Given $\Gamma \in \mathrm{Ess}(f)$ with $\Gamma = \mathrm{Graph}(\ell)$, we set

$$\Gamma^+ = \{(\theta, r) \in \boldsymbol{A} \mid r > \ell(\theta)\}, \quad \Gamma^- = \{(\theta, r) \in \boldsymbol{A} \mid r < \ell(\theta)\}. \tag{81}$$

By the Poincaré theory, every $\Gamma \in \mathrm{Ess}(f)$ admits a rotation number in $\mathbb{T}$ for $f_{|\Gamma}$. One can choose a common lift to $\mathbb{R}$ for the rotation number of all circles, which yields a function $\rho : \mathrm{Ess}(f) \to \mathbb{R}$. This function is continuous and increasing, in the sense that if $\Gamma_i = \mathrm{Graph}\, \ell_i$, $i = 1, 2$ are invariant with $\ell_1 \leq \ell_2$, then $\rho(\ell_1) \leq \rho(\ell_2)$. Moreover, $\rho(\ell_1) < \rho(\ell_2)$ when $\ell_1 < \ell_2$.

Definition 33. Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be an area-preserving twist map of the annulus $\boldsymbol{A}$. Let $\ell_\bullet$ and $\ell^\bullet$ be two functions $\mathbb{T} \to]a, b[$ whose graphs $\Gamma(a)$ and $\Gamma^\bullet$ are in $\mathrm{Ess}(f)$. Then one says that the set

$$\mathscr{B} = \{(\theta, r) \mid \theta \in \mathbb{T}, \ell_\bullet(\theta) \leq r \leq \ell^\bullet(\theta)\}$$

is a *Birkhoff zone* when that there is no element $\Gamma = \mathrm{Graph}\, \ell \in \mathrm{Ess}(f)$ such that $\ell_\bullet \leq \ell \leq \ell^\bullet$ and $\ell \neq \ell_\bullet$, $\ell \neq \ell^\bullet$.

We now prove Lemma 13, which was used in Section 3

Proof of Lemma 13. The main property of a special twist map f, coming from the fact that no element of $\mathrm{Ess}(f)$ has rational rotation, is that two distinct elements of $\mathrm{Ess}(f)$ are disjoint; see [34], Section 13.2. As a consequence, the rotation number $\rho : \mathrm{Ess}(f) \to \mathbb{R}$ is a homeomorphism onto its image $\mathcal{R} = \rho(\mathrm{Ess}(f))$, by compactness of $\mathrm{Ess}(f)$. The boundaries of the Birkhoff zones are sent by ρ on the boundaries of the maximal intervals in the complement $\mathrm{Rot} \setminus \rho(\mathrm{Ess}(f))$, where $\mathrm{Rot} = [\rho(\Gamma(a)), \rho(\Gamma(b))]$ is the rotation interval of f. Our claim easily follows. □

We can now state a second easy lemma on special twist maps and domains associated with right or left splitting arcs.

Lemma 34. *Consider an essential circle $\Gamma \in \mathrm{Ess}(\varphi)$, $\Gamma \subset \boldsymbol{A} \setminus \Gamma(a)$, and a right (resp. left) splitting arc ζ based on Γ, with domain $D(\zeta)$. Consider an essential circle $\Gamma(a) \subset \boldsymbol{A}$ such that $\tilde{\zeta}$ is contained in the domain $\Gamma(a)^+$ above $\Gamma(a)$. Then for $x \in D(\zeta)$ there exists a positively (resp. negatively) tilted arc γ with $\gamma(0) \in \Gamma(a)$ and $\gamma(1) = x$, whose image does not intersect the union $\Gamma \cup \tilde{\zeta}$.*

The following easy result on negatively tilted arcs is used several times in our constructions.

Lemma 35. *Let Γ be an essential circle of $\boldsymbol{A}$ which is the graph of a ν-Lipshitz function $\ell : \mathbb{T} \to [0, 1]$, and let B be a ν-ball centered on Γ. Then for any $z \in \Gamma^+ \cap B$, there exists a negatively tilted arc based on Γ and ending at z, whose image is contained in B.*

The proof of the following lemma is immediate.

Lemma 36. *Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be an area-reserving twist map. Let $\Gamma^{\pm}$ be two non-intersecting essential invariant circles contained in $\boldsymbol{A}$. Then for any continuous curves C and C' which intersect both circles $\Gamma^{\pm}$, the positive orbit of C under f intersects C'.*

We refer to [39] for the proofs of the following two results from Birkhoff's theory.

Lemma 37. *Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be an area-preserving twist map and let Γ be an essential invariant circle for f. The inverse image $f^{-1} \circ \gamma$ of a positively tilted arc γ based on Γ is a positively tilted arc based on Γ. The direct image $f \circ \gamma$ of a negatively tilted arc γ emanating from Γ is a negatively tilted arc based on Γ.*

Given a point $x \in \boldsymbol{A}$, we define the lower vertical $V^-(x)$ as the vertical segment joining a point of the lower boundary of $\boldsymbol{A}$ to x.

Lemma 38. *Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be an area-preserving twist map. Let $\Gamma \in \mathrm{Ess}(f)$. Let X be a connected closed subset of $\boldsymbol{A}$ which disconnects the annulus $\boldsymbol{A}$ and such that $X \subset \Gamma^+$. Let $x \in \boldsymbol{A}$ be such that there exists a positively tilted arc γ and a negatively tilted arc η, both based on Γ and ending at x, such that the images of γ and η do not intersect X. Then the vertical $V^-(x)$ does not intersect X.*

The following strong connecting lemma appeared with a different proof in [22].

Proposition 39. *Let $f : \boldsymbol{A} \to \boldsymbol{A}$ be a (not necessarily special) area-preserving twist map. Let $\Gamma(a)$ and $\Gamma^\bullet$ be the boundary components of some Birkhoff zone of instability for f. Fix a pair of open sets $V_\bullet$, $V^\bullet$ which intersect $\Gamma(a)$ and $\Gamma^\bullet$ respectively, with moreover $V_\bullet \subset (\Gamma^\bullet)^-$. Then there exist a point $z \in V_\bullet$ and an integer $n \geq 0$ such that $f^n(z) \in V^\bullet$. Moreover the integer n can be chosen arbitrarily large.*

Proof. Set

$$U = \bigcup_{n\geq 0} f^n(\Gamma(a)^- \cup V_\bullet) = \Gamma(a)^- \cup \Big(\bigcup_{n\geq 0} f^n(V_\bullet)\Big),$$

so that U is a connected and f-invariant neighborhood of $\partial_\bullet \boldsymbol{A}$, which satisfies

$$U \subset (\Gamma^\bullet)^-.$$

Hence the frontier $\Gamma := \mathrm{Fr}\,\mathcal{U}$ of its associated filled subset is in $\mathrm{Ess}(f)$ and satisfies $\Gamma(a) \leq \Gamma \leq \Gamma^\bullet$. Therefore $\Gamma = \Gamma(a)$ or $\Gamma = \Gamma^\bullet$. The former equality is impossible by construction, so $\Gamma = \Gamma^\bullet$.

As a consequence, $\Gamma^\bullet \subset \mathrm{Fr}\,\mathcal{U} \subset \mathrm{Fr}\,U$, so there exists an integer $n \geq 0$ such that

$$f^n(V_\bullet) \cap V^\bullet \neq \varnothing,$$

which proves our claim. Finally, observe that by choosing arbitrarily small open subsets $W_\bullet \subset V_\bullet$, $W^\bullet \subset V^\bullet$ and applying the previous result to the pair $W_\bullet$, $W^\bullet$, one can ensure that the integer n can be chosen arbitrarily large. □

Appendix C. Normally hyperbolic shadowing

For the convenience of the reader, we add a proof of the normally hyperbolic shadowing lemma, whose main ingredient is the Poincaré recurrence theorem and which closely follows [23; 24]. Let d stand for the product metric on $\mathbb{A}^2$.

Theorem 40. *Fix $f \in \mathscr{F}^\kappa$ with κ so that the statements of the last section hold. Fix g in $B^\kappa(f, \varepsilon(f))$ and fix an orbit $x_0, \dots, x_n$ of the polysystem (φ_g, ψ_g) on $\mathscr{A}_g$. Then for any $\delta > 0$ there is an orbit $z_0, \dots, z_N$ of g in $\mathbb{A}^2$ such that $d(z_0, x_0) < \delta$ and $d(z_N, x_n) < \delta$. One can moreover choose z_0 so that for each $i \in \{0, \dots, n\}$, there is an $m(i)$ with*

$$d(g^{m(i)}(z_0), x_i) < \delta. \tag{82}$$

Since φ_g has compact support and preserves the symplectic area on $\mathscr{A}_g$, by the Poincaré recurrence theorem almost every point of $\mathscr{A}_g$ is positively and negatively recurrent for φ_g. In the following we use *recurrent* as a shorthand for *positively and negatively recurrent.*

The other main tool of the proof is the following λ-lemma.

Lemma (normally hyperbolic inclination lemma). *Fix $f \in \mathscr{F}^\kappa$ with κ so that the statements of the last section hold, and fix g in $B(f, \varepsilon(f))$. Let $(j_x)_{x \in \mathscr{A}_g}$ be a continuous family of C^1 parametrizations of the local unstable manifolds attached to $\mathscr{A}_g$, that is, a C^0 map $j : \mathscr{A}_g \times [-1, 1] \to W^-(\mathscr{A}_g)$ such that, setting $j_x = j(x, \cdot)$,*

$$j_x(0) = x, \quad j_x([-1, 1]) \subset W^-(x), \tag{83}$$

and j_x is C^1. Then for any C^1 submanifold Δ of $\mathbb{A}^2$ which intersects $W^+(\mathscr{A}_g)$ transversely in $\mathbb{A}^2$ at some point $\xi \in W^+(x)$, there exist a sequence $(\Delta_n)_{n \in \mathbb{N}}$ such that

$$\xi \in \Delta_n \subset \Delta \quad \forall n \in \mathbb{N}, \tag{84}$$

and for $n \in \mathbb{N}$, a C^1 diffeomorphism $\ell_n : [-1, 1] \to g^n(\Delta_n)$ such that

$$\lim_{n \to \infty} \|\ell_n - j_{g^n(x)}\|_{C^0} = 0. \tag{85}$$

We refer to [52] for a proof with detailed estimates in the compact setting, which directly applies here thanks to our compactness assumption on the support of g.

Proof of Theorem 40. We will write φ, ψ instead of φ_g, ψ_g. Fix an orbit $x_0, \dots, x_n$ of the polysystem (φ, ψ) on $\mathscr{A}_g$ and fix $\delta > 0$. We fix a tubular neighborhood $\mathscr{N}$ of $\mathscr{A}_g$ in $\mathbb{A}^2$ such that $\mathscr{N} \cap W^-(\mathscr{A}_g)$ is invariant by g^{-1} and for each $z \in \mathscr{N} \cap W^-(\mathscr{A}_g)$ with $z \in W^-(y)$

$$d(g^{-1}(z), g^{-1}(y)) < d(z, y). \tag{86}$$

Setting $\tau_0 = \varphi$ and $\tau_1 = \psi$, by definition, there exists a sequence $\omega_0, \dots, \omega_{n-1}$ in $\{0, 1\}$ such that, for $0 \leq j \leq n-1$,

$$x_{j+1} = \tau_{\omega_j}(x_j). \tag{87}$$

Choose $r > 0$ small enough so that if $D_0 = \mathscr{A}_g \cap B(x_0, r)$ and if

$$D_{j+1} = \tau_{\omega_j}(D_j) \quad \text{for} \quad 0 \leq j \leq n-1, \tag{88}$$

then $D_j \subset \mathscr{A}_g \cap B(x_j, \delta/2)$ for $0 \leq j \leq n$ (which is possible by continuity of both maps τ_j).

We will prove the existence of an orbit $(y_j)_{1 \leq j \leq n}$ of (τ_0, τ_1) associated with the same sequence (ω_j), such that the point y_j belongs to D_j and is recurrent for $\tau_0 = \varphi$, and the existence of a sequence of balls $(B_j)_{0 \leq j \leq n}$ of $\mathbb{A}^2$ which satisfy the following two properties:

(C_j) For $0 \leq j \leq n$, B_j is centered at some point $z_j \in W^-(y_j) \cap \mathscr{N}$ and $B_j \subset B(y_j, \delta/2)$.

(T_j) For $0 \leq j \leq n-1$, $\exists m_j > 0$ such that $g^{m_j}(B_j) \subset B_{j+1}$.

We will construct these objects backwards, by finite induction. It is enough to prove that given some recurrent point $y_{j+1} \in D_{j+1}$ together with a ball B_{j+1} satisfying (C_{j+1}), one can find a recurrent point $y_j \in D_j$, a ball B_j satisfying (C_j) and a positive m_j which satisfies (T_j).

3. Assume first that $x_{j+1} = \varphi(x_j)$, so $D_{j+1} = \varphi(D_j)$. By assumption, the point $y_{j+1} \in D_{j+1}$ is recurrent for φ, hence the point $y_j = \varphi^{-1}(y_{j+1})$ is in D_j and is recurrent for φ too. By (C_{j+1}), the ball B_{j+1} is centered at some $z_{j+1} \in W^-(y_{j+1})$. By our assumption on $W^-(\mathscr{A}_g) \cap \mathscr{N}$ and since g coincides with φ on $\mathscr{A}_g$, setting $z_j = g^{-1}(z_{j+1})$,

$$d(z_j, y_j) = d(g^{-1}(z_{j+1}), g^{-1}(y_{j+1})) < d(z_{j+1}, y_{j+1}) < \tfrac{\delta}{2}. \tag{89}$$

Therefore, by continuity of g, there exists a ball B_j centered at z_j and contained in $B(y_j, \delta/2)$ such that $g(B_j) \subset B_{j+1}$.

4. Assume now that $x_{j+1} = \psi(x_j)$, so that $D_{j+1} = \psi(D_j)$. Let R_j and R_{j+1} be the full-measure subsets of D_j and D_{j+1} formed by the recurrent points for φ. Since ψ is measure preserving, $R_{j+1} \cap \psi(R_j)$ is a full measure subset of D_{j+1}. Therefore, there exists a recurrent point $\bar{y}_j \in R_j$ such that $\bar{y}_{j+1} = \psi(\bar{y}_j)$ is recurrent, and so close to y_{j+1} that, by continuity of the unstable foliation, the leaf $W^-(\bar{y}_{j+1})$ intersects the ball B_{j+1}. By definition of ψ and by the last item in Lemma 7, the submanifold $\Delta = W^-(\bar{y}_j)$ intersects $W^+(\mathscr{A}_g)$ transversely in $\mathbb{A}^2$ at some point $\xi \in W^+(\bar{y}_{j+1})$. Apply the inclination lemma to Δ in the neighborhood of ξ, together with the positive recurrence property of $\bar{y}_{j+1}$: there exists an arbitrarily large integer m' such that $g^{m'}(\Delta)$ intersects B_{j+1}. Fix

$$z \in g^{m'}(\Delta) \cap B_{j+1}, \tag{90}$$

then

$$g^{-m'}(z) \in \Delta \subset W^-(\bar{y}_j). \tag{91}$$

Now, by definition of $W^-(\bar{y}_j)$ and since $\bar{y}_j$ is negatively recurrent, there is an (arbitrarily large) integer m'' such that

$$d(g^{-m''}(g^{-m'}(z)), g^{-m''}(\bar{y}_j)) < \delta/2 \quad \text{and} \quad g^{-m''}(\bar{y}_j) \in D_j. \tag{92}$$

Set $y_j = g^{-m''}(\bar{y}_j)$, so that y_j is recurrent and the point $z_j = g^{-(m''+m')}(z) \in W^-(y_j)$ satisfies

$$d(y_j, z_j) < \delta/2 \quad \text{and} \quad g^{(m''+m')}(z_j) = z \in B_{j+1}. \tag{93}$$

Hence by continuity there exists a ball B_j centered at z_j such that conditions (C_j) and (T_j) are satisfied.

5. As a consequence, there exists a sequence of integers $(m_i)_{1\leq \leq n}$ such that for $1 \leq i \leq n$

$$g^{m_i} \circ \cdots \circ g^{m_1}(B_0) \subset B_i.$$

By construction, any $z_0 \in B_0$ satisfies our statement. □

Appendix D. A global Hamiltonian flow-box theorem

We refer to [46] for the necessary definitions and results in symplectic geometry. The proof of the following global form of the Hamiltonian flow-box theorem is immediate.

Lemma 41. *Let (M^{2m}, Ω) be a symplectic manifold with Poisson bracket $\{\cdot, \cdot\}$, and fix a Hamiltonian $H \in C^\infty(M)$ with complete vector field X_H.*

• *Let Λ be a codimension 1 submanifold of M, transverse to X_H, such that there exists an open interval $I \subset \mathbb{R}$ with $0 \in I$, for which the restriction of Φ_H to $I \times \Lambda$ is an embedding. Set*

$$\mathscr{D} = \Phi_H(I \times \Lambda) \tag{94}$$

and let $T : \mathscr{D} \to \mathbb{R}$ be the transition time function defined by

$$\Phi_H(-T(x), x) \in \Lambda, \quad \forall x \in \mathscr{D}. \tag{95}$$

Then T is C^∞, $\{H, T\} = 1$ and $\Lambda = T^{-1}(0)$, so X_T is tangent to Λ.

• *Assume moreover that there exist an open interval J and $\boldsymbol{e}_0 \in J$ such that, setting*

$$\Lambda_{\boldsymbol{e}_0} = H^{-1}(\boldsymbol{e}_0) \cap \Lambda,$$

the flow of X_T is defined on $J \times \Lambda_{\boldsymbol{e}_0}$ and satisfies

$$\Lambda = \Phi_T(J \times \Lambda_{\boldsymbol{e}_0}). \tag{96}$$

Then the form $\Omega_{\boldsymbol{e}_0}$ induced by Ω on $\Lambda_{\boldsymbol{e}_0}$ is symplectic, and the map

$$\begin{aligned} \boldsymbol{\chi} : (I \times J) \times \Lambda_{\boldsymbol{e}_0} &\to \mathscr{D} \\ ((t, \boldsymbol{e}), x) &\mapsto \Phi_H(t, \Phi_T(\boldsymbol{e} - \boldsymbol{e}_0, x)) \end{aligned} \tag{97}$$

is a C^∞ symplectic diffeomorphism on its image, where $(I \times J) \times \Lambda_{\boldsymbol{e}_0}$ is equipped with the form

$$(d\boldsymbol{e} \wedge dt) \oplus \Omega_{\boldsymbol{e}_0}. \tag{98}$$

Moreover

$$H \circ \boldsymbol{\chi}((t, \boldsymbol{e}), x) = \boldsymbol{e}, \quad \forall (t, \boldsymbol{e}, x) \in (I \times J \times \Lambda_{\boldsymbol{e}_0}), \tag{99}$$

and

$$\boldsymbol{\chi}^*(X_H) = \frac{\partial}{\partial t}. \tag{100}$$

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jean-pierre.marco@imj-prg.fr *Sorbonne Université, Paris, France*

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Hamiltonian ODE, homogenization, and symplectic topology

FRAYDOUN REZAKHANLOU

This article is based on a course the author gave in fall of 2018 at UC Berkeley, in connection with the MSRI program *Hamiltonian systems*, *from topology to applications through analysis*. In this article we explore the connection between the Hamiltonian ODEs and Hamilton–Jacobi PDEs, and give an overview of some of the existing techniques for the question of homogenization. We also discuss stochastic formulations of several classical problems in symplectic geometry.

1. Introduction

Hamiltonian systems of ordinary differential equations appear in celestial mechanics to describe the motion of planets. They are also used in statistical mechanics to model the dynamics of particles in a fluid, gas or many other microscopic models. It was known to Liouville that the flow of a Hamiltonian system preserves the volume. Poincaré observed that the Hamiltonian flows are *symplectic*; they preserve certain *symplectic area* of two dimensional surfaces. Various *symplectic rigidity phenomena* offer ways to take advantage of the symplecticity of Hamiltonian flows.

Writing q and p for the position and momentum coordinates respectively, a Hamiltonian function $H(q, p)$ represents the total energy associated with the pair (q, p). We regard a Hamiltonian system associated with H *completely integrable* if there exists a symplectic change of coordinates $(q, p) \mapsto (Q, P)$, such that our

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Hamiltonian system in new coordinates is still Hamiltonian system that is now associated with a Hamiltonian function $\overline{H}(P)$. For completely integrable systems the coordinates of $P = P(q, p)$ are conserved and the set of (q, p) at which $P(q, p)$ takes a fixed vector is an invariant set for the flow of our system. These invariant sets are homeomorphic to tori in many classical examples of completely integrable systems. According to *Kolmogorov–Arnold–Moser* (*KAM*) *theory*, many of the *invariant tori* survive when a completely integrable system is slightly perturbed. *Aubry–Mather theory* constructs a family of invariant sets provided that the Hamiltonian function is convex in the momentum variable. These invariant sets lie on the graph of the gradient of certain scalar-valued functions. A. Fathi [10] uses *viscosity solutions* of the Hamilton–Jacobi PDE associated with the Hamiltonian function H to construct Aubry–Mather invariant measures; see also [3]. Recently there have been several interesting works to understand the connection between Aubry–Mather theory and *symplectic topology*. The hope is to use tools from symplectic topology to construct interesting invariant sets/measures for Hamiltonian systems associated with nonconvex Hamiltonian functions.

Most of the aforementioned works on Hamiltonian systems are done when the Hamiltonian function is defined on the cotangent bundle of a compact manifold. A prime example is when $p, q \in \mathbb{R}^d$, with H periodic in q-variable, so that we may regard H as a function that is defined on $T^*\mathbb{T}^d = \mathbb{T}^d \times \mathbb{R}^d$. To go beyond the periodic case, we may take a Hamiltonian function that is *quasiperiodic* with respect to q. In fact there is a probabilistic generalization of quasiperiodic condition by selecting H randomly according to a probability measure $\mathbb{P}$ that is invariant with respect to spatial shifts: $\tau_a H(q, p) = H(q + a, p)$. As it turns out the Hamiltonian $\overline{H}$ can be obtained from H by a scaling limit that is called *homogenization*.

In these notes we will explore the connection between Hamilton–Jacobi PDE, homogenization, Hamiltonian ODE and symplectic topology.

1A. ***Hamiltonian ODE.*** In Euclidean setting a Hamiltonian system associated with a C^2 Hamiltonian function $H : \mathbb{R}^{2d} \to \mathbb{R}$ is the ODE

$$\dot{x} = X_H(x) := J\nabla H(x), \tag{1-1}$$

where

$$J := \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

with I denoting the $d \times d$ identity matrix. Writing $x = (q, p)$ with $q, p \in \mathbb{R}^d$, the system (1-1) means

$$\dot{q} = H_p(q, p), \quad \dot{p} = -H_q(q, p).$$

We write $\phi_t^H(x)$ for the flow of the vector field X_H. Poincaré discovered that the form

$$(\phi_t^H)^*(\bar{\alpha}am) - \bar{\alpha}am,$$

is exact for $\bar{\alpha}am = p \cdot dq$. As a consequence $(\phi_t^H)^*(\bar{\alpha}m) = \bar{\alpha}m$, where

$$\bar{\alpha}m := d\bar{\alpha}am = \sum_{i=1}^{d} dp_i \wedge dq_i.$$

This means that if $A(x,t) = (d\phi_t^H)_x$, then

$$\bar{\alpha}m(A(x,t)v, A(x,t)w) = \bar{\alpha}m(v,w) \quad \text{or} \quad A(x,t)^* J A(x,t) = J.$$

More generally, we can define *Hamiltonian vector fields* on any *symplectic manifold*. By a symplectic manifold we mean a pair (M,ω) with M a smooth manifold, and ω a nondegenerate closed 2-form on M. Given a smooth function $H : M \to \mathbb{R}$, we define the vector field $X_H = X_H^\omega$ as the unique vector field such that

$$i_{X_H}\omega = -dH.$$

In particular, $\mathcal{L}_{X_H}\omega = 0$, which implies the following identity for its flow

$$(\phi_t^H)^*\omega = \omega.$$

When $\omega = \bar{\alpha}m$, and $M = \mathbb{R}^{2d}$, we have $X_H^{\bar{\alpha}m} = J\nabla H$.

Given a vector field X on a manifold M, we write ψ_t^X for its flow. Given C^1 scalar-valued function $f : M \to \mathbb{R}$, we define its *Lie derivative* with respect to X by

$$\mathcal{L}_X f(x) = \tfrac{d}{dt} f(\psi_t(x))\big|_{t=0} = (df)_x(X(x)). \tag{1-2}$$

More generally, if $u(x,t) = f(\psi_t(x))$, then

$$u_t = \mathcal{L}_X u.$$

where u_t denotes the partial derivative of u with respect to t. From this, we learn that a function $f \in C^1(M;\mathbb{R})$ is *conserved* along the flow of X if and only if $\mathcal{L}_X f = 0$. In the case of a Hamiltonian vector field $X = X_H$, the Lie derivative $\mathcal{L}_X f$ is the *Poisson bracket* of H and f:

$$\{H,f\} := \mathcal{L}_{X_H} f = (df)(X_H) = -\omega(X_f, X_H) = \omega(X_H, X_f).$$

1B. ***Completely integrable systems.*** We may call a Hamiltonian ODE completely integrable if we have a sufficiently explicit formula for its solutions. One strategy to achieve this is by finding enough conservation laws. As it turns out, a Hamiltonian system on a manifold M is completely integrable if it has d many independent conservation laws that do not *interact* with each other. Note that if

$f_1, \dots, f_k : M \to \mathbb{R}$ are C^2 functions such that $\{H, f_i\} = 0$, $i = 1, \dots, k$, then the set

$$M_P = \{x \in M : (f_1(x), \dots, f_k(x)) = P\},$$

is invariant for the flow

$$x \in M_P \Longrightarrow \phi_t(x) \in M_P.$$

We recall a classical result of Liouville and Arnold; see for example [2].

Theorem 1.1. *Assume that there are C^2 functions $f_1, \dots, f_d : M \to \mathbb{R}$ such that the following conditions hold*:

- $\{H, f_i\} = \{f_i, f_j\} = 0$ *for all i and j.*
- *For $P \in \mathbb{R}^d$, the corresponding set M_P is compact.*
- *For each $x \in M_P$, the vectors $X_{f_1}(x), \dots, X_{f_d}(x)$ are linearly independent.*

Then each such M_P is homeomorphic to a d-dimensional torus. Moreover, the motion of X_H on M_P is conjugate to a linear motion. In other words, there exists a symplectic diffeomorphism $\Psi : \mathbb{T}^d \times \mathbb{R}^d \to M$ such that $\Psi^{-1} \circ \phi_t^H \circ \Psi$ is the flow of a Hamiltonian ODE for which the Hamiltonian function is independent of position.

Remark 1.2. (i) For an example, assume that $M = T^*\mathbb{T}^d = \mathbb{T}^d \times \mathbb{R}^d$, and consider a Hamiltonian function H that is independent of q. If we think of a torus as $[0, 1]^d$ with $0 = 1$, then the motion is given by $x(t) = x + tv \pmod 1$, for some vector $v = \nabla H(p) \in \mathbb{R}^d$. Depending on the vector v, we may have a periodic or *quasiperiodic* orbit. (The latter means that the closure of the orbit is a k-dimensional linear subtorus for some $k > 1$.)

(ii) The set M_P is an example of a *Lagrangian submanifold*. This means that $\dim M_P = d$ and $\omega \restriction_{M_P} = 0$. The latter follows from

$$\omega(X_{f_i}, X_{f_j}) = \{f_i, f_j\} = 0,$$

and the independence of $\{X_{f_i}(x)\}_{i=1}^d$, for every $x \in M_P$.

(iii) When $f_1 = H$, let us present a sketch of the proof of the Arnold–Liouville theorem. If we define $\phi_t : M \to M$, $t = (t_1, \dots, t_d) \in \mathbb{R}^d$ by

$$\phi_t(x) = \phi_{t_1}^{f_1} \circ \cdots \circ \phi_{t_d}^{f_d},$$

then $\phi_t(M_P) \subseteq M_P$. On the other hand, if we pick some point $a \in M_P$ and set $\varphi(t) = \phi_t(a)$, then $\varphi : \mathbb{R}^d \to M_P$, and the set

$$\Gamma = \{t \in \mathbb{R}^d : \varphi(t) = \varphi(0) = a\},$$

is a subgroup of $(\mathbb{R}^d, +)$. Indeed the compactness of M_P and the linear independence of $\{X_{f_i}(x)\}_{i=1}^d$ imply that the subgroup Γ is discrete. That is, there are vectors $v_1, \dots, v_d$, such that

$$\Gamma = \{n_1 v_1 + \cdots + n_d v_d : n_1, \dots, n_d \in \mathbb{Z}\}.$$

Hence the quotient $\mathbb{R}^d/\Gamma$ is a torus and the map φ yields a homeomorphism $\hat{\varphi} : \mathbb{R}^d/\Gamma \to M_P$. Moreover, assuming that $f_1 = H$, then ϕ_s^H is conjugate to the map $(t_1, \dots, t_d) \mapsto (t_1 + s, \dots, t_d)$. If we use the basis $(v_1, \dots, v_d)$ for $\mathbb{R}^d$, we can then show that ϕ_s^H is conjugate to a linear motion. Writing Q for the coordinates of $\mathbb{R}^d/\Gamma \equiv \mathbb{T}^d$, we have a homeomorphism $\Psi^P = \hat{\varphi} : \mathbb{T}^d \to M_P$. As we vary P, we obtain a map

$$\Psi : T^*\mathbb{T}^d = \mathbb{T}^d \times \mathbb{R}^d \to M.$$

We think of $\Psi(Q, P) = x$ as a parametrization of M. Setting $\overline{H}(P) = H(x) = H(\Psi(Q, P))$, for $x \in M_P$, we obtain a new Hamiltonian function $\overline{H} : T^*\mathbb{T}^d \to \mathbb{R}$ that is independent of Q. The motion of $\hat{\phi}_t(Q(0), P(0)) := (Q(t), P(t))$ may be defined by

$$\hat{\phi}_t := \Psi^{-1} \circ \phi_t^H \circ \Psi.$$

We already know that $Q(t)$ is a linear motion and that $P(t) = P(0)$. We may regard this motion as a solution to the Hamiltonian ODE

$$\dot{Q} = \nabla \overline{H}(P), \qquad \dot{P} = 0.$$

In summary, we have seen that for a completely integrable Hamiltonian ODE, we can find a change of coordinates that turns our system to a linear motion. That is, there exists a diffeomorphism Ψ such that

$$\phi_t^{\overline{H}} = \Psi^{-1} \circ \phi_t^H \circ \Psi, \qquad \overline{H} = H \circ \Psi, \tag{1-3}$$

for a Hamiltonian function H that is independent of position. Recall that both ϕ_t^H and $\phi_t^{\overline{H}}$ are symplectic. It is no surprise that the change of coordinates map Ψ is also symplectic. As the following proposition indicates, a symplectic change of coordinates always transforms a Hamiltonian system to another Hamiltonian system.

Proposition 1.3. *Let (M, ω) and (M', ω') be two symplectic manifolds and assume that $\Psi : M' \to M$ is a diffeomorphism such that $\Psi^*\omega = \omega'$. Let $H : M \to \mathbb{R}$ be a Hamiltonian function on M, and let ϕ_t^H be the flow of X_H^ω. Then*

$$\hat{\phi}_t := \Psi^{-1} \circ \phi_t^H \circ \Psi,$$

is the flow of the vector field $X_{\overline{H}}^{\omega'}$ for $\overline{H} = H \circ \Psi$.

We refer to [13; 19; 24] for an introduction to symplectic geometry.

1C. *Kolmogorov–Arnold–Moser (KAM) theory.* We may take a small perturbation of a completely integrable system and wonder whether or not some of the invariant tori persist. It turns out that for a small perturbation, an invariant torus persists if the *action variable* $\nabla H(P)$ is sufficiently irrational; see for example [32].

Theorem 1.4. *Assume that* $H : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ *is of the form*

$$H^\varepsilon(q, p) = H^0(p) + \varepsilon K(q, p),$$

with $\det D^2 H_0 \neq 0$ *and* K *real analytic. Then for every* $\tau, \gamma > 0$, *there exists* $\varepsilon_0 = \varepsilon_0(\tau, \gamma) > 0$ *such that if* $\nabla H^0(p)$ *satisfies a* ***Diophantine condition*** *of the form*

$$n \in \mathbb{Z}^d \setminus \{0\} \Longrightarrow |n \cdot \nabla H^0(p)| \geq \gamma |n|^{-\tau},$$

then the vector field X_{H^ε} *has a quasiperiodic orbit of velocity* $\nabla H^0(p)$, *whenever* $|\varepsilon| \leq \varepsilon_0$.

Remark 1.5. It is worth mentioning that if we set

$$D(\gamma, \tau) = \{v \in \mathbb{R}^d : |v \cdot n| \geq \gamma |n|^{-\tau} \text{ for all } n \in \mathbb{Z}^d \setminus \{0\}\},$$

then the set $D(\tau) = \cup_{\gamma>0} D(\gamma, \tau)$ is of full measure whenever $\tau > d - 1$. This is because, the complement of $D(\gamma, \tau)$, restricted to a bounded set, has a volume of order $O(\gamma |n|^{-\tau-1})$, and

$$\sum_{n \neq 0} |k|^{-\tau-1} < \infty,$$

if and only if $\tau + 1 > d$.

1D. *Generating function.* Note that a Hamiltonian vector field is very special as it is fully determined by a scalar-valued function, namely its Hamiltonian function. As it turns out, the symplectic maps are also locally determined by scalar-valued functions known as *generating functions*. To explain this, take an $\bar{\alpha}m$-symplectic map $\psi(q, p) = (Q, P)$, and observe that since $\psi^* \bar{\alpha}m = \bar{\alpha}m$, we can find a scalar-valued function S such that

$$p \cdot dq - P \cdot dQ = dS. \tag{1-4}$$

Normally we think of S as a function of (q, p) or (Q, P). However, it is more convenient to think of S as a function of other pairs. For example under some nondegeneracy assumption (for example if $Q_p(q, p)$ is invertible so that we can locally solve $Q(q, p) = Q$ implicitly for $p = p(q, Q)$), we may regard $S = S(q, Q)$ as a function of the pair (q, Q). Under such circumstances, (1-4) implies

$$S_q(q, Q) = p, \quad -S_Q(q, Q) = P, \quad \psi(q, S_q(q, Q)) = (Q, -S_Q(q, Q)). \tag{1-5}$$

The scalar-valued functions S is an example of a generating function for the symplectic map ψ. Since there are other type of generating functions that we may consider for a symplectic map, let us refer to S as a *generating function of type I* (in short GFI).

Alternatively, we may set $W = p \cdot q - S$, and regard W as a function of (Q, p) so that (1-4) means

$$W_p(Q, p) = q, \quad W_Q(Q, p) = P, \quad \psi(W_p(Q, p), p) = (Q, W_Q(Q, p)).$$

The function W is another example of a generating function for the symplectic map ψ and we will refer to it as a *generating function of type II* (in short GFII). Another popular choice for a generating function is $W' = W'(q, P)$ that will be referred to as a *generating function of type III* (in short GFIII).

If ψ is the change of coordinates transformation of a completely integrable system, we have

$$\bar{H}(P) = H(q, p) = H(q, W'_q(q, P)).$$

This means that for each fixed P, the function $q \mapsto W'(q, P)$ is a solution to a *Hamilton–Jacobi equation* (*HJE*) associated with H. Thinking of $\mathbb{T}^d \times \mathbb{R}^d$, as $T^*\mathbb{T}^d$, we interpret $W'_q(q, P)$ as a 1-form on the torus for each P. If we write $W'(q, P) = q \cdot P + w^P(q)$ and assume that $w^P : \mathbb{T}^d \to \mathbb{R}$, is periodic, then our HJE reads as

$$H(q, P + (dw^P)_q) = \bar{H}(P). \tag{1-6}$$

We think of $\alpha^P = P + dw^P$ as a closed 1-form that belongs to the cohomology class of the constant (closed) form P.

1E. ***Weak KAM theory.*** In the classical KAM theory, we consider a small perturbation of a nondegenerate Hamiltonian function $H_0(p)$ that depends on p only. We have learned that the majority of the invariant tori of unperturbed systems persist for a sufficiently small perturbation. However some invariant tori could be destroyed after a small perturbation. In fact Arnold constructed an example of a perturbed integrable system, in which chaotic orbits — resulting from the breaking of unperturbed KAM tori — coexist with the invariant tori of KAM theorem. This phenomenon is known as *Arnold diffusion*. A natural question is whether or not we can construct a family of invariant sets $(M_P : P \in \mathbb{R}^d)$ for perturbed systems that come from the invariant tori of the unperturbed system and still carry some of their features. Aubry and Mather constructed such family for the so-called *twist maps* (these maps are the analog of Hamiltonian systems when $d = 1$ and time is discrete). The generalization of Aubry–Mather invariant sets to higher dimensions was achieved by Mather, Mañé and Fathi. They prove the existence of interesting invariant (action-minimizing) sets, which generalize KAM tori, and which continue to exist even after KAM tori disappearance.

Aubry–Mather theory replaces the condition of being close to an integrable Hamiltonian with the *Tonelli condition*. We say that a Hamiltonian function $H : \mathbb{T}^d \times \mathbb{R}^d \to \mathbb{R}$ is Tonelli, if the following conditions are true:

- $H(q, p)$ is C^2, and the matrix $H_{pp}(q, p)$ is positive definite for every (q, p).
- $|p|^{-1} H(q, p) \to \infty$ as $|p| \to \infty$, uniformly in q.

According to Aubry–Mather and Mather–Mane–Fathi theory, for each P, there exists a constant $\overline{H}(P)$, a Lipschitz function $w^P : \mathbb{T}^d \to \mathbb{R}$, and an invariant measure μ^P for ϕ^H such that:

- The function w^P solves the HJE (1-6) in a suitable weak sense.
- The support of the measure μ^P is a subset of

$$M_P = \{(q, P + (dw^P)_q) : q \in \mathbb{T}^d\}.$$

Note that we only require the function w^P to be Lipschitz and not everywhere differentiable. This is because the HJE (1-6) does no possess classical solutions in general. One remedy for this is to consider certain generalized solutions. In fact if we consider the so called *viscosity solutions*, then (1-6) always has at least one Lipschitz solution for each P. This was established by Lions, Papanicolaou and Varadhan [17] in 1987. We then modify the definition of M_P with

$$M_P = \{(q, P + (dw^P)_q) : q \in \mathbb{T}^d,\ w^P \text{ differentiable at } q\}. \tag{1-7}$$

1F. ***From torus to general closed manifolds.*** We may replace the torus with any sufficiently smooth manifold M in weak KAM theory. Now our Hamiltonian function H is a C^2 function on the cotangent bundle T^*M. The manifold T^*M carries a standard symplectic form $\omega = d\lambda$ with λ defined as

$$\lambda_{(q,p)}(a) = p_q((d\pi)_{(q,p)} a),$$

where $\pi : T^*M \to M$ is the projection $\pi(q, p) = q$ to the base point, and its derivative $(d\pi)_{(q,p)} : T_{(q,p)} T^*M \to T_q M$ projects onto tangent vectors. Recall that in the case of a torus, we know that the (1-6) has at least one solution by [17]. This existence result has been extended to arbitrary closed manifold and convex Hamiltonian by Albert Fathi [10].

Theorem 1.6. *Let M be a smooth closed manifold and assume that $H : T^*M \to \mathbb{R}$ is a Tonelli Hamiltonian. Then for every closed form α, there exists a unique constant $\overline{H}(\alpha)$, and a Lipschitz function $w : M \to \mathbb{R}$ such that w satisfies*

$$H(q, \alpha_q + (dw)_q) = \overline{H}(\alpha), \tag{1-8}$$

in viscosity sense.

Because of the uniqueness of $\overline{H}$, it is clear that if we add an exact form to α, the value of $\overline{H}$ does not change. Abusing the notation slightly, we may define $\overline{H}$ on the space $H^1(M)$ of the cohomology classes of 1-forms and write $\overline{H}([\alpha])$ in place of $\overline{H}(\alpha)$. Alternatively, for each $P \in H^1(M)$, we may fix a representative $\bar{\alpha}^P$ in class P and search for a Lipschitz $w^P : M \to \mathbb{R}$ such that $\alpha^P = \bar{\alpha}^P + dw^P$. Even when we fix the representative, the function w^P may not be unique. Given a choice of w^P, we define an invariant set M' by

$$M' = \{(q, \bar{\alpha}_q^P + (dw^P)_q) : q \in M, w^P\{\text{ differentiable at } q\}. \tag{1-9}$$

1G. ***From torus to stochastic Hamiltonian and homogenization.*** Weak KAM theory à la Fathi employs the HJE (1-6) in order to construct interesting invariant measures for the corresponding Hamiltonian ODE. It turns out that HJE can be used to model certain *deterministic and stochastic growths*. More precisely, imagine that we have an interface that separates different phases and this interface is represented by a graph of function $u(\,\cdot\,, t) : \mathbb{R}^d \to \mathbb{R}$ at time t. Suppose that the growth rate of this interface depends on the position q, and the inclination of the interface u_q. Mathematically speaking, u satisfies a HJE of the form

$$u_t + H(q, u_q(q, t)) = 0, \tag{1-10}$$

for a Hamiltonian function $H : \mathbb{R}^{2d} \to \mathbb{R}$. We think of (1-10) as the microscopic equation describing the evolution of the interface. If a large parameter n represents the ratio between the macro and micro scales, then

$$u^n(q, t) = n^{-1} u(nq, nt),$$

is the corresponding macroscopic height above that macro position q at the macro time t. We observe that u^n now solves

$$u_t^n + H^n(q, u_q^n(q, t)) = 0, \tag{1-11}$$

where

$$H^n(q, p) = (\gamma_n H)(q, p) := H(nq, p).$$

A *homogenization* occurs if the limit

$$\bar{\alpha}(q, t) = \lim_{n\to\infty} u^n(q, t),$$

exists whenever the limit

$$g(q) := \lim_{n\to\infty} u^n(q, 0),$$

exists. As it turns out, in many examples of interest, the limit $\bar{\alpha}$ satisfies a simpler HJE of the form

$$\begin{cases} \bar{\alpha}_t + \overline{H}(\bar{\alpha}_q) = 0, \\ \bar{\alpha}(q, 0) = g(q). \end{cases} \tag{1-12}$$

In fact we may use (1-6) to guess that when H is periodic in q, then $\overline{H}$ that appears in (1-12) coincides with $\overline{H}$ that appears in (1-6). This is because if w^P is a periodic function that satisfies (1-6), and we choose $u(q,0) = P\cdot q + w^P(q)$ as the initial condition for (1-10), then $u(q,t) = P\cdot q - t\overline{H}(P) + w^P(q)$, and

$$\bar{\alpha}(q,t) = \lim_{n\to\infty} u^n(q,t) = P\cdot q - t\overline{H}(P),$$

which solves (1-12).

We may wonder whether a weak KAM theory can be achieved for $H : \mathbb{R}^{2d} \to \mathbb{R}$ that is not necessarily periodic. Let us denote by $\mathcal{H}$ the set of all C^1 Hamiltonian functions $H : \mathbb{R}^{2d} \to \mathbb{R}$. For homogenization question, there are two relevant group actions on $\mathcal{H}$, namely the spacial translation and scaling. More precisely we set

$$\tau_a H(q,p) = H(q+a,p), \quad \gamma_n H(q,p) = H(nq,p),$$

for $a \in \mathbb{R}^d$ and $n \in \mathbb{R}^+$. We certainly have

$$\tau_a \circ \tau_b = \tau_{a+b}, \quad \gamma_m \circ \gamma_n = \gamma_{mn}.$$

We are interested to know for what Hamiltonian $H \in \mathcal{H}$ we have weak KAM theory and homogenization. Let us make a comment on bounded continuous functions K of the position variable. For $K : \mathbb{R}^d \to \mathbb{R}$, we define the translation operator $\tau_a K(q) = K(q+a)$ as before. We note that if a function K is periodic in q, then the set

$$\{\tau_a K : a \in \mathbb{R}^d\},$$

is homeomorphic to a d-dimensional torus. More generally, let us take a function $\hat{K} : \mathbb{T}^N \to \mathbb{R}$, and a $N \times d$ matrix A. We then set $K(q) = \hat{K}(Aq)$, which is an example of a *quasiperiodic* function. In fact the closure of the set

$$\Gamma(K) := \{\tau_a K : a \in \mathbb{R}^d\},$$

with respect to the uniform topology is

$$\Gamma(\hat{K}) := \{\hat{K}(\cdot + b) : b \in \mathbb{R}^N\},$$

if the following condition holds:

$$n \in \mathbb{Z}^N \setminus \{0\} \Longrightarrow nA \neq 0.$$

In general a bounded continuous function $K : \mathbb{R}^d \to \mathbb{R}$ is called *almost periodic* if the set $\Gamma(K)$ is precompact in $C_b(\mathbb{R}^d)$ with respect to the uniform topology.

We regard the group $\{\tau_a : a \in \mathbb{R}^d\}$ as a d-dimensional dynamical system on $\mathcal{H}$. A probability measure $\mathbb{P}$ on $\mathcal{H}$ is *translation invariant and ergodic* if the following conditions are met:

- For every Borel set $\mathcal{A} \subset \mathcal{H}$, and $a \in \mathbb{R}^d$, we have $\mathbb{P}(\tau_a \mathcal{A}) = \mathbb{P}(\mathcal{A})$.
- If a Borel set $\mathcal{A}$ is invariant i.e., $\tau_a \mathcal{A} = \mathcal{A}$ for all $a \in \mathbb{R}^d$, then $\mathbb{P}(\mathcal{A}) \in \{0, 1\}$.

We may wonder whether or not the weak KAM theory or homogenization are applicable to generic Hamiltonian functions in the support of an invariant ergodic measure. The hope is that Birkhoff ergodic theorem would make up for the lack of compactness that has played an essential role when we considered a cotangent bundle of a compact manifold in Section 1F.

1H. ***Variational techniques.*** Homogenization questions and the existence of interesting invariant measures are closely related to the existence of special orbits of the Hamiltonian ODEs. Such existence questions also play central role in several recent developments in symplectic topology. (A prime example is *Floer homology* that was formulated by Floer in order to prove *Arnold's conjecture*.) Hamilton discovered a variational description for the solutions of Hamiltonian systems. More specifically, we may reduce the existence of special orbits of (1-1) to the existence of a critical point of a suitable *action functional*. To explain this, let us assume that (M, ω) is a symplectic manifold with $\omega = d\lambda$. We also write Γ_T for the space of C^1 functions $x : [0, T] \to T^*M$. Given a Hamiltonian function $H : T^*M \times [0, T] \to \mathbb{R}$, we define $\mathcal{A} = \mathcal{A}_H : G_T \to \mathbb{R}$ by

$$\mathcal{A}(\gamma) = \mathcal{A}_H^T(\gamma) := \int_0^T [\lambda_{\gamma(t)}(\dot{\gamma}(t)) - H(\gamma(t), t)]\, dt. \tag{1-13}$$

The form $\lambda^H = \lambda - H\, dt$ is known as the *Poincaré–Cartan* form. We note that if we regard $d\lambda^H = \omega + dt \wedge dH$ as a form on $T^*M \times \mathbb{R}$, and $X_H = (X_H, 1)$, then

$$i_{\hat{X}_H} d\lambda^H = i_{X_H}\omega + dH = 0.$$

Moreover, if we take a variation of a path with fixed end points, for example

$$w : [0, T] \times [0, \delta] \to T^*M, \quad (t, \theta) \mapsto w(t, \theta),$$

with

$$\begin{aligned} w(t, 0) &= \gamma(t), & w(0, \theta) &= w(0, 0), \\ w(T, \theta) &= w(T, 0), & w_\theta(t, 0) &= v(t), \end{aligned}$$

then

$$
\begin{aligned}
-\frac{d}{d\theta}\int_{w(\,\cdot\,,\theta)}\lambda\Big|_{\theta=0} &= \lim_{h\to 0} h^{-1}\Big[\int_{w(\,\cdot\,,0)}\lambda-\int_{w(\,\cdot\,,h)}\lambda\Big]\\
&= \lim_{h\to 0} h^{-1}\int_{w([0,T]\times[0,h])}\omega\\
&= \lim_{h\to 0} h^{-1}\int_0^h\int_0^T \omega_w(w_t, w_\theta)\,dt\,d\theta\\
&= \int_0^T \omega_\gamma(\dot\gamma, v)\,dt.
\end{aligned}
$$

(Note that the orientation of w must be compatible with $\gamma = w(\,\cdot\,,0)$ for Stokes theorem to apply.) This in turn implies

$$
\begin{aligned}
\frac{d}{d\theta}\mathcal{A}_H^T(w(\,\cdot\,,\theta))\Big|_{\theta=0} &= -\int_0^T (i_{\dot\gamma}\omega + dH)_\gamma(v)\,dt\\
&= -\int_0^T (i_{\dot\gamma - X_H(\gamma)}\omega)_\gamma(v)\,dt. \qquad (1\text{-}14)
\end{aligned}
$$

Hence, if we restrict $\mathcal{A}$ to the set of curves with the same end points, then its *critical points* are the orbits of X_H. In fact the *critical values* of $\mathcal{A}$ solve the corresponding Hamilton–Jacobi PDE. To explain this, first we argue that the action functional can be used to produce generating functions for ϕ_T^H. Indeed if we define $\lambda_H^T : T^*M \to \mathbb{R}$, by

$$
\lambda_H^T(x) = \mathcal{A}_H(\eta_T^x), \qquad \text{where } \eta_T^x(t) = \phi_t^H(x) \text{ for } t \in [0, T], \qquad (1\text{-}15)
$$

then λ_H^T is a generating function for ϕ_T^H.

Proposition 1.7. *For every $T \ge 0$ and any Hamiltonian H, we have*

$$
d\lambda_H^T = (\phi_T^H)^*\lambda - \lambda. \qquad (1\text{-}16)
$$

Proof. Set

$$
A(x) = \int_{\eta_T^x}\lambda, \qquad B(x) = \int_0^T H(\eta_T^x(t), t)\,dt.
$$

Take any $(\tau(\theta) : 0 \le \theta \le \delta)$ with $\tau(0) = x$ and $\dot\tau(0) = v \in T_xM$. Set $y(t,\theta) = \phi_{-t}^H(\tau(\theta))$,

$$
\Theta_h = \{y(t,\theta) : 0 \le t \le T, 0 \le \theta \le h\},
$$

and use Stokes' theorem to assert that for $h \in (0, \delta)$,

$$h^{-1}\int_0^h\int_0^T \omega_y(y_t, y_\theta)\,dt\,d\theta = h^{-1}\int_{\Theta_h} d\lambda$$
$$= h^{-1}\left[\int_{\eta^{\tau(0)}}\lambda - \int_{\eta^{\tau(h)}}\lambda + \int_{\varphi\circ\tau(\cdot)}\lambda - \int_{\tau(\cdot)}\lambda\right],$$
$$h^{-1}\int_0^h\int_0^T (i_{X_H}\omega)_y(y_\theta)\,dt\,d\theta = h^{-1}\left[\int_{\eta^{\tau(0)}}\lambda - \int_{\eta^{\tau(h)}}\lambda + \int_{\tau(\cdot)}(\varphi^*\lambda - \lambda)\right],$$

where $\varphi = \phi_T^H$. Sending $h \to 0$ yields

$$-(dB)_x(v) = -(dA)_x(v) + (\varphi^*\lambda - \lambda)_x(v).$$

This is exactly (1-16). □

Let us assume that $M = \mathbb{R}^{2d}$, $\omega = \bar{\alpha}m$, and that H is a C^2 Hamiltonian function with D^2H uniformly bounded. With the aid of Proposition 1.7 we may define a GFI of ϕ_t^H by

$$S(q(t), t; q) := \int_0^t [p(s)\cdot\dot{q}(s) - H(q(s), p(s), s)]\,ds, \tag{1-17}$$

where $(q(s), p(s)) = \phi_s^H(q(0), p(0))$. Hence

$$\begin{aligned} \phi_t^H(q, -S_q(Q, t; q)) &= (Q, S_Q(Q, t; q)),\\ q(0) &= q,\\ q(t) &= Q,\\ p(t) &= S_Q(Q, t; q). \end{aligned}$$

Differentiating both sides of (1-17) with respect to t yields

$$S_t(Q, t; q) + S_Q(Q, t; q)\cdot\dot{q} = p(t)\cdot\dot{q}(t) - H(q(t), p(t), t).$$

As a result,

$$S_t(Q, t; q) + H(Q, S_Q(Q, t; q), t) = 0. \tag{1-18}$$

Similarly if we set $W = S + q\cdot p$, and regard $W(Q, t; p)$ as a function of (Q, p), then

$$W(q(t), t; p(0)) = p(0)\cdot q(0) + \int_0^t [p(s)\cdot\dot{q}(s) - H(q(s), p(s), s)]\,ds.$$

Differentiating both sides with respect to t yields

$$W_t(q(t), t; p(0)) + W_Q(q(t), t; p(0))\cdot\dot{q}(t) = p(t)\cdot\dot{q}(t) - H(q(t), p(t), t).$$

This yields

$$W_t(Q,t;\,p)+H(Q,W_Q(Q,t;\,p),t)=0, \tag{1-19}$$

because $W_Q(q(t),t;\,p(0))=p(t)$.

Remark 1.8. (i) In particular, if H is 1-periodic in t, $T=1$, and we define $\mathcal{A}$ on the space of 1-periodic paths (loops), then the critical points of $\mathcal{A}$ correspond to the periodic orbits of X_H. Floer uses the gradient flow equation

$$w_s=-\partial\mathcal{A}(w), \tag{1-20}$$

to prove the existence of periodic orbits by showing that

$$\lim_{s\to\infty} w(\,\cdot\,,s),$$

exists. Here the gradient is defined with respect to the L^2 inner product, which guarantees that (1-20) is an elliptic (in fact Cauchy–Riemann type) PDE. One may use the elliptic regularity of the solutions to obtain the compactness of path w in a suitable Sobolev space.

(ii) When H is a Tonelli Hamiltonian, it is more convenient to work with an action functional that is expressed in terms of the Legendre transform of H. To explain this, let us assume that there exists a C^2 function $L:TM\to\mathbb{R}$, $L=L(q,v)$, that is convex in the velocity v, and that the transformation $\mathbb{L}:TM\to T^*M$,

$$\mathbb{L}(q,v)=(q,L_v(q,v)), \tag{1-21}$$

is a C^1 diffeomorphism with

$$p=L_v(q,v)\quad\text{if and only if}\quad v=H_p(q,p).$$

(Here we identify $(T_qM)^{**}$ with T_qM.) The *Lagrangian* function L and the Hamiltonian function H are related to each other by Legendre transform

$$L(q,v)=\sup_{p\in T_q^*M}(p(v)-H(q,p)),\qquad H(q,p)=\sup_{v\in T_qM}(p(v)-L(q,v)).$$

Moreover

$$H\circ\mathbb{L}(q,v)=L_v(q,v)(v)-L(q,v).$$

Given a C^1 path $\alpha:[0,T]\to M$, we may define,

$$\mathcal{L}(\alpha):=\int_0^T L(\alpha,\dot\alpha)\,dt.$$

Note that if $x(t)=\phi_t^H(a)$ is a solution of (1-1), then

$$\lambda_x(\dot x)-H(x)=p_q((d\pi)_x(\dot x))-H(q,p)=p_q(\dot q)-H(q,p)=L(q,\dot q).$$

Hence

$$\mathcal{A}(x(\,\cdot\,)) = \int_0^T (\lambda_x(\dot{x}) - H(x))\,dt = \int_0^T L(q,\dot{q})\,dt = \mathcal{L}(q(\,\cdot\,)).$$

By a classical work of Tonelli, we have the following results:

- If we regard the action functional $\mathcal{L}$ as a function on paths $\alpha : [0, T] \to M$ with specified endpoints, then $\mathcal{L}$ has a minimizer $q(\,\cdot\,)$. As a consequence, this minimizer is a critical point of $\mathcal{L}$, and satisfies the Euler–Lagrange equation
$$\frac{d}{dt} L_v(q,\dot{q}) = L_q(q,\dot{q}). \tag{1-22}$$
- The corresponding path $x(t) = \mathbb{L}(q(t), \dot{q}(t))$ satisfies equation (1-1).

1I. ***Discrete models.*** Any symplectic map ψ from a symplectic manifold to itself serves as an example of a discrete analog of a Hamiltonian flow. We will be mainly interested in those symplectic diffeomorphisms for which a global generating function exists. For example, we may assume that a generating function of the first kind exists, i.e., (1-5) holds for some $S(q, Q)$ (with a slight abuse of notation we use the letter S for our generating function as in Section 1D). In the Euclidean setting, we may write $S(q, Q) =: L(q, Q - q)$. If $L(q, v)$ is bounded below and has a superlinear growth at infinity in the *velocity* variable v, we call the corresponding map ψ a twist map and the corresponding dynamical model is a generalization of the *Frenkel–Kontorova model*. Given a sequence $\boldsymbol{q} = (q_0, q_1, \dots, q_n)$, we define its *action* by

$$\mathcal{A}(\boldsymbol{q}) = \sum_{i=1}^{n} S(q_{i-1}, q_i) = \sum_{i=1}^{n} L(q_{i-1}, q_i - q_{i-1}).$$

The critical points of $\mathcal{A}$ correspond to the orbits of ψ. As we will see in Section 2, we may use the minimizers of $\mathcal{A}$ to construct interesting orbits of ψ.

We may also consider a generating function $W(Q, p) = Q \cdot p - w(Q, p)$ of type III so that

$$\psi(Q - w_p(Q, p), p) = (Q, p - w_Q(Q, p)).$$

In other words,

$$Q = q + w_p(Q, p), \qquad P = p - w_Q(Q, p),$$

which should be regarded as a discrete analog of a Hamiltonian ODE, with the function w playing the role of the Hamiltonian function.

Example 1.9 (standard map). Consider the Hamiltonian function $H(q, p) = \frac{1}{2}|p|^2 + V(q)$ for a C^2 potential function $V : \mathbb{T}^d \to \mathbb{R}$. The corresponding Hamiltonian equations are

$$\dot{q} = p, \quad \dot{p} = -\nabla V(q).$$

For a discrete version of these equations, we consider a map $\psi(q, p) = (Q, P)$ with

$$P = p - \nabla V(q), \quad Q = q + P.$$

This corresponds to a symplectic map associated with the generating function

$$S(q, Q) = \tfrac{1}{2}|Q - q|^2 - V(q).$$

2. Twist maps and their generalizations

The origin of the twist maps goes back to Poincaré's work on area-preserving maps on annulus that he encountered in his work on 3-body problem of celestial mechanics. Before embarking on studying twist maps, we give an overview of circle diffeomorphisms and their rotation numbers.

Definition 2.1. (i) Regarding $\mathbb{S}^1$ as the interval $[0, 1]$ with $0 = 1$, let $f : bS^1 \to \mathbb{S}^1$ be an orientation preserving homeomorphism. Its *lift* $F = \ell(f)$ is an increasing map $F : \mathbb{R} \to \mathbb{R}$ such that $f(x) = F(x) \pmod 1$, and F can be written as $F(x) = x + G(x)$, for a 1-periodic function $G : \mathbb{R} \to \mathbb{R}$. We may also regard G as a map on the circle: $g : bS^1 \to \mathbb{R}$, $g(x) = G(x)$ for $x \in [0, 1)$.

(ii) We define $\pi : \mathbb{R} \to \mathbb{S}^1$ by $\pi(x) = e^{2\pi i x}$. For f and F as in (i), we define its rotation number

$$\rho(F) = \lim_{n\to\infty} n^{-1} F^n(x), \quad \rho(f) = \pi(\rho(F)). \tag{2-1}$$

(iii) Given $\rho \in [0, 1)$, we write r_ρ for a rotation of the circle through the angle ρ. Its lift R_ρ is given by $R_\rho(x) = x + \rho$.

(iv) We write $D(\tau)$ for the set of numbers that satisfy a *Diophantine condition of type* τ. More precisely, $\rho \in D(\tau)$ if and only if there exists a positive constant c such that for every $r, s \in \mathbb{Z}$,

$$\left|\rho - \frac{r}{s}\right| \geq \frac{c}{|s|^\tau}.$$

Theorem 2.2 (Poincaré). *Let $f : bS^1 \to \mathbb{S}^1$ be an orientation preserving homeomorphism and write F for its lift. Then the following statements are true*:

(i) *The rotation number always exists and is independent of* x.

(ii) f *has a fixed point if and only if* $\rho(f) = 0$.

(iii) $\pm\rho(F) > 0$ *if and only if* $\pm(F(x) - x) > 0$.

(iv) *Let* (r, s) *be a pair of coprime positive integers. Then* f *has a* (r, s)*-periodic orbit* (*this means that* $F^s(x) = F(x) + r$ *for* $F = \ell(f)$), *if and only if* $\rho(f) = r/s$.

(v) *If* $\rho(f) \notin \mathbb{Q}$, *then the set* $\Omega_\infty(x)$ *of the limit points of the sequence* $\{f^n(x) : n \in \mathbb{N}\}$ *is independent of* x, *and is either* $\mathbb{S}^1$ *or nowhere dense.*

Proof. We only prove (i) and refer to [14] for the proof of the other parts.

By induction, we can readily show that if $F(x) = x + g(x)$ for a periodic function g, then $F^n(x) = x + G_n(x)$ for a periodic function G_n that is simply given by

$$G_n(x) = \sum_{i=0}^{n-1} G(F^i(x)) = \sum_{i=0}^{n-1} g(f^i(x)). \tag{2-2}$$

Since F^n is increasing, we learn that if $0 \le y \le x < 1$, then

$$x + G_n(x) = F^n(x) \ge F^n(y) = y + G_n(y) \quad \text{or} \quad G^n(y) - G^n(x) \le x - y < 1.$$

From this and 1-periodicity of G_n we deduce that $G^n(y) - G^n(x) < 1$ for all x and y. Hence

$$G_{m+n}(x) = G_m(x) + G_n(F^m(x)) \le G_m(x) + G_n(x) + 1.$$

This means that the sequence $\{a_n = G_n(x)\}$ is *almost* subadditive (more precisely, the sequence $\{a_n + 1\}$ is subadditive). From this we deduce

$$\rho(x) = \lim_{n\to\infty} n^{-1} G_n(x) = \lim_{n\to\infty} n^{-1}(F_n(x) - x) = \lim_{n\to\infty} n^{-1} F_n(x),$$

exists. From the last equality we learn that the limit ρ is nondecreasing, whereas the first equality implies that ρ is 1-periodic. This is possible only if $\rho(x)$ is a constant function. $\square$

Theorem 2.3. *Let* f *and* F *be as in Theorem 2.2*:

(i) (*Denjoy*) *If* $f \in C^1$ *with* f' *a function of bounded variation, and* $\rho = \rho(f) \notin \mathbb{Q}$, *then there exists a homeomorphism* h *such that* $f = h^{-1} \circ r_\rho \circ h$.

(ii) (*Herman* [12]) *If* $f \in C^{2+\alpha}$ *with* $\alpha \in [0, 1)$, *and* $\rho(F) \in D(\tau)$ *for some* $\tau > 2$, *then* h *in part* (*i*) *is in* $C^{1+\alpha}$. (*See Definition 2.1*(*iv*) *for the definition of* $D(\tau)$.)

Remark 2.4. (i) Let us write H, F, and $R_\rho(x) = x + \rho$, for the lifts of the maps h, f and r_ρ, respectively. Since the Lebesgue measure is invariant for R_ρ, and $F \circ H^{-1} = H^{-1} \circ R_\rho$, we learn that for any 1-periodic continuous function $\zeta : \mathbb{R} \to \mathbb{R}$,

$$\int \zeta \circ F \, dH = \int \zeta \, dH.$$

In other words, the measure μ with $\mu[0, x] = H(x)$ is invariant for f. Hence part (ii) is equivalent to the statement that if $f \in C^{2+\alpha}$, then the dynamical system associated with f is (uniquely) ergodic with an invariant measure that has a C^α density with respect to Lebesgue measure.

(ii) In terms of the invariant measure, the rotation number can be express as

$$\rho(f) = \int g \, d\mu,$$

by (2-1), (2-2) and the ergodic theorem.

(iii) Define $\mathcal{F}$ to be the set of continuous increasing functions $F : \mathbb{R} \to \mathbb{R}$ such that

$$\sup_x |F(x) - x| < \infty.$$

Write $F(x) = x + G(x)$, and define a translation operator that translates G:

$$(\tau_a F)(x) = F(x + a) - a = x + G(x + a).$$

Let $\mathbb{P}$ be a τ-invariant ergodic probability measure on $\mathcal{F}$. Then one can show that there exists a constant $\rho(\mathbb{P})$ such that

$$\lim_{n\to\infty} n^{-1} F^n(x) = \rho(\mathbb{P}),$$

for $\mathbb{P}$-almost all choices of F.

We next study *cylinder maps*.

Definition 2.5. (i) Let $\varphi : bS^1 \times [-1, 1] \to \mathbb{S}^1 \times [-1, 1]$, be an orientation preserving homeomorphism. Its *lift* $\ell(\varphi) = \Phi : \mathbb{R} \times [-1, 1] \to \mathbb{R} \times [-1, 1]$ is a homeomorphism such that

$$\varphi(x) = \Phi(x) \pmod 1,$$

and Φ can be written as $\Phi(q, p) = (q, 0) + \Psi(q, p)$, for a continuous $\Psi : \mathbb{R} \times [-1, 1] \to \mathbb{R} \times [-1, 1]$, that is 1-periodic function in q-variable.

(ii) An orientation-preserving diffeomorphism $\varphi : bS^1 \times [-1, 1] \to \mathbb{S}^1 \times [-1, 1]$ is called a *twist map* if the following conditions are met:

(a) φ (or equivalently its lift Φ) is area-preserving.

(b) If we define $\Phi^\pm$ by $(\Phi^\pm(q), \pm 1) = \Phi(q, \pm 1)$, then $\pm(\Phi^\pm(x) - x) > 0$. Equivalently, $\pm\rho(\Phi^\pm) > 0$.

Our main result about twist maps is the following:

Theorem 2.6 (Poincaré and Birkhoff). *Any twist map has at least two fixed points.*

Poincaré established Theorem 2.6 provided that φ has a global generating function. Such a generating function exists if φ is a *monotone twist map*. To explain Poincare's argument, let us formulate a condition on $\Phi = \ell(\varphi)$ that would guarantee the existence of a global generating function $S(q, Q)$ for Φ.

Definition 2.7. A C^1 area-preserving map φ or its lift $\Phi(q, p) = (Q(q, p), P(q, p))$ is called *positive* twist if $Q_p(q, p) > 0$ for all (q, p). We say φ is *negative* twist if φ^{-1} is a positive twist. We say that φ is a *monotone* twist, if φ either positive or negative twist.

Proposition 2.8. *Let Φ be a monotone twist map. Then there exists a C^2 function $S : U \to \mathbb{R}$ with*

$$U = \{(q, q') : Q(q, -1) \le q' \le Q(q, +1)\}$$

such that

$$\Phi(q, -S_q(q, Q)) = (Q, S_Q(q, Q)).$$

Moreover

$$S(q+1, Q+1) = S(q, Q), \quad S_{qQ} < 0. \tag{2-3}$$

Proof. The image of the line segment $\{q\} \times [-1, 1]$ under Φ is a curve γ with parametrization $\gamma(p) = (Q(q, p), P(q, p))$. By the monotonicity, the relation $Q(q, p) = Q$ can be inverted to yield $p = p(q, Q)$ which is increasing in Q. The set $\gamma([-1, 1])$ can be viewed as a graph of the function

$$Q \mapsto P(q, p(q, Q))$$

with $Q \in [Q(q, -1), Q(q, +1)]$. The antiderivative of this function yields $S(q, Q)$. This can be geometrically described as the area of the region Δ between the curve $\gamma([-1, 1])$, the line $P = -1$, and the vertical line $\{q\} \times [-1, 1]$. We now apply Φ^{-1} on this region. The line segment $\{Q\} \times [-1, 1]$ is mapped to a curve $\hat{\gamma}([-1, 1])$ which coincides with a graph of a function $q \mapsto p(q, Q)$. Since Φ is area preserving the area of $\Phi^{-1}(\Delta)$ is $S(q, Q)$. From this we deduce that $S_Q = -p$. Here we have used the fact that Φ^{-1} is a (negative) twist map; indeed if we write $\Phi^{-1}(Q, P) = (\hat{q}(Q, P), \hat{p}(Q, P))$, then

$$(\Phi^{-1})' = \begin{bmatrix} \hat{q}_Q & \hat{q}_P \\ \hat{p}_Q & \hat{p}_P \end{bmatrix} = \begin{bmatrix} Q_q & Q_p \\ P_q & P_p \end{bmatrix}^{-1} = \begin{bmatrix} P_p & -Q_p \\ -P_q & Q_q \end{bmatrix}$$

which implies that $\hat{q}_P = -Q_p < 0$.

The periodicity (2-3) is an immediate consequence of $\Phi(q+1, p) = \Phi(q, p) + (1, 0)$;

$$\Phi(\{q+1\} \times [-1, 1]) = \Phi(\{q\} \times [-1, 1]) + (1, 0).$$

As for the second assertion in (2-3), recall that $p(q, Q)$ is increasing in Q. Hence

$$S_{qQ} = -p_Q < 0. \qquad \square$$

We now show how the existence of a generating function can be used to prove the existence of fixed points.

Proof of Theorem 2.6 for a monotone twist map. Define $L(q) = S(q, q)$. We first argue that a critical point of L corresponds to a fixed point of Φ. Indeed, if $L'(q^0) = 0$, then $S_q(q^0, q^0) + S_Q(q^0, q^0) = 0$. Since $\Phi(q^0, -S_q(q^0, q^0)) = (q^0, S_Q(q^0, q^0))$, we deduce that $\Phi(q^0, y^0) = (q^0, y^0)$ for $y^0 = -S_q(q^0, q^0) = S_Q(q^0, q^0)$. On the other hand, by (2-3), we have that $L(q+1) = L(q)$. Either L is identically constant which yields a continuum of fixed points for Φ, or L is not constant. In the latter case, L has at least two distinct critical points, namely a maximizer and minimizer. These yield two distinct critical points of ϕ. $\square$

See for example [19] for a proof of Theorem 2.6 for general twist maps.

To see Poincaré–Birkhoff's theorem within a larger context, we interpret it in the following way: since $0 \in (\rho(\Phi^-), \rho(\Phi^+))$, then φ has at least two orbits in the interior of the cylinder that are associated with 0 rotation number, namely fixed points. In fact an analogous result is true for periodic orbits that is in the same spirit as Theorem 1.1(iv).

Theorem 2.9 (Birkhoff). *Let $\varphi : bS^1 \times [-1, 1] \to \mathbb{S}^1 \times [-1, 1]$, be an area and orientation preserving C^1-diffeomorphism. If $r/s \in (\rho(\Phi^-), \rho(\Phi^+))$ is a rational number with r and s coprime, then φ has at least two (r, s)-periodic orbits in the interior of $\mathbb{S}^1 \times [-1, 1]$.*

We may wonder whether a similar strategy as in the proof of Theorem 2.6 can be used to prove Theorem 2.9 when φ is a monotone area-preserving map. Indeed if Φ is a monotone twist map, then we can associate with it a variational principle which is the discrete analog of the principle of least action, as can be seen in the following proposition.

Proposition 2.10. *Let Φ be a monotone twist map with generating function S. Fix an integer $n \geq 2$:*

(i) *Given q and $Q \in \mathbb{R}$, define*

$$L(q_1, q_2, \ldots, q_{n-1}; q, Q) = \sum_{j=0}^{n-1} S(q_j, q_{j+1}),$$

with $q_0 = q$, *and* $q_n = Q$. *Then* $(q_1, q_2, \ldots, q_{n-1})$ *is a critical point of* $L(\,\cdot\,; q, Q)$ *if and only if there exist* $p_0, p_1, \ldots, p_n$ *such that* $\Phi(q_j, p_j) = (q_{j+1}, p_{j+1})$ *for* $j = 0, 1, 2, \ldots, n-1$.

(ii) *Given a positive integer* r, *define*

$$K(q_0, q_1, \ldots, q_{n-1}) = S(q_{n-1}, q_0 + r) + \sum_{j=0}^{n-2} S(q_j, q_{j+1}).$$

Then $(q_0, q_1, \ldots, q_{n-1})$ *is a critical point of* K *if and only if there exist* $p_0, p_1, p_2, \ldots, p_n$ *such that* $\Phi(q_j, p_j) = (q_{j+1}, p_{j+1})$ *for* $j = 0, \ldots, n-1$, *with* $q_n = q_0 + r$.

Proof. We only prove (ii) because (i) can be proved by a verbatim argument. Let $(q_0, \ldots, q_{n-1})$ be a critical point and set $q_n = q_0 + r$. We also set $p_j = -S_q(q_j, q_{j+1})$. The result follows because if $P_j = S_Q(q_j, q_{j+1})$, then

$$K_{q_j} = p_j - P_{j-1}, \quad \Phi(q_j, p_j) = (q_{j+1}, P_j),$$

for $j = 0, 1, 2, \ldots, n-1$. □

As we mentioned earlier, Theorem 2.9 for monotone twist maps can be established with the aid of Proposition 2.10. See, for example, [14] or [11] for a reference.

Remark 2.11. Naturally we are led to the following question: Can we find an orbit of φ associated with such $\rho \in (\rho(\Phi^-), \rho(\Phi^+))$? The answer to this question is affirmative and this is the subject of the *Aubry–Mather theorem*. For any irrational $\rho \in (\rho(\Phi^-), \rho(\Phi^+))$, There exists an invariant set on the cylinder that in some sense has the rotation number ρ. This invariant set q-projects onto either a Cantor-like subset of S^1 or the whole S^1. The invariant set lies on a graph of a Lipschitz function defined on S^1. These invariant sets are known as *Aubry–Mather sets*.

Arnold formulated an influential conjecture that is a vast generalization of Theorem 2.6 to higher dimensions. Given a Hamiltonian function $H : M \times \mathbb{R} \to \mathbb{R}$ on a closed symplectic manifold (M, ω), we may wonder whether or not the corresponding Hamiltonian vector field $X_H = X_H^\omega$ has T-periodic orbits for a given period T. *Arnold's conjecture* offers a nontrivial lower bounds on the number of such periodic orbits. To convince that such a question is natural and important, let us examine this question when the Hamiltonian function is time-independent first. We note that for the autonomous X_H we can even find rest points (or constant orbits) and there is a one-one correspondence between the constant orbits of X_H and the critical points of H. We can appeal to the following classical theories in algebraic topology to obtain sharp universal lower bounds on the number of critical points of a smooth function on M where M is a smooth closed manifold. Let us write $\mathrm{Crit}(H)$ for the set of critical points of $H : M \to \mathbb{R}$:

(i) According to Lusternik–Schnirelmann (LS) theorem,

$$\sharp\,\mathrm{Crit}(H) \geq c\ell(M), \tag{2-4}$$

where $c\ell(M)$ denotes the *cuplength* of M.

(ii) According to Morse theory, for a Morse function H,

$$\sharp\,\mathrm{Crit}(H) \geq \sum_k \beta_k(M), \tag{2-5}$$

where $\beta_k(M)$ denotes the k-th *Betti's number* of M.

According to Arnold's conjecture, the analogs of (2-4) and (2-5) should be true for the nonautonomous Hamiltonian functions provided that we count 1-periodic orbits of X_H in place of constant orbits. For the sake of comparison, we may regard (2-4) and (2-5) as a lower bound on the number of 0-periodic orbits when H is 0-periodic in t. In Arnold's conjecture, we replace 0-periodicity with 1-periodicity. Note that if H is 1-periodic in time, then $\phi^H_{t+1}(x) = \phi^H_t(x)$ for all t if and only if $\phi^H_1(x) = x$. To this end, we define

$$\mathbb{F}\mathrm{ix}(H) := \{x \in M : \phi^H_1(x) = x\} =: \mathrm{Fix}(\phi^H_1). \tag{2-6}$$

Arnold's conjecture. *Let (M, ω) be a closed symplectic manifold and let $H : M \times [0, \infty) \to \mathbb{R}$ be a smooth Hamiltonian function that is 1-periodic in the time variable. Then*

$$\sharp\,\mathbb{F}\mathrm{ix}(H) \geq c\ell(M). \tag{2-7}$$

Moreover, if $\varphi := \phi^H_1$ is nondegenerate in the sense that $\det(d\varphi - id)_x \neq 0$ for every $x \in \mathrm{Fix}(\varphi)$, then

$$\sharp\,\mathbb{F}\mathrm{ix}(H) \geq \sum_k \beta_k(M). \tag{2-8}$$

We now describe a strategy for tackling Arnold's conjecture under some additional conditions on M: We may establish the Arnold's conjecture by studying the set of critical points of $\mathcal{A}_H : G \to \mathbb{R}$, where Γ is the space of 1-periodic $x : bS^1 \to M$ and

$$\mathcal{A}_H(x(\,\cdot\,)) = \int_w \omega - \int_{\mathbb{S}^1} H(x(t), t)\, dt. \tag{2-9}$$

where $w : bD \to M$ is any extension of $x : bS^1 \to M$ to the unit disc $\mathbb{D}$. Note that the right-hand side of (2-9) would be independent of the extension w if the symplectic form ω is *aspherical* i.e., $\int_{f(\mathbb{S}^2)} \omega = 0$ for every smooth map

$f : bS^2 \to M$. We may try to apply LS and Morse theory to the functional $\mathcal{A}_H$ in order to get lower bounds on $\sharp\mathbb{F}ix(H)$. Of course we cannot apply either Morse theorem (2-5) or LS theorem (2-4) to $\mathcal{A}_H$ directly because Γ is neither compact nor finite-dimensional. However in the case of a torus or the cotangent bundle of a torus (namely $M = \mathbb{T}^d \times \mathbb{R}^d$), we may reduce the dimension to a finite (possibly very large) number by using *generalized generating functions*; see [11] for example. In fact, one can show that ϕ_t^H has a type II or III generating function (as we discussed in Section 1H and 1I) provided that t is sufficiently small. We then use the group property of the flow to write

$$\varphi = \phi_1^H = \psi_1 \circ \cdots \circ \psi_N,$$

where each ψ_i has a generating function. This can be used to build a generalized generating function for φ à la Chaperon [7]. We may establish Arnold's conjecture with the aid of generalized generating functions in some cases. Arnold's conjecture was established by Conley and Zehnder when $M = \mathbb{T}^{2d}$.

Theorem 2.12. *Assume that $\varphi = \phi_1^H$, for a smooth Hamiltonian function $H : \mathbb{T}^{2d} \times \mathbb{R} \to \mathbb{R}$ such that $H(x, t+1) = H(x, t)$ for every $(x, t) \in \mathbb{T}^{2d} \times \mathbb{R}$. Then φ has at least $2d + 1$ fixed points.*

We first prove Theorem 2.12, when the map ϕ has a global generating function. Before embarking on this, we make some observations and state some definitions.

For our purposes, it is more convenient to think of the Hamiltonian function as a function $H : \mathbb{R}^{2d} \times \mathbb{R} \to \mathbb{R}$ that is 1-periodic in all the coordinates of (x, t). (With a slight abuse of notion, this Hamiltonian function is also denoted by H.) The flow of this Hamiltonian function is denoted by $\Phi_t^H : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. Note that $\Phi := \Phi_1^H$ is a lift of φ of Theorem 2.12.

Definition 2.13. (i) Let us write $\mathcal{H} = \mathcal{H}(\mathbb{R}^{2d})$ for the space of C^2 Hamiltonian functions $H : \mathbb{R}^{2d} \times \mathbb{R} \to \mathbb{R}$. For each $a = (b, c) \in \mathbb{R}^d \times \mathbb{R}^d$, we define

$$\begin{aligned}(\tau_b H)(q, p, t) &= H(q+b, p, t),\\ (\eta_c H)(q, p, t) &= H(q, p+c, t),\\ (\theta_a H)(q, p, t) &= H(q+b, p+c, t).\end{aligned}$$

(ii) We write $\mathcal{C}^1$ for the set of C^1 maps $\Phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$. We set $\mathcal{F}(\Phi) = \Phi - id$, where id denotes the identity map. We write $\mathcal{S}$ for the set of symplectic diffeomorphism $\Phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ and set $\tilde{\mathcal{S}} = \mathcal{F}(\mathcal{S})$. For $a \in \mathbb{R}^{2d}$, the translation operators $\theta_a : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ and $\theta_a, \theta_a' : c\mathcal{C}^1 \to \mathcal{C}^1$ are defined by

$$\theta_a(x) = x + a, \quad \theta_a F = F \circ \theta_a, \quad \theta_a' = \mathcal{F}^{-1} \circ \theta_a \circ \mathcal{F},$$

for $x \in \mathbb{R}^{2d}$ and $F \in \mathcal{C}^1$. Note that for $\Phi \in \mathcal{C}^1$,

$$(\theta'_a \Phi)(x) = (\theta_{-a} \circ \Phi \circ \theta_a)(x) = \Phi(x+a) - a.$$

(iii) Let Φ be a symplectic diffeomorphsim with

$$\Phi(q,p) = (Q(q,p), P(q,p)).$$

We say that Φ is *exact* if for every $p \in \mathbb{R}^d$, the map $q \mapsto Q(q,p)$ is a diffeomorphism of $\mathbb{R}^d$. We write $\hat{q}(Q,p)$ for the inverse:

$$Q(q,p) = Q \Leftrightarrow q = \hat{q}(Q,p).$$

We also set $\hat{P}(Q,p) = P(q(Q,p),p)$, and

$$\widehat{\Phi}(Q,p) = (\hat{q}(Q,p), \hat{P}(Q,p)), \quad \widetilde{\Phi}(Q,p) = (\hat{P}(Q,p), \hat{q}(Q,p)).$$

Proposition 2.14. (i) *We have* $\mathcal{F}(\theta'_a \Phi) = \theta_a \mathcal{F}(\Phi)$, *and*

$$\phi^{\theta_a H} = \theta_{-a} \circ \phi^H \circ \theta_a = \theta'_a \phi^H. \tag{2-10}$$

In particular, if H is 1*-periodic, i.e., $\theta_n H = H$, for all $n \in \mathbb{Z}^{2d}$, and $\Phi = \phi_1^H$, then $\mathcal{F}(\Phi)$ is also* 1*-periodic.*

(ii) *For every exact Φ, and $a \in \mathbb{R}^d$, we have*

$$\widehat{\theta'_a \Phi} = \theta'_a \widehat{\Phi}.$$

In particular, if $\mathcal{F}(\Phi)$ is 1*-periodic, then so is $\mathcal{F}(\widehat{\Phi})$.*

(iii) *Assume that $\Phi \in \mathcal{S}$ is exact. Then there exists a C^2 function $W : \mathbb{R}^{2d} \to \mathbb{R}$ such that $\widetilde{\Phi} = \nabla W$.*

(iv) *If $\mathcal{F}(\Phi)$ is* 1*-periodic, with*

$$\int_{\mathbb{T}^{2d}} \mathcal{F}(\Phi)(x)\, dx = 0,$$

then

$$W(Q,p) = Q \cdot p - w(Q,p),$$

for a function w that is 1*-periodic.*

Proof. (i) The proof of $\mathcal{F}(\theta'_a \Phi) = \theta_a \mathcal{F}(\Phi)$ is straightforward and is omitted. The claim (2-10) is an immediate consequence of the fact that if $y(\cdot)$ is an orbit of $X_{\theta_a H}$, then $x(\cdot) = \theta_{-a} y(\cdot) = y(\cdot) - a$ is an orbit of X_H.

(ii) Fix $a = (b,c) \in \mathbb{R}^{2d}$. Let us define

$$\begin{aligned} \Phi^a(q,p) &:= (\theta'_a \Phi)(q,p) = (Q^a(q,p), P^a(q,p)), \\ \widehat{\Phi}^a(Q,p) &= (\hat{q}^a(Q,p), \hat{P}^a(Q,p)). \end{aligned}$$

We certainly have

$$Q(q+b,\,p+c)-b=Q^a(q,\,p)=Q\Leftrightarrow \hat{q}^a(Q,\,p)=q,$$
$$Q(q+b,\,p+c)=Q+b\Leftrightarrow \hat{q}(Q+b,\,p+c)=q+b.$$

Hence $\hat{q}^a(Q,\,p)=\hat{q}(Q+b,\,p+c)-b$. On the other hand

$$\begin{aligned}\hat{P}^a(Q,\,p)&=P^a(\hat{q}^a(Q,\,p),\,p)\\&=P(\hat{q}^a(Q,\,p)+b,\,p+c)-c\\&=P(\hat{q}(Q+b,\,p+c),\,p+c)-c\\&=\hat{P}(Q+b,\,p+c)-c,\end{aligned}$$

as desired.

(iii) Since Φ is symplectic, we have

$$\begin{aligned}d(\hat{P}\cdot dQ+\hat{q}dp)&=d(\hat{P}\cdot dQ+d(p\cdot\hat{q})-p\cdot d\hat{q})\\&=d(\hat{P}\cdot dQ-p\cdot d\hat{q})\\&=d(P\cdot dQ-p\cdot dq)\\&=0.\end{aligned}$$

Hence, there exists a function $W=W(Q,\,p)$ such that

$$dW=\hat{P}\cdot dQ+\hat{q}\cdot dp.$$

As a result, $\nabla W=\widetilde{\Phi}$.

(iv) Define

$$\hat{G}:=\mathcal{F}(\widehat{\Phi}),\quad w(Q,\,p):=Q\cdot p-W(Q,\,p),\quad \widehat{\nabla}w:=(w_p,\,w_Q).$$

We certainly

$$\begin{aligned}(Q,\,p)+\hat{G}(Q,\,p)&=\nabla W(Q,\,p)\\&=(W_p(Q,\,p),\,W_Q(Q,\,p))\\&=(Q-w_p(Q,\,p),\,p-w_Q(Q,\,p))\\&=(Q,\,p)-\widehat{\nabla}w(Q,\,p).\end{aligned}$$

In summary, $\hat{\nabla}w=-G$. By (ii) we know that $\hat{G}$ is a 1-periodic function. We wish to show that w is also a 1-periodic function. For this, it suffices to show

$$\int_{[0,1]^{2d}}\hat{\nabla}w(y)\,dy=-\int_{[0,1]^{2d}}\hat{G}(y)\,dy=0.$$

(Here $y = (Q, p)$.) To verify this, observe that if

$$A := (B, C) := \int_{[0,1]^{2d}} \hat{G}(y)\, dy, \quad B, C \in \mathbb{R}^d,$$

then there exists a C^2 periodic function $v(Q, p)$ such that $\hat{G} - A = -\hat{\nabla} v$, or

$$\hat{P}(Q, p) = C + p - v_Q(Q, p), \quad \hat{q} = B + Q - v_p(Q, p).$$

On the other hand, by assumption,

$$\begin{aligned} 0 &= \int_{[0,1]^{2d}} G(q, p)\, dq\, dp \\ &= \int_{[0,1]^{2d}} (Q(q, p) - q, P(q, p) - p)\, dq\, dp \\ &= \int_{[0,1]^{2d}} (Q - \hat{q}(Q, p), \hat{P}(Q, p) - p) \det(\hat{q}_Q(Q, p))\, dQ\, dp \\ &= \int_{[0,1]^{2d}} (v_p(Q, p) - B, C - v_Q(Q, p)) \det(I - v_{Qp}(Q, p))\, dQ\, dp \\ &= (-B, C) + \int_{[0,1]^{2d}} J\nabla v(Q, p) \det(I - v_{Qp}(Q, p))\, dQ\, dp, \end{aligned}$$

where I denotes the $(2d) \times (2d)$ identity matrix. We are done if we can show

$$\int_{[0,1]^{2d}} \nabla v(Q, p) \det(I - v_{Qp}(Q, p))\, dQ\, dp = 0. \tag{2-11}$$

The proof of this is left as an exercise. □

Exercise. Verify (2-11).

With the aid of Proposition 2.14, we can establish Theorem 2.12 when Φ (the lift of φ) is exact in the sense of Definition 2.13(iii). The proof can be carried out in exactly the same way that we proved Theorem 2.6 for monotone twist maps. To go beyond exact maps, we first express $\Phi = \Phi_H^1$ as a finite composition of exact maps and use their generating functions to construct a (generalized) generating function of type II for Φ.

Proposition 2.15. *Let Φ_i, $i = 1, \ldots, k$, be k exact symplectic diffeomorphisms with generating functions $W^i(Q, p) = Q \cdot p - w^i(Q, p)$, $i = 1, \ldots, k$, respectively. Let $\Phi = \Phi_k \circ \cdots \circ \Phi_1$:*

(i) *With $p_0 = p$, $q_k = Q$, and $\xi = (q_1, p_1, \ldots, q_{k-1}, p_{k-1})$, define*

$$W(Q, p; \xi) = \sum_{i=1}^{k} W^i(q_i, p_{i-1}) - \sum_{i=1}^{k-1} q_i \cdot p_i =: Q \cdot p + w(Q, p; \xi).$$

Then

$$W_\xi(Q, p; \xi) = 0 \Longrightarrow \Phi(W_p(Q, p; \xi), p) = (Q, W_Q(Q, p; \xi)). \tag{2-12}$$

In particular, if the full derivative ∇W of W with respect to its arguments Q, p and ξ vanishes at some point $(\bar\alpha, \bar\alpha, \bar\xi)$, then $(\bar\alpha, \bar\alpha)$ is a fixed point of Φ.

(ii) *Given $\boldsymbol{x} = (x_0, \dots, x_{k-1})$, $x_0 = (q_0, p_0), \dots, x_{k-1} = (q_{k-1}, p_{k-1})$, define*

$$\mathcal{A}^k(\boldsymbol{x}) = \sum_{i=1}^{k} W^i(q_i, p_{i-1}) - \sum_{i=1}^{k} q_i \cdot p_i,$$

with $x_0 = x_k = (q_k, p_k)$. (In other words, $\mathcal{A}^k$ is defined for k-periodic sequences.) Then any critical point $\boldsymbol{x}$ of $\mathcal{A}^k$ yields an orbit $\Phi_i(x_{i-1}) = x_i$, $i = 1, \dots, k$. In particular $x_0 = x_k$ is a fixed point of Φ.

Proof. (i) If we write $\hat q_{i-1} = W^i_p(q_i, p_{i-1})$, and $\hat p_i = W^i_Q(q_i, p_{i-1})$, then $\Phi_i(\hat q_{i-1}, p_{i-1}) = (q_i, \hat p_i)$. On the other hand, for $i = 1, \dots, k-1$,

$$\begin{aligned} W_{q_i}(Q, p; \xi) &= \hat p_i - p_i, & W_{p_i}(Q, p; \xi) &= \hat q_i - q_i, \\ W_p(Q, p; \xi) &= W^1_p(q_1, p) = \hat q_0, & W_Q(Q, p; \xi) &= W^k_Q(Q, p_k). \end{aligned}$$

From this, we can readily deduce (2-12).

(ii) As in part (i),

$$\begin{aligned} \mathcal{A}^k_{q_i}(\boldsymbol{x}) &= \hat p_i - p_i, & \mathcal{A}^k_{p_i}(\boldsymbol{x}) &= \hat q_i - q_i, \\ \mathcal{A}^k_{q_k}(\boldsymbol{x}) &= \hat p_k - p_k, & \mathcal{A}^k_{p_0}(\boldsymbol{x}) &= \hat q_0 - q_0 \end{aligned}$$

for $i = 1, \dots, k-1$. Hence at a critical point we have $\Phi_i(x_{i-1}) = x_i$ for $i = 1, \dots, k$. This completes the proof. □

Remark 2.16. Note that $\mathcal{A}^k$ can be written as

$$\mathcal{A}^k(\boldsymbol{x}) = \sum_{i=1}^{k} (p_{i-1} \cdot (q_i - q_{i-1}) - w^i(q_i, p_{i-1})),$$

which is a discrete variant of (1-17).

Proof of Theorem 2.12 (sketch). For some sufficiently large k, we can find exact symplectic diffeomorphisms Φ_i, $i = 1, \dots, k$, such that $\Phi = \Phi_k \circ \cdots \circ \Phi_1$. In Proposition 2.15(ii), we found a one-to-one correspondence between a fixed point x_0 of Φ, and a critical point $\boldsymbol{x} = (x_0, \dots, x_{k-1})$ of $\mathcal{A}^k$. Observe that from Proposition 2.14(iv) we know that $w^1, \dots, w^k$ are periodic. Let us write

$\mathcal{A}^k = \mathcal{A}_0^k - \boldsymbol{w}$, where

$$\mathcal{A}_0^k(\boldsymbol{x}) = \sum_{i=1}^{k} p_{i-1} \cdot (q_i - q_{i-1}), \quad \boldsymbol{w}(x) = \sum_{i=1}^{k} w^i(q_i, p_{i-1}).$$

To ease the notation, let us write $z_i = x_i - x_{i-1} = (q_i', p_i')$, and $\boldsymbol{z} = (z_1, \dots, z_{k-1})$. Since $x_k = x_0$, we may rewrite $\mathcal{A}_0^k$ as

$$\mathcal{A}_0^k(\boldsymbol{x}) = \sum_{i=1}^{k} (p_{i-1} - p_0) \cdot (q_i - q_{i-1}) = \sum_{i=1}^{k} (p_{i-1}' + \dots + p_1') \cdot q_i',$$

$$\begin{aligned}\mathcal{A}_0^k(\boldsymbol{x}) &= -\sum_{i=1}^{k} (p_i - p_{i-1}) \cdot q_i = -\sum_{i=1}^{k} (p_i - p_{i-1}) \cdot (q_i - q_0) \\ &= -\sum_{i=1}^{k} (q_i' + \dots + q_1') \cdot p_i'.\end{aligned}$$

Using this, we can express $\mathcal{A}_0^k(\boldsymbol{x})$ as $2^{-1} B\boldsymbol{z} \cdot \boldsymbol{z}$, for a matrix $B = [B_{ij}]_{i,j=1}^{k-1}$, with each B_{ij} a $(2d) \times (2d)$ matrix. We may express B as

$$B = \begin{bmatrix} 0 & C \\ -D & 0 \end{bmatrix},$$

with both C and D invertible. Hence B is nonsingular. Since for each $m \in \mathbb{Z}^{2d}$,

$$\mathcal{A}^k(x_0 + m, \dots, x_{k-1} + m) = \mathcal{A}^k(x_0, \dots, x_{k-1}),$$

we can write

$$\mathcal{A}^k(\boldsymbol{x}) = \tfrac{1}{2} B\boldsymbol{z} \cdot \boldsymbol{z} + \hat{\boldsymbol{w}}(x_0, \boldsymbol{z}),$$

for a bounded C^2 function $\hat{\boldsymbol{w}}(x_0, \boldsymbol{z})$ that is periodic in x_0. Let us $\boldsymbol{y} = (x_0, \boldsymbol{z})$, and $\mathcal{B}(\boldsymbol{y})$ for $\mathcal{A}^k(\boldsymbol{x})$ in these new coordinates. Observe that $\mathcal{B} : \mathbb{T}^{2d} \times \mathbb{R}^{2d(k-1)} \to \mathbb{R}$ is a bounded perturbation of a nondegenerate quadratic function $\boldsymbol{z} \mapsto 2^{-1} B\boldsymbol{z} \cdot \boldsymbol{z}$. We may study the set of critical points of $\mathcal{B}$ by analyzing the corresponding gradient flow $\dot{\boldsymbol{y}} = -\nabla \mathcal{B}(\boldsymbol{y})$. Equivalently,

$$\dot{\boldsymbol{z}} = B\boldsymbol{z} + \hat{\boldsymbol{w}}_{\boldsymbol{z}}(x_0, \boldsymbol{z}), \quad \dot{x}_0 = \hat{\boldsymbol{w}}_{x_0}(x_0, \boldsymbol{z}). \tag{2-13}$$

If we write $\psi_t(\boldsymbol{y})$ for the flow of (2-13), and X for the set $\boldsymbol{y}$ such that the corresponding orbit $(\psi_t(\boldsymbol{y}) : t \in \mathbb{R})$ is bounded, then X inherits the topology of $\mathbb{T}^{2d}$. To explain this, observe that $X = \mathbb{T}^{2d} \times \{0\}$, when $\hat{\boldsymbol{w}} = 0$. In general, the projection map $(x_0, \boldsymbol{z}) \mapsto x_0$ from X to $\mathbb{T}^{2d}$ induces an injective map from the *Cech homology* of $\mathbb{T}^{2d}$ to the Cech homology of X. This allows us to deduce that (2-13) has at least $2d+1$ many constant solution; we refer to [13] for more details. □

Remark 2.17. (i) The full proof of Theorem 2.12 as we sketched above can be found in [19]. A similar proof has been used in [13] by studying critical points of the operator $\mathcal{A}_H$ of (1-13) directly.

(ii) A variant of Theorems 2.6 and 2.12 can be proved when the periodicity of $\Phi - id$ is replaced with almost periodicity, or even when $\Phi - id$ is selected randomly according to a translation invariant probability measure; see [20; 21] for more details.

Exercises. (i) Let $b : \mathbb{R} \to \mathbb{R}$ be a positive 1-periodic function and write ϕ_t for the flow of the ODE $\dot{x} = b(x)$. Find the rotation number of this ODE by evaluating the following limit:

$$\lim_{t\to\infty} t^{-1}(\phi_t(x) - x).$$

Also, find a strictly increasing function $K : \mathbb{R} \to \mathbb{R}$ such that

$$K \circ \phi_t \circ K^{-1},$$

is a translation.

(ii) Define $\tau_a b(x) = b(x+a)$, and write $\mathcal{B}$ for the set of uniformly positive Lipschitz function $b : \mathbb{R} \to \mathbb{R}$. Let $\mathbb{P}$ be a τ-invariant ergodic probability measure on $\mathcal{B}$. For each b, write $\phi_t(x; b)$ for the flow of the ODE $\dot{x} = b(x)$. Show that $\mathbb{P}$-almost surely, the limit

$$\lim_{t\to\infty} t^{-1}(\phi_t(x; b) - x),$$

exists for every x. Evaluate this limit.

3. Discrete type Hamilton–Jacobi equation

In Section 2 we learned how the critical points of the action functional yield the orbits of the corresponding dynamical system. In this chapter we focus on the critical values of the action functional. We also examine how the stochasticity can play a role. We may choose the generating function randomly according to a probability law, or add some noise to the dynamics.

3A. ***Frenkel–Kontorova model.*** Imagine that we have a sequence of symplectic maps $(\Phi_i : i \in \mathbb{N})$ such that each Φ_i has a type I generating function $S^i(q, Q)$, so that

$$\Phi_i(q, S^i_q(q, Q)) = (Q, -S^i_Q(q, Q)).$$

We may define a dynamical system with orbits $(x_0, x_1, \dots, x_n, \dots)$;

$$x_{i+1} = \Phi_{i+1}(x_i) \quad \text{or} \quad x_n = \Phi_n \circ \cdots \circ \Phi_1(x_0).$$

If $\Phi_i = \Phi$ is independent of i, then we have an autonomous dynamical system with $x_n = \Phi^n(x_0)$. Under some type of nondegeneracy assumptions on the generating functions, we may regard our system as a second order dynamical system in q components. By this we mean that if $(x_n : n = 0, 1, \dots)$ is an orbit with $x_i = (q_i, p_i)$, then $(q_n : n = 0, 1, \dots)$ is an orbit of the dynamical system with the rule $q_n = F_n(q_{n-2}, q_{n-1})$, where F_n is implicitly defined by

$$S_Q^{n-1}(q_{n-2}, q_{n-1}) + S_q^n(q_{n-1}, q_n) = 0. \tag{3-1}$$

Moreover, given q and Q, we can find an orbit $(q_0, \dots, q_n)$, with $q_0 = q$, $q_n = Q$, if and only if $(q_1, \dots, q_{n-1})$ is a critical point of

$$\mathcal{S}^n(q_1, \dots, q_{n-1}; q, Q) = \sum_{i=1}^{n} S^i(q_{i-1}, q_i).$$

For the construction of invariant measures, we may consider the following variation: given a continuous function $g : \mathbb{R}^d \to \mathbb{R}$, consider

$$\mathcal{S}^n(q_0, q_1, \dots, q_{n-1}; g; Q) = g(q_0) + \mathcal{S}^n(q_1, \dots, q_{n-1}; q_0, Q).$$

Given q and Q, a critical point of $\mathcal{S}^n(q_0, q_1, \dots, q_{n-1}; g; Q)$ yields an orbit $(x_0, \dots, x_n)$ of our dynamical system with the properties

$$p_0 = -S_q^1(q_0, q_1) = \nabla g(q_0), \quad p_n = S_Q^n(q_{n-1}, Q).$$

As we mentioned in Section 2, it is more convenient to write $S^i(q, Q) = L^i(q, Q - q)$. Because of some of the examples we have in mind, it is quite natural to assume that

$$\liminf_{|v|\to\infty} \inf_q |v|^{-1} L^i(q, v) = \infty. \tag{3-2}$$

Note that this condition is satisfied for a standard map associated with $L(q, v) = |v|^2/2 - V(q)$, for a bounded C^1 function V. Assuming (3-2) is valid for each S^i, we define two operators

$$(\mathcal{T}_i g)(Q) = \inf_q (g(q) + S^i(q, Q)), \quad (\widehat{\mathcal{T}}_i g)(q) = \sup_Q (g(Q) - S^i(q, Q)), \tag{3-3}$$

on the space Λ of Lipschitz functions $g : \mathbb{R}^d \to \mathbb{R}$. Note that if $S(q, Q)$ is a generating function for Φ, then $S'(q, Q) = -S(Q, q)$ is a generating function for Φ^{-1}. We will see later that $\mathcal{T}_i g \in \Lambda$ when $g \in \Lambda$. Observe

$$u_n(Q) := (\mathcal{T}_n \circ \cdots \circ \mathcal{T}_1)(g)(Q) = \inf_{q_0, \dots, q_{n-1}} (g(q_0) + \mathcal{S}^n(q_1, \dots, q_{n-1}; q_0, Q)).$$

We regard

$$u_n = \mathcal{T}_n(u_{n-1}), \quad u_0 = g,$$

as a discrete variant of the (time inhomogeneous) HJE, where g is the initial data. Similarly,

$$u_{-n} = \widehat{\mathcal{T}}_n(u_{1-n}), \quad \hat{u}_0 = g,$$

is a discrete HJE with final condition $u_0 = g$. In particular, when $S^i = S$ is independent of i, we simply have $u_n = \mathcal{T}^n(g)$, and $u_n = \widehat{\mathcal{T}}^n(g)$, where

$$\begin{aligned} u(Q) &:= (\mathcal{T}g)(Q) = \inf_q (g(q) + S(q, Q)), \\ \hat{u}(q) &:= (\widehat{\mathcal{T}}g)(q) = \sup_Q (g(Q) - S(q, Q)). \end{aligned} \tag{3-4}$$

If we assume that $L(q, v) = S(q, q+v)$ has a superlinear growth at infinity, then the inf in (3-4) can be replace with min.

Assumption 3.1. There exists constants c_0, c_1 and $\delta > 0, \alpha > 1$ such that

$$\begin{aligned} &\inf_q L(q, v) \geq \delta |v|^\alpha - c_0, \quad \sup_q L(q, 0) \leq c_1, \\ &\sup_q \sup_{|v|\leq \ell} |L(q+z, v) - L(q, v)| \leq c_2(\ell)|z|. \end{aligned} \tag{3-5}$$

Proposition 3.2. *Assume that* (3-5) *holds and that* $|g(q') - g(q)| \leq \ell |q' - q|$ *for all* q, q'. *Then*

$$(\mathcal{T}g)(Q) = \min_{q : |Q-q| \leq \ell'} (g(q) + S(q, Q)), \tag{3-6}$$

$$|u(Q') - u(Q)| \leq \ell'' |Q' - Q|, \tag{3-7}$$

for $\ell' = c_0 + c_1 + (\delta^{-1}(\ell+1))^{1/(\alpha-1)}$ *and* $\ell'' = \ell + c_2(\ell')$.

Proof. Observe

$$g(q) + S(q, Q) \geq g(Q) - \ell|Q - q| + \delta |Q - q|^\alpha - c_0.$$

Hence

$$g(Q) + S(Q, Q) \leq g(q) + S(q, Q),$$

if $c_0 + c_1 \leq \delta |v|^\alpha - \ell |v|$, for $v = Q - q$. Then note that $\delta |v|^\alpha - \ell |v| \geq |v|$ if $|v| \geq (\delta^{-1}(\ell+1))^{1/(\alpha-1)}$. This implies (3-6).

If $u(Q) = g(q) + L(q, Q - q)$ for some Q with $|Q - q| \leq \ell'$, then for $q' = q + Q' - Q$,

$$\begin{aligned} u(Q') &\leq g(q') + L(q', Q - q) \\ &\leq g(q) + L(q, Q - q) + \ell |Q' - Q| + c_2(\ell')|Q' - Q| \\ &= u(Q) + (\ell + c_2(\ell'))|Q' - Q|, \end{aligned}$$

which proves (3-7). $\square$

We now describe some plausible applications of the operators $\mathcal{T}$ and $\widehat{\mathcal{T}}$ for finding invariant sets for the dynamical system associated with the transformation Φ. Recall that by Proposition 3.2, for each Q, there exists a point q such that

$$u(Q) := (\mathcal{T}g)(Q) = g(q) + S(q, Q).$$

Let us write $q = q(Q)$ for a minimizer in (3-4), which could be multivalued. If g is differentiable at q, then we have $\nabla g(q) + S_q(q, Q) = 0$, and if we write $A(q, Q) = g(q) + S(q, Q)$, then $A_q(q, Q) = 0$ when $q = q(Q)$. For now let us assume that the function $q(\,\cdot\,)$ is single-valued and differentiable at Q. Under such assumptions, u is differentiable at Q, and

$$\nabla u(Q) = A_q(q, Q)\nabla q(Q) + A_Q(q, Q) = S_Q(q, Q).$$

As a result,

$$\Phi(q, g(q)) = (Q, \nabla u(Q)). \tag{3-8}$$

This suggests that if U solves the discrete Hamilton–Jacobi equation $\mathcal{T}(U) = U + c$ for a constant c (or equivalently $\nabla\mathcal{T}(U) = \nabla U$ at any differentiability point of U), then the set

$$\mathrm{Gr}(U) = \{(q, \nabla U(q)) : U \text{ differentiable at } q\},$$

may serve as an invariant set for Φ. We will discuss the relevance of the equation $\mathcal{T}(U) = U + c$ and $\widehat{\mathcal{T}}(U) = U + c'$ to the question of homogenization in Section 5.

3B. ***Type II generating function.*** If we consider a symplectic map with a type II generating function $W(Q, p) = Q \cdot p - w(Q, p)$, then a candidate for the action is

$$A(q, p; Q) = A(x; Q) = g(q) + W(Q, p) - q \cdot p = g(q) + (Q - q) \cdot p - w(Q, p).$$

Let us assume that both g and w are differentiable functions. Given Q, at any critical point $x = (q, p)$ of A we have

$$0 = A_q(q, p; Q) = \nabla g(q) - p, \quad 0 = A_p(q, p; Q) = W_p(Q, p) - q.$$

Imagine that we can find a function $x(\,\cdot\,)$ such that $A_x(x(Q); Q) = 0$. If the function $x(\,\cdot\,)$ is differentiable at some $\bar{\alpha}$, then $u(Q) := A(x(Q); Q)$ is also differentiable at $\bar{\alpha}$, and

$$\nabla u(\bar{\alpha}) = A_x(x(\bar{\alpha}); \bar{\alpha})(\nabla x)(\bar{\alpha}) + W_Q(\bar{Q}, \bar{\alpha}) = W_Q(\bar{\alpha}, \bar{\alpha}),$$

where $x(\bar{\alpha}) = (\bar{\alpha}, \bar{\alpha})$. From this and $\Phi(W_p(\bar{\alpha}, \bar{\alpha}), \bar{\alpha}) = (\bar{\alpha}, W_Q(\bar{\alpha}, \bar{\alpha}))$ we deduce

$$\Phi(\bar{\alpha}, \nabla g(\bar{\alpha})) = (\bar{\alpha}, \nabla u(\bar{\alpha})).$$

In the case of type I generating function, we simply take the minimum of the action when L is bounded below (see (3-4)). This is no longer the case for type II generating function. For example if Φ is a lift of a symplectic map on the torus, then w is periodic and A is a periodic perturbation of the quadratic function $A^0(x;\, Q); = (Q-q)\cdot p$. Since 0, the only critical point of A^0 is a saddle point, the best we can hope for is that given Q, the function $A(\,\cdot\,;\, Q)$ has a saddle point which is of the same type as the type 0 is for $A^0(\,\cdot\,;\, Q)$. Now imagine that we come up with a universal way of *selecting* a critical value of A no matter what g is. This critical value yields an operator

$$\mathcal{V}(g)(Q) = A(x(Q);\, Q),$$

where $x(Q)$ is our selected critical point. A solution to the equation $\mathcal{V}(U) = U + c$, for a constant c, may be used to construct invariant sets of the map Φ.

More generally, assume that $\Phi = \Phi_k \circ \cdots \circ \Phi_1$ and each Φ_i has a generating function $W^i(q_i, p_{i-1}) = q_i \cdot p_{i-1} - w^i(q_i, p_{i-1})$. Then Φ has a (generalized) generating function of the form

$$\begin{aligned} W(q_k, p_0;\, \xi) &= W(q_k, p_0;\, q_1, p_1, \ldots, q_{k-1}, p_{k-1}) \\ &= q_1 \cdot p_0 + \sum_{i=2}^{k} p_{i-1}\cdot(q_i - q_{i-1}) - \sum_{i=1}^{k} w^i(p_{i-1}, q_i). \end{aligned}$$

Recall that by (2-12),

$$W_\xi(q_k, p_0;\, \xi) = 0 \Longrightarrow \Phi(W_{p_0}(q_k, p_0;\, \xi), p_0) = (q_k, W_{q_k}(q_k, p_0;\, \xi))$$

Given an initial data g, we set

$$\begin{aligned} A(\xi';\, q_k) &= A(q_1, p_1, \ldots, q_{k-1}, p_{k-1};\, q_k) \\ &= g(q_0) - p_0 \cdot q_0 + W(q_k, p_0;\, \xi) \\ &= g(q_0) + \sum_{i=1}^{k} (p_{i-1}\cdot(q_i - q_{i-1}) - w^i(p_{i-1}, q_i)), \end{aligned}$$

where $\xi' = (q_0, p_0, \xi)$. To study the orbits of the map Φ, we may search for a function $\xi'(q_k)$ such that $A_{\xi'}(\xi'(q_k);\, q_k) = 0$ for every q_k. Setting $u_k(q_k) = A(q_k;\, \xi'(q_k))$, we have

$$p_0 = \nabla g(q_0), \qquad \Phi(q_0, p_0) = (q_k, \nabla u_k(q_k)),$$

provided that g is differentiable at q_0, and ξ' is differentiable at q_k. In Section 4, we will address the question of selecting the critical point ξ'.

3C. ***Gibbs measures.*** There is a viscous variant of the discrete HJE that is related to the orbits (or rather realizations) of a Markov chain. Given $S : M \times M \to \mathbb{R}$, recall the action function $\mathcal{S}^n$ of Section 3A Instead of minimizing $\mathcal{S}^n$, we define a probability measure on M^{n-1} that favors states $\boldsymbol{q}^n = (q_1, \dots, q_{n-1})$ of lower *energy* $\mathcal{S}^n$. This measure depends on a positive parameter $\beta > 0$ that represents the *inverse temperature*. More precisely, we define a *Gibbs measure* $\mathbb{P}_n(\,\cdot\,) = \mathbb{P}_n(\,\cdot\,; q, Q; \beta)$ on M^{n-1} as

$$\mathbb{P}(d\boldsymbol{q}^n) = Z_n(q, Q)^{-1} \exp(-\beta \mathcal{S}^n(\boldsymbol{q}^n; q, Q)) \prod_{i=1}^{n-1} \nu(dq_i),$$

where $\nu(dq)$ is a finite *reference measure* (for example a volume form associated with a metric when M is a Riemannian manifold), and Z is the normalizing constant:

$$Z_n(q, Q) = \int_{M^{n-1}} \exp(-\beta \mathcal{S}^n(\boldsymbol{q}^n; q, Q)) \prod_{i=1}^{n-1} \nu(dq_i).$$

This constant is finite if for example

$$\sup_{a,b\in M} \int_M \exp(-\beta S^i(a, q) - \beta S^{i+1}(q, b))\, \nu(dq) < \infty$$

for every i. For simplicity, let us assume that $S^i = S$ for all i. Now, if we attempt to normalize our measure inductively, we need to calculate

$$Z(q_{n-2}, Q) := \int_M \exp(-\beta S(q_{n-2}, q_{n-1}) - \beta S(q_{n-1}, Q))\, \nu(dq_{n-1}),$$

which depends on q_{n-2}. Dividing the integrand by $Z(q_{n-2}, Q)$ would alter S. To avoid this, observe that if we replace $S(q, Q)$ with $S(q, Q) + u(Q) - u(q)$, then the corresponding Gibbs measure would not be affected (it only changes the normalizing constant). Motivated by this, we define

$$\mathcal{R}_\beta(h)(g)(Q) = \int_M e^{-\beta S(q,Q)} h(Q)\, \nu(dQ),$$
$$\mathcal{R}^*_\beta(h)(g)(Q) = \int_M e^{-\beta S(q,Q)} h(q)\ \nu(dq).$$

The operator $\mathcal{R}^*_\beta$ is the adjoint of $\mathcal{R}_\beta$ with respect to the inner product

$$\langle h, k\rangle = \int_M hk\, d\nu.$$

The celebrated Krein–Rutman theorem (an infinite-dimensional generalization of Perron–Frobenius theorem) offers a way of modifying S so that we can normalize our measure inductively.

For simplicity, let us assume that M is a compact metric space.

Theorem 3.3. *The largest eigenvalue $\lambda'_\beta = e^{\beta\lambda_\beta}$ of $\mathcal{R}_\beta$ is positive and λ'_β satisfies $\lambda'_\beta \geq |\lambda'|$ for any other eigenvalue λ'. Moreover λ'_β is simple, and there exist functions $u_\beta, u^*_\beta : M \to \mathbb{R}$ such that*

$$\mathcal{R}_\beta(e^{\beta u_\beta}) = e^{\beta\lambda_\beta} e^{\beta u_\beta}, \quad \mathcal{R}^*_\beta(e^{-\beta u^*_\beta}) = e^{\beta\lambda_\beta} e^{-\beta u^*_\beta}.$$

See, for example, [16] for a proof of Theorem 3.3 and the Krein–Rutman theorem. Motivated by Theorem 3.3, we set

$$\begin{aligned} \hat{S}(q, Q) &:= S(q, Q) - (u_\beta(Q) - u_\beta(q)) + \lambda_\beta, \\ p(q, dQ) &:= p(q, Q)\, \nu(dQ) := \exp(-\beta \hat{S}(q, Q))\, \nu(dQ). \end{aligned}$$

By Theorem 3.3, the *kernel* $p(q, dQ)$ is a probability measure for each q. Using this kernel, we may define a Markov chain $\boldsymbol{q} = (q_0, q_1, \dots, q_n, \dots)$ such that

$$\mathbb{P}^q(q_n \in A \mid q_0, \dots, q_{n-1}) = \int_A p(q_{n-1}, dq_n), \quad q_0 = q,$$

for every measurable set $A \subseteq M$. Here $\mathbb{P}^q$ is a probability measure on the set of sequences $\boldsymbol{q}$ with $q_0 = q$. Hence

$$\begin{aligned} \mathbb{P}^q(q_1 \in A_1, \dots, q_n \in A_n) &= \int_{A_1} \cdots \int_{A_n} \prod_{i=1}^n p(q_{i-1}, dq_i) \\ &= \int_{A_1} \cdots \int_{A_n} \exp\Big(-\sum_{i=1}^n \beta \hat{S}(q_{i-1}, q_i)\Big) \prod_{i=1}^n \nu(dq_i). \end{aligned}$$

Writing $\mathbb{P}^q_n(dq_1, \dots, dq_n)$ for the n-dimensional marginal of $\mathbb{P}^q$, we deduce

$$\mathbb{P}_n(dq_1, \dots, dq_{n-1}; q, Q) = \mathbb{P}^q_n(dq_1, \dots, dq_n \mid q_n = Q).$$

Also, if we define

$$\hat{\mathcal{T}}_\beta(g) = \beta^{-1} \log \mathcal{R}_\beta(e^{\beta g}),$$

then

$$u_n = \hat{\mathcal{T}}_\beta(u_{n-1}),$$

is a discrete analog of viscous HJE. Note that we always have $\hat{\mathcal{T}}_\beta(g) \leq \hat{\mathcal{T}}(g)$. In fact

$$\lim_{\beta \to \infty} \hat{\mathcal{T}}_\beta(g) = \hat{\mathcal{T}}(g),$$

if for example $\nu(U) > 0$ for every nonempty open subset U of M: If

$$U_\delta(q) = \{Q \in M : g(Q) - S(q, Q) \geq \hat{\mathcal{T}}(q) - \delta\},$$

for $q \in M$, and $\delta > 0$, then $U_\delta(q)$ is a nonempty open set, and

$$\hat{\mathcal{T}}_\beta(g)(q) \geq \hat{\mathcal{T}}(g)(q) - \delta + \beta^{-1} \log \nu(U_\delta(q)) \to \hat{\mathcal{T}}(g)(q) - \delta,$$

as $\beta \to \infty$.

In the same vein, we set

$$\mathcal{T}_\beta(g) = -\beta^{-1} \log \mathcal{R}^*_\beta(e^{-\beta g}),$$

so that

$$u_{-n} = \mathcal{T}_\beta(u_{1-n}),$$

is a discrete analog of backward viscous HJE. Also

$$\lim_{\beta \to \infty} \mathcal{T}_\beta(g) = \mathcal{T}(g). \tag{3-9}$$

We note

$$\hat{\mathcal{T}}(u_\beta) = u_\beta + \lambda_\beta, \quad \mathcal{T}(u^*_\beta) = u^*_\beta - \lambda_\beta,$$

which is the analog of (3-7). Moreover, the eigenfunctions $e^{\beta u_\beta}$, and $e^{-\beta u^*_\beta}$, can be used to find an invariant measure for our Markov chain. For this, observe that if we look for an invariant measure of the form $d\mu = Z^{-1} e^h \, d\nu$, the function h must satisfy

$$e^{h(Q)} = \int e^{h(q)} p(q, Q) \, \nu(dq) = e^{\beta(u_\beta(Q) - \lambda_\beta)} R^*_\beta(e^{h - \beta u_\beta})(Q),$$

which holds, if we choose h so that $e^{h - \beta u_\beta} = e^{-\beta u^*_\beta}$. Hence for an invariant measure, we may choose a measure of the form

$$\mu(dq) = Z^{-1} e^{\beta(u_\beta - u^*_\beta)(q)} \, dq,$$

where Z is the normalizing constant.

As (3-9) indicates, the zero-temperature limit of our Gibbs measure $\mathbb{P}$ is associated with the Frenkel–Kontorova model of Section 3A. We refer to Anantharaman [1] for some deep results regarding the type of limiting measure we obtain as $\beta \to \infty$.

4. Variational and viscosity solutions

In Section 1H we learned that critical points of the action functional $\mathcal{A}_H$ are the orbits of the Hamiltonian ODE associated with the Hamiltonian function H. This was used in Section 2 to prove the existence of periodic orbits. We also argued that the *critical values* of $\mathcal{A}_H$ yield solutions to HJE associated with the

Hamiltonian function H. Though our derivations of the HJEs (1-18) and (1-19) were rather formal. For example, the derivation of (1-18), requires the existence a global C^1 generating function which is hardly the case. In this section, we focus on the HJE and try to figure out how generalized solutions can be constructed. Insisting on constructing a solution as a critical value of the action $\mathcal{A}_H$ would lead to the notion of *variational solutions* to HJEs. However, HJE also appears as a model of stochastic growth. Statistical mechanical considerations suggest an alternative strategy for constructing solutions: We may add a small viscous term to the HJE to guarantee the existence of a global solution, and then send the viscosity to 0. This yields the notion of *viscosity solutions*. Surprisingly viscosity solutions may differ from variational solutions when the Hamiltonian function is not convex in the momentum variables. As we saw in Sections 1E–1F, solutions to HJE may be used to construct invariant measures for the corresponding Hamiltonian ODE. This has been the case for Tonelli Hamiltonians. For such Hamiltonians viscosity solutions coincide with variational solutions. One may hope to use variational solutions to come up with an analog of weak KAM theory for nonconvex Hamiltonian. Viterbo's work [31] settles the question of homogenization for such Hamiltonian functions.

4A. ***Variational solutions.*** Let $\Phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be a symplectic map with a generating function $W(Q, p) = Q \cdot p - w(Q, p)$. In Section 3B we learned that if g is a C^1 function, and

$$A(q_0, p_0, \dots, q_{n-1}, p_{n-1}; q_n; g) = g(q_0) + \sum_{i=1}^{k} (p_{i-1} \cdot (q_i - q_{i-1}) - w(q_i, p_{i-1})),$$

then a critical point of A yields an orbit $x_i = (q_i, p_i) = \Phi^i(x_0)$, $i = 1, \dots, n$, with $x_0 = (q_0, p_0)$, and $p_0 = \nabla g(q_0)$. Motivated by this, let us define

$$\mathcal{W}_n(x_0) = \sum_{i=1}^{n} (p_{i-1} \cdot (q_i - q_{i-1}) - w(q_i, p_{i-1})),$$

where $x_i = \Phi^i(x_0)$ for $i = 1, \dots, n$. In other words, $\mathcal{W}_n(x_0)$ denotes the action at time n of an orbit that starts from x_0. We then set

$$\begin{aligned}\mathcal{F}_n(g) = \{(Q, g(q) + \mathcal{W}_n(q, \nabla g(q))) : q \in \mathbb{R}^d, \Phi^n(q, \nabla g(q)) \\ = (Q, P) \text{ for some } P \in \mathbb{R}^d\}.\end{aligned}$$

We may extend the definition of $\mathcal{F}_n$ to Lipschitz g. Recall that Λ denotes the set of Lipschitz functions $g : \mathbb{R}^d \to \mathbb{R}$.

Definition 4.1. (i) Given $g \in \Lambda$, we write $\hat{\partial} g(q)$ for the set of vectors p such that there exists a sequence q_k for which the following conditions hold:

$$\nabla g(q_k) \text{ exists} \quad \text{and} \quad q = \lim_{k\to\infty} q_k,\ p = \lim_{k\to\infty} \nabla g(q_k).$$

The convex hull of the set $\hat{\partial} g(q)$ is denoted by $\partial g(q)$.

(ii) Given $g \in \Lambda$, we set

$$\mathcal{F}_n(g) = \{(q_n, g(q_0) + \mathcal{W}_n(q_0, p_0)) : q_0 \in \mathbb{R}^d,\ p_0 \in \partial g(q_0),\ \Phi^n(q_0, p_0) = (q_n, p_n)\}.$$

(iii) By a *variational solution* associated with Φ, we mean a collection of operators $\mathcal{V}_n = \mathcal{V}_n^w : L \to \Lambda$, $n \in \mathbb{N}$ with the following properties:

- $\mathcal{V}_n(g + c) = \mathcal{V}_n(g) + c$ for each n and every constant $c \in \mathbb{R}$.
- For $g, g' \in \Lambda$ with $g \le g'$, we have $\mathcal{V}_n(g) \le \mathcal{V}_n(g')$.
- For every $g \in \Lambda$, and $n \in \mathbb{N}$,

$$\{(q, \mathcal{V}_n(g)(q)) : q \in \mathbb{R}^d\} \subseteq \mathcal{F}_n(g).$$

In the same fashion, variational solutions of the HJE (1-10) are defined. For this, let us assume that $H : \mathbb{R}^{2d} \to \mathbb{R}$ is a C^2 Hamiltonian function such that $D^2 H$ is uniformly bounded. For this H, the corresponding flow Φ^H is well-defined. Recall that for $\gamma : [0, t] \to \mathbb{R}^{2d}$, with $\gamma(s) = (q(s), p(s))$, the action is defined by

$$\mathcal{A}_t(\gamma) = \mathcal{A}_t^H(\gamma) = \int_0^t [p \cdot \dot{q} - H(\gamma)]\, ds.$$

Definition 4.2. (i) We set $\phi^H_{[0,t]}(a)$ for the restriction of the flow $\phi_s^H(a)$ to the interval $[0, t]$. Given $a \in \mathbb{R}^{2d}$, we define

$$A_t^H(a) = \mathcal{A}_t^H(\phi^H_{[0,t]}(a)).$$

(ii) Given a Lipschitz function g, we set

$$\mathcal{F}_t(g) = \{(q(t), g(q_0) + A_t^H(q_0, p_0)) : q_0 \in \mathbb{R}^d,\ p_0 \in \partial g(q_0),\ \phi_t^H(q_0, p_0) = (q(t), p(t))\}.$$

(iii) By a *variational solution* of (1-10), we mean a collection of operators $\mathcal{V}_t = \mathcal{V}_t^H : L \to \Lambda$, $t \in [0, \infty)$ with the following properties:

- $\mathcal{V}_0$ is identity, and $\mathcal{V}_t(g + c) = \mathcal{V}_t(g) + c$ for each t and every constant $c \in \mathbb{R}$.
- For $g, g' \in \Lambda$ with $g \le g'$, we have $\mathcal{V}_t(g) \le \mathcal{V}_t(g')$.
- For every $g \in \Lambda$, and $t \in [0, \infty)$,

$$\{(q, \mathcal{V}_t(g)(q)) : q \in \mathbb{R}^d\} \subseteq \mathcal{F}_t(g).$$

When H is independent of q, then

$$\phi_t^H(q,p) = (q + t\nabla H(p), p), \quad A_t^H(q,p) = t(p\cdot\nabla H(p) - H(p)).$$

As a result, $\mathcal{F}_t$ can simply be described as

$$\begin{aligned}\mathcal{F}_t(g) &= \{(q+t\nabla H(p), g(q)+t(p\cdot\nabla H(p)-H(p))) : q\in\mathbb{R}^d,\ p\in\partial g(q)\}\\ &= \{(Q, g(q)+p\cdot(Q-q)-tH(p))\\ &\qquad\qquad : Q\in\mathbb{R}^d,\ Q-q = t\nabla H(p),\ p\in\partial g(q)\}\\ &= \{(Q, A^t(x;Q;g)) : Q\in\mathbb{R}^d, 0\in\partial_x A^t(x;Q;g)\},\end{aligned}\tag{4-1}$$

where $A^t(q,p;Q;g) = A^t(x;Q;g) = g(q) + p\cdot(Q-q) - tH(p)$.

Before examining some examples in dimension one, we define a type of discontinuity of u_q that will be relevant as we compare variational solutions with *viscosity solutions*.

Definition 4.3. Let $H:\mathbb{R}\to\mathbb{R}$ be a continuous function. We say that a pair of momenta (p^-, p^+) satisfies the *Oleinik condition with respect to H*, if either $p^- > p^+$, and the graph of the restriction of H to $[p^+, p^-]$ is above the chord connecting $(p^-, H(p^-))$ to $(p^+, H(p^+))$, or $p^- < p^+$, and the graph of the restriction of H to $[p^-, p^+]$ is below the chord connecting $(p^-, H(p^-))$ to $(p^+, H(p^+))$.

Example 4.4. Assume $d = 1$ and the Hamiltonian function H is independent of q, and that the initial condition is given by $g(q) = p^- q\,\mathbb{1}(q\le 0) + p^+ q\,\mathbb{1}(q\ge 0)$. Set

$$\bar\alpha(p^-, p^+) := \frac{H(p^+) - H(p^-)}{p^+ - p^-}, \quad v^\pm := H'(p^\pm).$$

As we will see in this example,

$$u(q,t) = (p^-q - tH(p^-))\mathbb{1}(q\le t\bar\alpha) + (p^+q - tH(p^+))\mathbb{1}(q\ge t\bar\alpha),\tag{4-2}$$

provided that (p^-, p^+) satisfies the Oleinik condition with respect to H. The solution (4-2) is an example of a *shock wave*. Our expression for the *shock speed* $\bar\alpha$ is the celebrated *Rankine–Hugoniot formula*. On the other hand, if H is concave, then the initial condition g results in solution that is an example of a *rarefaction wave*. The details of our claims follow.

Set $K(p) = pH'(p) - H(p)$. Recall

$$\mathcal{F}_t(g) = \{(q + tH'(p), g(q) + tK(p)) : q\in\mathbb{R}, p\in\partial g(q)\}.$$

For example, if with $p^- > p^+$, then $\mathcal{F}_t(g) = \mathcal{F}_t^- \cup \mathcal{F}_t^0 \cup \mathcal{F}_t^+$, where

$$\begin{aligned}\mathcal{F}_t^- &= \{(q + tH'(p^-), p^- q + tK(p^-)) : q \le 0\}\\ &= \{(q, p^- q - tH(p^-)) : q \le tv_-\},\\ \mathcal{F}_t^+ &= \{(q + tH'(p^+), p^+ q + tK(p^+)) : q \ge 0\}\\ &= \{(q, p^+ q - tH(p^+)) : q \ge tv_+\},\\ \mathcal{F}_t^0 &= \{(tH'(p), tK(p)) : p \in [p^+, p^-]\}.\end{aligned}$$

Note

$$\mathcal{F}_t^\pm = t\mathcal{F}_1^\pm =: t\mathcal{F}^\pm, \quad \mathcal{F}_t^0 = t\mathcal{F}_1^0 =: t\mathcal{F}^0.$$

Hence we only need to determine $\mathcal{F}^{\cdot} = \mathcal{F}_1^{\cdot}$. To analyze $\mathcal{F}^{\cdot}$ further, we examine several cases:

(i) Assume that H is strictly convex, or equivalently H' is increasing. We then set $L = K \circ (H')^{-1}$, which is simply the Legendre transform of H. Moreover $v^- > v^+$, and

$$\mathcal{F}^0 = \{(v, L(v)) : v \in [v^+, v^-]\}.$$

Note that $\mathcal{F}^\pm$ are lines that intersect at the point $(\bar{\alpha}, \bar{\alpha})$ where $\bar{\alpha} = p^\pm \bar{\alpha} - H(p^\pm)$. Clearly the only continuous function $u(\cdot)$ such that the graph of u is a subset of $\mathcal{F}(g)$ is

$$u(q) = (p^- q - H(p^-))\mathbb{1}(q \le \bar{\alpha}) + (p^+ q - H(p^+))\mathbb{1}(q \ge \bar{\alpha}).$$

This yields the solution $u(q, 1) = u(q)$ when $t = 1$. For general t we simply have (4-2). Observe that $g = \min\{g^-, g^+\}$, with $g^\pm(q) = qp^\pm$, and $\mathcal{V}_t(g) = \min\{\mathcal{V}_t(g^-), (g^+)\}$. This strong form of monotonicity is true for any pair of initial data $g^\pm$, and is a consequence of the convexity of H.

(ii) If H is strictly concave, then H' is decreasing. As before, we set $L = K \circ (H')^{-1}$, which is now concave. It may be defined by

$$L(v) = \min_{p \in [p^+, p^-]} (vp - H(p)).$$

Moreover, $v^- < v^+$, and

$$\mathcal{F}^0 = \{(v, L(v)) : v \in [v^-, v^+]\}.$$

In fact $\mathcal{F}_t(g)$ is the graph of a function $\hat{u}(\cdot, t)$ that is given by

$$\begin{aligned}u(q, t) = (p^- q - tH(p^-))\mathbb{1}(q \le tv^-) + (p^+ q - tH(p^+))\mathbb{1}(q \ge tv^+)&\\ + tL(q)\mathbb{1}(tv^- \le q \le tv^+).&\end{aligned}$$

What we have is an example of a rarefaction wave.

(iii) We now relax the convexity assumption of part (i) to the Oleinik condition. More precisely, we assume that the graph of $H : [p^+, p^-] \to \mathbb{R}$ lies below the chord connecting $(p^+, H(p^+))$ to $(p^-, H(p^-))$. We claim that under Oleinik condition, the only possible u with its graph subset of $\mathcal{F}_1(g) = \mathcal{F}(g)$, is given by (4-2). For this, it suffices to show that no point of $\mathcal{F}^0$ can reach the set below the graph of u. Indeed by Oleinik condition

$$\frac{H(p) - H(p^+)}{p - p^+} \le \bar{\alpha} = \frac{H(p^+) - H(p^-)}{p^+ - p^-} \le \frac{H(p^-) - H(p)}{p^- - p},$$

for every $p \in [p^+, p^-]$. Hence

$$\bar{\alpha} \le q \implies \frac{H(p) - H(p^+)}{p - p^+} \le q \implies p^+ q - H(p^+) \le pq - H(p),$$
$$\bar{\alpha} \ge q \implies \frac{H(p^-) - H(p)}{p^- - p} \ge q \implies p^- q - H(p^-) \le pq - H(p).$$

As a result, we must have

$$u(q) \le \min_{p \in [p^+, p^-]} (pq - H(p)),$$

for every q. This means that the set $\mathcal{F}^0$ lies above the graph of u. On the other hand, if for some point $(H'(p), pH'(p) - H(p))$ lies on the graph of $\hat{u}$ for some $p \in [p^+, p^-]$, then either

$$\bar{\alpha} \le q = H'(p) = \frac{H(p) - H(p^+)}{p - p^+} \quad \text{or} \quad \bar{\alpha} \ge q = H'(p) = \frac{H(p^-) - H(p)}{p^- - p}.$$

By Oleinik condition, we must have $\bar{\alpha} = q$, which implies that the only possible intersection point between the graph of u and $\mathcal{F}^0$ is the corner point of the graph of u. This completes the proof of our claim.

(iv) Assume that $H(p^+) = H(p^-) = H'(p^-) = 0$, $H'(p^+) < 0$, and $H(p) < 0$ for every $p \in (p^+, p^-)$. We also assume that there exists $p_0 \in (p^+, p^-)$, such that H is convex in $[p^+, p_0]$, and that H is concave in the interval $[p_0, p^-]$. Clearly the Oleinik condition is satisfied. We note that $\mathcal{F}^-$ ends at the origin, $\mathcal{F}^+$ passes through the origin, and $\mathcal{F}^0$ has two concave and convex pieces that are tangent to $\mathcal{F}^-$ and $\mathcal{F}^+$ respectively. The shock location is the origin, and $u(q, t) = g(q)$ for all $t \ge 0$.

As Example 4.4 indicates, we may have a simple formula for the variational solution when H is convex in momentum variable. Note that the action can be expressed in terms of the Lagrangian because when $\dot{x} = J\nabla H(x)$ for $x = (q, p)$, then

$$p \cdot \dot{q} - H(q, p) = L(q, \dot{q}).$$

In fact in this case the variational solution is given by the Lax–Oleinik formula; see [27; 28] for reference.

Theorem 4.5. *For a Tonelli Hamiltonian function H, we have*

$$\mathcal{V}_t^H(g)(Q) = \inf\{g(q(0)) + \int_0^t L(q, \dot{q})\, ds : q(\cdot) \in C^1[0, t], q(t) = Q\}. \quad (4\text{-}3)$$

In particular if H is convex and independent of q, we may use (4-3) and (4-1) to write

$$\begin{aligned}\mathcal{V}_t^H(g)(Q) &= \inf_q \left(g(q) - tL\left(\frac{Q-q}{t}\right)\right) \\ &= \inf_q \sup_p (g(q) + p \cdot (Q-q) - tH(p)) \\ &= \inf_q \sup_p A^t(q, p; Q; g). \end{aligned} \quad (4\text{-}4)$$

This formula is not surprising; after all we are looking for a critical value of $A^t(\cdot\,; Q; g)$, which is a concave function in p. So it is natural to try a simple minimax critical value that happens to be finite when H is convex.

In fact if we set $t = 1$, then the role of q and p are of the same flavor. Because of this, we may wonder whether or not we have a simple formula for a variational solution when, for example g is concave. This is indeed the case as the following result confirms; see for example [27].

Theorem 4.6. *Assume that H is independent of q and has a superlinear growth as $|p| \to \infty$, and g is Lipschitz and concave. Then*

$$\mathcal{V}_t^H(g)(Q) = \inf_p \sup_q (g(q) + p \cdot (Q-q) - tH(p)). \quad (4\text{-}5)$$

The identity (4-5) is known as *Hopf's formula* and can be rewritten as

$$\mathcal{V}_t^H(g)(Q) = \inf_p (p \cdot Q - g^\dagger(p) - tH(p)) = (g + tH)^\dagger(Q), \quad (4\text{-}6)$$

where we have used $\dagger$ for the Legendre transform:

$$g^\dagger(p) = \inf_q (p \cdot q - g(q)).$$

Note that $(g + tH)^\dagger$ is always well-defined and concave, even when H is not concave. If g is convex instead, then (4-5) and (4-6) change to

$$\mathcal{V}_t^H(g)(Q) = \sup_p \inf_q (g(q) + p \cdot (Q-q) - tH(p)) = (g^* + tH)^*(Q), \quad (4\text{-}7)$$

where we have used $*$ for the *other* Legendre transform:

$$g^*(p) = \sup_q (p \cdot q - g(q)).$$

Example 4.7. (i) If the graph of H over $[p^+, p^-]$ consists of a collection of concave and convex pieces, then the set $\mathcal{F}^0$ is a union of the graphs of the Legendre transforms of such pieces. However, when $g(q) = \min\{p^- q, p^+ q\}$ with $p^+ < p^-$, then g is concave, and the corresponding function u depends only the concave hull of the restriction of H to $[p^+, p^-]$. Indeed from (4-6), and the elementary fact that $g^\dagger(p) = -\infty\mathbb{1}(p \notin [p^+, p^-])$, we deduce

$$u(q, 1) = u(q) = \min_{p\in[p^+,p^-]} (pq - H(p)) = \min_{p\in[p^+,p^-]} (pq - \hat{H}(p)),$$

where $\hat{H}$ denotes the concave hull of the restriction of H to $[p^+, p^-]$. Note that the graph of H is below the chord connecting $(p^+, H(p^+))$ to $(p^-, H(p^-))$, if and only if the concave hull of the restriction of H to $[p^+, p^-]$ is this cord. If this is the case, then the Oleinik condition is satisfied, and we have a shock.The solution is simply given by

$$u(q) = \min_{p\in[p^+,p^-]} (pq - H(p)) = \min\{p^- q - H(p^-), p^+ q - H(p^+)\},$$

as in (4-2). In general the graph of u can have pieces that lie on $\mathcal{F}^0$. In order to have a feel for how complex u could be, imagine that there are points p_1, p_2, p_3 with $p^+ < p_1 < p_2 < p_3 < p^-$ such that $\hat{H} = H$ in the set $[p_1, p_2] \cup [p_3, p^-]$, and $\hat{H} \neq H$ in its complement. Then the graph of u would have two pieces of $\mathcal{F}^0$ associated with the intervals $[p_1, p_2]$ and $[p_3, p^-]$. More precisely we may express the graph of u as $F_1 \cup F_2 \cup F_3 \cup F_4$, where $F_1 = \mathcal{F}^-$, $F_4 \subset \mathcal{F}^+$, and

$$F_2 = \{(H'(p), K(p)) : p \in [p_3, p^-]\}, \quad F_3 = \{(H'(p), K(p)) : p \in [p_1, p_2]\},$$

where $K(p) = pH'(p) - H(p)$. The momentum $u' = u_q$ consists of two rarefaction waves associated with F_2 and F_3 that are separated by a shock. The rarefaction F_3 is separated from F_4 by a shock.

(ii) Let us now assume that $p^- < p^+$. Then g is convex and we may apply (4-7) to assert

$$u(Q, 1) = u(Q) = \max_{p\in[p^-,p^+]} (pQ - H(p)) = \max_{p\in[p^-,p^+]} (pQ - \tilde{H}(p)),$$

where $\tilde{H}$ denotes the convex hull of H. In particular if the graph of the restriction of H to $[p^-, p^+]$ is above the chord connecting $(p^-, H(p^-))$ to $(p^+, H(p^+))$, then $H(p^\pm) = \tilde{H}(p^\pm)$, and

$$u(q, t) = \max\{qp^+ - H(p^+), qp^- - H(p^-)\}.$$

In other words, the *Oleinik condition* is satisfied and we have a shock discontinuity.

4B. ***Viscosity solutions.*** We start with the definition of upper and lower derivatives:

Definition 4.8. Given a function $u : \mathbb{R}^k \to \mathbb{R}$, we write $\bar{\partial} u(z)$ for the set of vectors $a \in \mathbb{R}^k$ such that

$$\limsup_{h\to 0} |h|^{-1}(u(z+h) - u(z) - a \cdot h) \leq 0.$$

Equivalently, $a \in \bar{\partial} u(z)$ if and only if there exists a C^1 function $\varphi : \mathbb{R}^k \to \mathbb{R}$ such that $\varphi(a) = u(a)$, $\nabla\varphi(z) = a$, and $u \leq \varphi$. Similarly, $a \in \underline{\partial} u(z)$ if and only if

$$\liminf_{h\to 0} |h|^{-1}(u(z+h) - u(z) - a \cdot h) \geq 0.$$

Equivalently, $a \in \underline{\partial} u(z)$ if and only if there exists a C^1 function $\varphi : \mathbb{R}^k \to \mathbb{R}$ such that $\varphi(a) = u(a)$, $\nabla\varphi(z) = a$, and $u \geq \varphi$.

Remark 4.9. (i) Assume that $u : \mathbb{R}^k \to \mathbb{R}$ is continuous and there exists a C^1 surface Γ of codimension one such that u is C^1 on $\mathbb{R}^k \setminus \Gamma$. Near Γ, we write $u^\pm$ for the restriction of u on each side of Γ. We assume that $u^\pm$ are C^1 functions up to the boundary points on Γ. Pick a point on Γ. We wish to determine $\bar{\partial} u(a)$ in terms of $\nabla u^\pm(a)$. Assume that $v \in \bar{\partial} u(a) \neq \varnothing$. Let us write $T_a\Gamma$ for the tangent fiber at a to Γ, P_a for the orthogonal projection onto $T_a\Gamma$, and ν_a for the unit normal vector at a that points from $-$-side (on which u^- is defined) to the $+$-side (on which u^+ is defined). First take a smooth path $\gamma : (-\delta, \delta) \to \Gamma$ with $\gamma(0) = a$, $\dot{\gamma}(0) = \tau$. Using $v \in \bar{\partial} u(a)$, and

$$\left(\frac{d}{dt} u \circ \gamma\right)(0) = \nabla u^\pm(a) \cdot \tau,$$

we deduce that $\nabla u^\pm(a) \cdot \tau \leq v \cdot \tau$. This also being also true for $-\tau \in T_a\Gamma$ implies that $\nabla u^\pm(a) \cdot \tau = v \cdot \tau$. Hence $\nabla u^+(a) - \nabla u^-(a)$ is orthogonal to $T_a\Gamma$. This is not surprising and follows from the continuity of u; since $u^+ = u^-$ on Γ, the τ-directional derivative of u^+ and u^- coincide whenever $\tau \in T_a\Gamma$. Now if we vary a in the direction of ν_a or $-\nu_a$, we deduce

$$\nabla u^+(a) \cdot \nu_a \leq v \cdot \nu_a, \quad \nabla u^-(a) \cdot (-\nu_a) \leq v \cdot (-\nu_a).$$

Equivalently,

$$\nabla u^+(a) \cdot \nu_a \leq v \cdot \nu_a \leq \nabla u^-(a) \cdot \nu_a.$$

Hence, if $\bar{\partial} u(a) \neq \varnothing$, then $P_a \nabla u^+(a) = P_a \nabla u^-(a)$, $\nabla u^+(a) \cdot \nu_a \leq \nabla u^-(a) \cdot \nu_a$, and

$$\bar{\partial} u(a) = \{P_a \nabla u^\pm(a) + r\nu_a : r \in [\nabla u^+(a) \cdot \nu_a, \nabla u^-(a) \cdot \nu_a]\}.$$

Likewise, if $\underline{\partial} u(a) \neq \varnothing$, then $P_a \nabla u^+(a) = P_a \nabla u^-(a)$, $\nabla u^+(a) \cdot \nu_a \geq \nabla u^-(a) \cdot \nu_a$, and

$$\underline{\partial} u(a) = \{P_a \nabla u^{\pm}(a) + r\nu_a : r \in [\nabla u^-(a) \cdot \nu_a, \nabla u^+(a) \cdot \nu_a]\}.$$

In summary, we always have $P_a \nabla u^+(a) = P_a \nabla u^-(a)$, and there are three possibilities:

$$\begin{aligned}
&\nabla u^+(a) \cdot \nu = \nabla u^-(a) \cdot \nu \Longrightarrow \bar{\partial} u(a) = \underline{\partial} u(a) = \{\nabla u^{\pm}(a)\}, \\
&\nabla u^+(a) \cdot \nu < \nabla u^-(a) \cdot \nu \Longrightarrow \bar{\partial} u(a) \neq \varnothing, \underline{\partial} u(a) = \varnothing, \\
&\nabla u^+(a) \cdot \nu > \nabla u^-(a) \cdot \nu \Longrightarrow \bar{\partial} u(a) = \varnothing, \underline{\partial} u(a) \neq \varnothing.
\end{aligned}$$

(ii) Let $u : \mathbb{R}^k \to \mathbb{R}$ be a Lipschitz function. Even though the function u is differentiable at almost all points, it is plausible that $\bar{\partial} u(a) \cup \underline{\partial} u(a) = \varnothing$ at some point $a \in \mathbb{R}^k$ (as an example, consider $u(x_1, x_2) = |x_1| - |x_2|$, and $a = (0, 0)$). This would not be the case if u is *semiconvex/concave*. First observe that if for example u is convex, then

$$\underline{\partial} u(a) = \{p \in \mathbb{R}^k : u(z) - u(a) - p \cdot (z - a) \geq 0 \text{ for all } z \in \mathbb{R}^k\},$$

which is always nonempty. We say a function u is *semiconvex*, if $w(z) = u(z) + \ell|z|^2$ is convex for some $\ell \geq 0$. For such a function

$$\underline{\partial} u(a) = \{p - 2\ell a : p \in \underline{\partial} w(a)\},$$

which is also nonempty. In fact one can show that for a semiconvex function, we always have

$$\underline{\partial} u(a) = \partial u(a),$$

where ∂u was defined in Definition 4.1(i); see, for example, Cannarsa and Sinestrari [6] for a proof.

(iii) We can always approximate any Lipschitz function $u : \mathbb{R}^k \to \mathbb{R}$ by semiconvex/concave functions. For example, given $\delta > 0$, set

$$u^\delta(z) = \sup_y (u(y) - \delta^{-1}|z - y|^2).$$

Then one can show that u^δ is always semiconvex, and

$$u(z) \leq u^\delta(z) \leq u(z) + \sup_{r>0} (\ell r - \delta^{-1} r^2) = u(z) + 4^{-1}\ell^2\delta,$$

where ℓ is the Lipschitz constant of u. On the other hand if the supremum is achieved at $y_\delta(z)$, then for $p = 2\delta^{-1}(y_\delta(z) - z)$, we have

$$p \in \hat{\partial} u^\delta(z) \subseteq \underline{\partial} u^\delta(z), \quad p \in \bar{\partial} u(y_\delta(z)).$$

We must have $|p| \le \ell$ because for every a with $|a| = 1$, and $y = y_\delta(z)$,

$$-\ell \le \delta^{-1}(u(y+\delta a) - u(y)) \le p \cdot a.$$

In particular, $|y_\delta(z) - z| = O(\delta)$, which means that near each z, we can find y such that $\bar\partial u(y) \neq \varnothing$. In fact, it is well-known that there exists a one-to-one correspondence between the set of all maximizers $y_\delta(z)$, and the set $\hat\partial u^\delta(z)$; see, for example, [6]. As a result,

$$\bigcup_z \hat\partial u^\delta(z) \subseteq \bigcup_y \bar\partial u(y).$$

Definition 4.10. We say a uniformly continuous function $u : \mathbb{R}^d \times [0, \infty) \to \mathbb{R}$ is a *viscosity solution* of (1-10) if every $(p, r) \in \bar\partial u(q, t), t > 0$ satisfies $r + H(q, p) \le 0$, and every $(p, r) \in \underline{\partial} u(q, t), t > 0$ satisfies $r + H(q, p) \ge 0$.

Remark 4.11. (i) The theory of viscosity solutions offers a satisfactory notion of solution for (1-10) for two major reasons:

- Under some natural and mild conditions on H, and for a given Lipschitz function $g : \mathbb{R}^d \to \mathbb{R}$, there exists a unique viscosity solution to (1-10) that satisfies the initial condition $g(q) = u(q, 0)$. This allows us to define an operator $S_t^H g(q) := u(q, t)$ that enjoys the semigroup property $S_{t+s}^H = S_t^H \circ S_s^H$; see [8] for the proof of uniqueness. Later in Section 4E, we use game theory to construct viscosity solutions.
- Many stochastic interfaces in statistical mechanics can be described macroscopically by viscosity solutions of suitable HJEs; see for example [25; 22].

(ii) When H is convex in the momentum variable, then any semiconcave weak solution is also a viscosity solution. Simply because $\bar\partial u(z)$ is the convex hull of $\hat\partial u(z)$, and the set

$$A(q) := \{(p, r) : r + H(q, p) \le 0\},$$

is convex.

Exercise. Assume that $d = 1$ and u is a (continuous) viscosity solution of (1-10). Let U be an open set in $\mathbb{R} \times (0, \infty)$ and assume that u is C^1 in $U \setminus \Gamma$, where

$$\Gamma = \{(a(t), t)) : t \in (t_0, t_1)\} \subset U,$$

with $a : (t_0, t_1) \to \mathbb{R}$ a C^1 function. Assume that $u = u^+$ and u^-, on the right and left side of Γ in U and both $u^\pm$ solve (1-10) classically. Use Remark 4.9 to show the following:

- $\dot a(t) = H[u_q^+(a(t), t), u_q^-(a(t), t)]$.
- The pair $(u_q^-(a(t), t), u_q^+(a(t), t))$ satisfies the Oleinink condition for every $t \in (t_1, t_2)$.

4C. ***Viscosity solution versus variational solution.*** In Example 4.4(i), (iii), (iv), and Example 4.7, we have variational solutions for which u_q has shock discontinuities. In all these examples, the jump discontinuity of u_q satisfies an Oleinik condition. However it is known that in general Oleinik condition could be violated for a variational solution. Several explicit examples have been discovered for such a violation. The following recent example is due to V. Roos [27]. This example is constructed by performing a small perturbation to our Example 4.4(iv).

Theorem 4.12. *Assume $d = 1$, $H \in C^2$ is independent of q, and that H'' is uniformly bounded. Assume that $p^+ < p^-$, $H(p^+) = H(p^-) = H'(p^-) = 0 > H''(p^-)$, and $H(p) < 0$ for every $p \in (p^+, p^-)$. Let $f \in C^2$ be a Lipschitz, strictly convex function such that f'' is uniformly bounded, and $f(0) = f'(0) = 0$. Assume that the initial condition g is of the form*

$$g(q) = p^- q \mathbb{1}(q \le 0) + (p^+ q + f(q))\mathbb{1}(q \ge 0).$$

Then there exist $t_0 > 0$ and a continuous function $q : [0, t_0) \to \mathbb{R}$ such that $q(0) = 0$, and for every $t \in [0, t_0)$, there exists a point $q(t) > 0$ such that for every variational solution u, the function $u_q(q, t)$ is discontinuous at $q(t)$. Moreover the Oleinik condition is violated at $q(t)$.

Proof. Step 1 As before, $\mathcal{F}_t(g) = \mathcal{F}_t^+ \cup \mathcal{F}_t^0 \cup \mathcal{F}_t^-$, where

$$\begin{aligned}
\mathcal{F}_t^+ &=: t\mathcal{G}_t = \{t(q + H'(g'(tq)), t^{-1}g(tq) + K(g'(tq))) : q \ge 0\},\\
\mathcal{F}_t^- &= \mathcal{F}^- = \{(q, qp^-) : q \le 0\},\\
\mathcal{F}_t^0 &= t\mathcal{F}^0 = \{t(H'(p), K(p)) : p \in [p^+, p^-]\}.
\end{aligned}$$

Note that the sets $\mathcal{F}^-$ and $\mathcal{F}^0$ are independent of f and coincide with what we had in Example 4.4(iv). Let us write

$$\mathcal{F}^+ = \{(q, qp^+ - H(p^+)) : q \ge H'(p^+)\} = \{(q, qp^+) : q \ge H'(p^+)\},$$

which is what we get when $f = 0$ and $t = 1$.

We now examine the set $\mathcal{F}_t^+$. We claim that for $t \in (0, t_0)$, with

$$t_0 = [\sup_p |H''(p)| \sup_q |f''(q)|]^{-1}, \tag{4-8}$$

the set $\mathcal{F}_t^+$ is a graph of a convex function that is above $t\mathcal{F}^+$, and is tangent to $t\mathcal{F}^+$ at its end point. For convexity, observe that if

$$a(q) = q + H'(g'(tq)), \quad b(q) = t^{-1}g(tq) + K(g'(tq)),$$

then $a'(q) = 1 + tH''(g'(tq))g''(tq) = 1 + tH''(g'(tq))f''(tq) > 0$, and

$$b'(q) = g'(tq) + tg'(tq)H''(g'(tq))g''(tq) = g'(tq)a'(tq).$$

Hence the slope of $\mathcal{F}_t^+$ at the point $t(a(q), b(q))$ is $g'(tq)$. Since both a' and g' are increasing, $\mathcal{F}_t^+$ is convex. At $q = 0$ the slope is p^+, which means that the line $t\mathcal{F}^+$ is tangent to $\mathcal{F}_t^+$ at its end point $t(a(0), b(0))$, hence it lies above this line.

<u>Step 2</u> For small $\delta > 0$, the set

$$\hat{\mathcal{F}}_t^0 := t\hat{\mathcal{F}}^0 := \{t(H'(p), K(p)) : p \in [p^- - \delta, p^-]\} \subset \mathcal{F}_t^0,$$

is a graph of concave function that starts from the origin and lies below a line of slope p^- that passes through the origin. We claim that the set $\mathcal{F}_t^+$ will intersect $\hat{\mathcal{F}}_t^0$ at some point $t(a(q^t), b(q^t))$, $q^t > 0$, for small and positive t. To see this, let us compare the set $\mathcal{G}_t$ with $\hat{\mathcal{F}}^0$. The set $\mathcal{G}_t$ is above $\mathcal{F}^+$ and tangent to $\mathcal{F}^+$ at its end point. Moreover, since

$$g'(tq) = p^+ + f'(tq) = p^+ + o(1), \quad t^{-1}g(tq) = qp^+ + t^{-1}f(tq),$$

we have that $\mathcal{G}_t^+ \to \mathcal{F}^+$ as $t \to 0$. This guarantees that the sets $\mathcal{G}_t$ and $\hat{\mathcal{F}}^0$ intersect at a some point $(a(q^t), b(q^t))$ near the origin for small $t > 0$, as desired.

<u>Step 3</u> The intersection point of the sets $\mathcal{F}_t^+$ and $\hat{\mathcal{F}}_t^0$ represents a corner of the variational solution $u(q, t)$ at $q = q(t) := ta(q^t)$. The left and right derivatives of $u(\cdot, t)$ at $q(t)$, are given by the slope of $\mathcal{F}_t^0$ and $\mathcal{F}_t^+$ at the point $t(a(q^t), b(q^t))$. The right derivative is given by $\tilde{p}^+ := g'(tq^t)$ as we showed in *step* 1. To calculate the left derivative, take $\tilde{p}^- \in [p^- - \delta, p^-]$, such that $H'(\tilde{p}^-) = a(q^t)$. We then have

$$b(q^t) = K(\tilde{p}^-) = \tilde{p}^- H'(\tilde{p}^-) - H(\tilde{p}^-),$$

and the tangent vector to $\hat{\mathcal{F}}_t^0$ at $(a(q^t), b(q^t))$ is $(H''(\tilde{p}^-), \tilde{p}^- H''(\tilde{p}^-))$, which has a slope $\tilde{p}^-$. It remains to show that the Oleinik condition is violated for the left and right momenta $\tilde{p}^-$ and $\tilde{p}^+$.

<u>Final step</u> For small t, we have $\tilde{p}^- = p^- + o(1)$, $\tilde{p}^+ = p^+ + o(1)$. So $\tilde{p}^- > \tilde{p}^+$. By $H'(\tilde{p}^-) = a(q^t) = q^t + H'(g'(tq^t))$, we know that $H'(\tilde{p}^+) = H'(\tilde{p}^-) - q^t$. Hence,

$$\begin{aligned}\tilde{p}^- H'(\tilde{p}^-) - H(\tilde{p}^-) &= b(q^t) = t^{-1}g(tq^t) + \tilde{p}^+ H'(\tilde{p}^+) - H(\tilde{p}^+)\\ &= t^{-1}g(tq^t) - \tilde{p}^+ q^t + \tilde{p}^+ H'(\tilde{p}^-) - H(\tilde{p}^+).\end{aligned}$$

Equivalently,

$$\begin{aligned}(\tilde{p}^- - \tilde{p}^+)H'(\tilde{p}^-) + H(\tilde{p}^+) - H(\tilde{p}^-) &= t^{-1}(g(tq^t) - g'(tq^t)tq^t)\\ &= t^{-1}(f(tq^t) - f'(tq^t)tq^t)\\ &=: t^{-1}\varphi(tq^t).\end{aligned}$$

We note that $\varphi(0) = 0$ and $\varphi'(q) < 0$ for $q > 0$ by convexity of f. As a result,

$$(\tilde{p}^- - \tilde{p}^+)H'(\tilde{p}^-) < H(\tilde{p}^-) - H(\tilde{p}^+). \tag{4-9}$$

This violates the Oleinik condition because $\tilde{p}^+ < \tilde{p}^-$. □

Since, at every discontinuity point (q, t) of $\hat{u}_q$, the Oleinik condition is always satisfied by the pair $(\hat{u}_q(q-, t), \hat{u}_q(q+, t))$, where $\hat{u}$ is a viscosity solution (see the exercise at the end of Section 4B), we deduce that the variational solution of Theorem 4.12 is not a viscosity solution. In Example 4.13 below, we make some additional assumptions on H, so that we can find a rather precise description for the viscosity solution $\hat{u}$ for small t, with H and g as in Theorem 4.12. This would allow us to show that the jump discontinuity of $\hat{u}_q$ occurs at a point $\hat{q}(t)$ such that $q(t) < \hat{q}(t)$ for small positive t. Moreover, $u(q, t) > \hat{u}(q, t)$ for $q \in (0, \hat{q}(t))$, and small positive t. The details follow.

Example 4.13. Let H and g be as in Theorem 4.12. Additionally, assume that H is concave near p^-, and for some $\delta, \delta_1, \delta_2 > 0$,

$$\{p \in [p^+, p^-] : H(p) \in [-\delta, 0]\} = [p^+, p^+ + \delta_1] \cup [p^- - \delta_2, p^-].$$

Choose $\delta^- \in (0, \delta_2]$, $\delta^+ \in (0, \delta_1]$ such that for each $p \in [p^+, p^+ + \delta^+]$, there exists a unique $\psi(p) \in [p^- - \delta^-, p^-]$ such that $\psi(p^+) = p^-$, and

$$H(p) - H(\psi(p)) = H'(\psi(p))(p - \psi(p)). \tag{4-10}$$

Let us write $\hat{u}$ for the viscosity solution with the initial condition g. We claim that $\hat{u}(\,\cdot\,, t)$ has a corner at some $\hat{q}(t)$ with the following properties: $\hat{q}(0) = 0$, and for small $t > 0$,

$$\hat{q}'(t) = H'(\hat{p}_-(t)), \quad \hat{p}_-(t) = \psi(\hat{p}_+(t)), \tag{4-11}$$

where $\hat{p}_\pm(t) = \hat{u}_q(\hat{q}(t), t)$ represent the left and right values of $\hat{u}_q$ at $\hat{q}(t)$. We now express $\hat{p}^+(t)$ in terms of $\hat{q}(t)$, so that the ODE (4-11) can be solved uniquely for the initial condition $\hat{q}(0) = 0$. For this, let us write $h : [\hat{p}_+, \infty) \to [0, \infty)$ for $(g')^{-1}$, so that $h(p_+) = 0$. Note if for some q, we have $\hat{q}(t) = q + tH'(g'(q))$, then $\hat{p}_+(t) = g'(q)$. Equivalently,

$$\hat{q}(t) = h(\rho) + tH'(\rho), \quad \hat{p}_+(t) = \rho.$$

Let us write $\ell(q,t)$ for the inverse of $\rho \mapsto h(\rho)+tH'(\rho)$, that is increasing and well-defined for small t. This gives us the formula

$$\hat{p}_+(t) = \ell(\hat{q}(t),t),$$

which allows us to express $\hat{p}_-(t)$ as a function of $\hat{q}(t)$. The function $\ell(q,t)$ can be expressed as $\ell = w_q$, where w solves the HJE with initial condition $g(q), q \geq 0$, and our formula for ℓ is compatible with (4-7). In particular

$$\ell_t + H'(\ell)\ell_q = 0.$$

We note that $\hat{q}'(0)=0$ but $\hat{q}'(t)>0$ for $t>0$ and small because $H'(p_-(t))>0$. On the other hand,

$$p'_+(t) = \ell_t(\hat{q}(t),t) + \ell_q(\hat{q}(t),t)\hat{q}'(t) = \ell_q(\hat{q}(t),t)(H'(\hat{p}_-(t)) - H'(\hat{p}_+(t))).$$

Since $\ell_q > 0$, $H'(\hat{p}_-(t))>0$, $H'(\hat{p}_+(t))<0$, we deduce that $\hat{p}_+(t)$ is increasing as a function of t. Since ψ is decreasing, we learn that $\hat{p}_-(t)$ is decreasing. On the other hand,

$$\hat{q}''(t) = H''(p^-(t))p'_-(t) > 0,$$

for small t. This means that $\hat{q}$ is convex. This is how the viscosity solution for short times look like:

- For $Q \geq \hat{q}(t)$ we have $\hat{u}(Q,t) = g(h(\rho)) + tK(\rho)$, where $\rho = \ell(Q,t)$.
- For $Q \leq 0$, we have $\hat{u}(Q,t) = p^- Q$.
- For $Q \in [0,\hat{q}(t)]$, we first set $Q(s,t) = \hat{q}(s) + (t-s)H'(\hat{p}_-(s))$, for $s \leq t$. We note that $Q_s = (t-s)H''(\hat{p}_-(s))\hat{p}'_-(s) > 0$, so that $s \mapsto Q(s,t)$ is increasing with $Q(0,t)=0$, $Q(t,t)=\hat{q}(t)$. Its inverse is denoted by $s(Q,t)$, and $\hat{u}(Q,t) = \hat{u}(\hat{q}(s),s) + (t-s)H'(\hat{p}_-(s))$, for $s = s(Q,t)$.

What we have constructed is a viscosity solution because it solves HJE outside the set $\{(\hat{q}(t),t) : t \in [0,\delta)\}$ for small δ, and on this set the Oleinik condition is satisfied. It also coincides with g initially. So $\hat{u}$ must be the unique viscosity solution.

For comparison, let us write u for the variational solution which has a corner at $q(t)$ with the left and right momenta at $q(t)$ given by $\tilde{p}^{\pm}(t)$ as we discussed in the proof of Theorem 4.12. Indeed by (4-10) and (4-9),

$$H(\hat{p}_+(t)) - H(\hat{p}_-(t)) - H'(\hat{p}_-(t))(\hat{p}_+(t) - \hat{p}_-(t)) = 0,$$
$$H(\tilde{p}^+(t)) - H(\tilde{p}^-(t)) - H'(\tilde{p}^-(t))(\tilde{p}^+(t) - \tilde{p}^-(t)) < 0,$$

for $t > 0$. In comparison,

$$\begin{aligned}
\hat{p}_-(t) &= \psi(\hat{p}_+(t)),\\
\tilde{p}^-(t) &> \psi\big(\tilde{p}^+(t)\big),\\
\hat{q}'(t) &= H'(\hat{p}_-(t)) = H'(\psi(\hat{p}_+(t))),\\
q'(t) &= H[\tilde{p}^+(t), \tilde{p}^-(t)] < H'(\psi(\tilde{p}^+(t))).
\end{aligned}$$

To the left and right of the discontinuity curve, both u_q and $\hat{u}_q$ are classical solutions that can be determined by the method of characteristics. Hence

$$\hat{p}_+(t) = \ell(\hat{q}(t), t), \quad \tilde{p}^+(t) = \ell(q(t), t).$$

Hence,

$$\hat{q}'(t) = H'(\psi(\ell(\hat{q}(t), t))), \quad q'(t) < H'(\psi(\ell(q(t), t))).$$

From this and $q(0) = \hat{q}(0) = 0$, we deduce that $\hat{q}(t) < q(t)$ for small $t > 0$. Note that $u(q,t) = \hat{u}(q,t)$ for $q \notin (0, \hat{q}(t))$. We claim that $\hat{u}(q,t) < u(q,t)$ if $q \in (0, \hat{q}(t))$, and t is small. As a preparation, we t show that if $\rho = u_q$ and $\hat{\rho} = \hat{u}_q$, then $\hat{\rho}(q,t) < \rho(q,t)$ for $q \in (0, \hat{q}(t))$. To verify this, we first consider the case $q \in (q(t), \hat{q}(t))$. For small t, $\rho(q,t) = \rho(q_0, 0) = g'(q_0)$ for some q_0 that is close to 0. Hence $\rho(q,t)$ is close to p^+. However, since such q is on the left side of the jump discontinuity for $\hat{\rho}$, we have $\hat{\rho}(q,t)$ is close to ρ^-, which is strictly larger than ρ^+. This implies that $\hat{\rho}(q,t) < \rho(q,t)$ for small t, and $q \in (q(t), \hat{q}(t))$. In the same fashion we can treat the case $q \in (0, q(t))$.

We are now ready to show that $\hat{u}(q,t) < u(q,t)$ if $q \in (0, \hat{q}(t))$, and t is small. Indeed for $q \in (0, \hat{q}(t))$,

$$\begin{aligned}
u(q,t) &= u(\hat{q}(t), t) - \int_q^{\hat{q}(t)} \rho(a,t)\,da\\
&= \hat{u}(\hat{q}(t), t) - \int_q^{q(t)} \rho(a,t)\,da\\
&> \hat{u}(\hat{q}(t), t) - \int_q^{\hat{q}(t)} \hat{\rho}(a,t)\,da\\
&= \hat{u}(q,t),
\end{aligned}$$

as desired.

As we have seen in the proof of Theorem 4.12, we can easily calculate a solution for small times if the second derivative of the initial data is uniformly bounded.

Proposition 4.14. *Assume that $D^2 H$ and $D^2 g$ are uniformly bounded, and g is C^1 and Lipschitz. Write u and $\hat{u}$ for variational and viscosity solution with initial condition g. Then there exists $t_0 > 0$ (with t_0 depending only on the uniform bounds on $D^2 H$ and $D^2 g$) such that for $t \in [0, t_0]$, we have*

$$u(Q, t) = \hat{u}(Q, t) = g(q(0)) + \int_0^t [p \cdot \dot{q} - H(q, p)]\, ds,$$

where $(q(s), p(s)) = \phi_s(q(0), \nabla g(q(0)))$ is the unique Hamiltonian orbit such that $q(t) = Q$.

The proof of Proposition 4.14 is rather straightforward and is carried out by showing that the map $a \mapsto q(a, t)$ is a homeomorphism for small t, where $q(a, t)$ is the q-component of $\phi_t(a, \nabla g(a))$; see [3] for details.

We saw in Example 4.13 that for the initial condition of Theorem 4.12, the variational solution dominates the viscosity solution. This indeed is always true as the following result of Bernard [4] confirms.

Theorem 4.15. *Assume that $D^2 H$ is uniformly bounded and g is Lipschitz. We also assume that $g \in C^2$, and that there exists a constant c_0 such that $D^2 g(q) \leq c_0 I$ for every $q \in \mathbb{R}^d$ (or more generally, g is semiconcave). Write $\hat{u}$ and u for viscosity and variational solution with initial condition g. Then there exists $t_1 > 0$ (with t_1 depending only on c_0 and the bound on $D^2 H$) such that the following statements are true for $t \in [0, t_1]$:*

(i) $\hat{u}(q, t) \leq u(q, t)$.

(ii) $u(q, t) = \inf\{z : (q, z) \in \mathcal{F}_t(g)\}$.

4D. ***Variational selectors.*** We now give a recipe for the construction of variational solutions in the discrete setting. A similar construction can be give for the continuous setting. We write Λ for the set of Lipschitz functions, and Λ_r for the set of $g \in \Lambda$ such that $|g(q) - g(q')| \leq r|q - q'|$. Recall that a variational solution $u_n(Q)$ is a critical value of

$$A(\boldsymbol{x}_n; Q; g) = g(q_0) + \sum_{i=1}^{n} [p_{i-1} \cdot (q_i - q_{i-1}) - w(p_{i-1}, q_i)],$$

where $q_n = Q$, and $\boldsymbol{x}_n = (x_0, \ldots, x_{n-1})$, with $x_i = (q_i, p_i) \in \mathbb{R}^{2d}$. We assume that $w : \mathbb{R}^{2d} \to \mathbb{R}$ is a C^1 and Lipschitz function. We may write $A = \ell + f$, where ℓ is a quadratic function and f is a Lipschitz function. Writing $\boldsymbol{x}_n = x = (q, p) \in \mathbb{R}^k$ for $k = 2nd$, then

$$\ell(x) = \tfrac{1}{2} Bx \cdot x = \sum_{i=1}^{n-1} p_{i-1} \cdot (q_i - q_{i-1}) - p_{n-1} \cdot q_{n-1},$$

where B is a matrix of the form

$$B = \begin{bmatrix} 0 & D \\ D^t & 0 \end{bmatrix},$$

where D is a matrix which has -1 on its main diagonal, 1 right below the main diagonal, and 0 elsewhere. As a result, ℓ is a nondegenerate quadratic form. Because of the very form of A, we make the following definition.

Definition 4.16. (i) We write $\mathcal{Q}_k$ for the set of nondegenerate quadratic functions $\ell : \mathbb{R}^k \to \mathbb{R}$. In other words, $\ell(x) = \frac{1}{2} Bx \cdot x$ for a nonsingular symmetric matrix B. We write $\Omega_k(\ell; r)$ for the set of functions $F : \mathbb{R}^k \to \mathbb{R}$ such that $F = \ell + f$ for some $f \in \Lambda_r$. We write

$$\mathcal{Q} = \bigcup_{k=1}^{\infty} \mathcal{Q}_k, \quad \Omega_k = \bigcup_{r=1}^{\infty} \bigcup_{\ell \in \mathcal{Q}_k} \Omega_k(\ell; r), \quad \Omega = \bigcup_{k=1}^{\infty} \Omega_k.$$

(ii) We call $\mathcal{C} : O \to \mathbb{R}$ a *variational selector* if it satisfies the following conditions:

(1) If $F \in \Omega$ and $F \in C^1$, then $\mathcal{C}(F) = F(\bar{\alpha})$, for some $\bar{\alpha}$ with $\nabla F(\bar{\alpha}) = 0$.
(2) If $f_1, f_2 \in \Lambda$, with $f_1 \le f_2$, and $\ell \in \mathcal{Q}$, then $\mathcal{C}(\ell + f_1) \le \mathcal{C}(\ell + f_2)$.
(3) $\mathcal{C}(F + c) = \mathcal{C}(F) + c$, for every $F \in \Omega$ and $c \in \mathbb{R}$.
(4) If $F \in \Omega$ is bounded below, then $\mathcal{C}(F) = \min F$.
(5) If $\psi : \mathbb{R}^k \to \mathbb{R}^k$ is a Lipschitz smooth diffeomorphism, and $F \in \Omega_k$, then $\mathcal{C}(F) = \mathcal{C}(F \circ \psi)$.
(6) If $F \in \Omega_k$, $\ell' \in \mathcal{Q}_{k'}$, and $F'(x, y) = F(x) + \ell'(y)$, then $\mathcal{C}(F') = \mathcal{C}(F)$.

Once a variational selector is known, then we can use it to construct a variational solution by setting

$$\mathcal{V}_n(g)(Q) = \mathcal{C}(A(\,\cdot\,; Q; g)). \tag{4-12}$$

As we mentioned before we use Lusternik–Schnirelmann (LS) theory to construct a selector; see for example [5] for more details. Before we give a precise recipe for $\mathcal{C}$, we make some remarks:

Proposition 4.17. (i) *If* $F \in \Omega_k(\ell; r)$, *with* $F = \ell + f$, $\ell(x) = 2^{-1} Bx \cdot x$, *and* $\nabla F(\bar{\alpha}) = 0$, *then*

$$|\bar{\alpha}| \le r\delta(\ell)^{-1}, \quad \textit{where } \delta(\ell) = \inf_{|x|=1} |Bx|.$$

(ii) *If* $\ell + f = \ell' + f'$, *for* $f, f' \in \Lambda$, $\ell, \ell' \in \mathcal{Q}_k$, *then* $\ell = \ell'$, *and* $f = f'$.

Proof. (i) At a critical point $\bar{\alpha}$ we have $B\bar{\alpha} = -\nabla f(\bar{\alpha})$, which implies

$$\delta(\ell)|\bar{\alpha}| \le |B\bar{\alpha}| = |\nabla f(\bar{\alpha})| \le r,$$

as desired.

(iii) If $\ell + f = \ell' + f'$, then $\ell'' = f''$, where $\ell'' = \ell' - \ell$, $f'' = f - f'$. Since f'' is Lipschitz, then $\ell'' = 0$. In fact if $\ell''(x) = B''x \cdot x$, and v is an eigenvector of B'' associated with eigenvalue λ, then $\varphi(t) = \lambda|v|^2t^2$ must be Lipschitz in t, which is impossible unless $\lambda|v|^2 = 0$. □

LS theory is normally applied to continuous maps $F : M \to \mathbb{R}$, for a compact manifold M. In our case the nondegeneracy of quadratic function ℓ makes up for the lack of compactness. A standard way to find a critical value of F is by designing a collection $\mathcal{F}$ of subsets of $\mathbb{R}^k$ such that

$$c(F, \mathcal{F}) = \inf_{A \in \mathcal{F}} \sup_A F,$$

is a critical value of F. This is guaranteed if the collection $\mathcal{F}$ satisfies the following property:

$$A \in \mathcal{F}, t > 0 \Longrightarrow \varphi_t^F(A) \in \mathcal{F},$$

where φ_t^F denotes the flow of the vector field $-\nabla F$. To have a universal collection $\mathcal{F}$ that works for all F, we assume two properties for $\mathcal{F}$:

(1) If $A \in \mathcal{F}$, and φ is a homeomorphism, then $\varphi(A) \in \mathcal{F}$.

(2) If $A \in \mathcal{F}$, and $A \subset B$, then $B \in \mathcal{F}$.

Note that the second property is harmless and can always be assumed because of the infimum over subsets of $A \in \mathcal{F}$ in the definition of c. Its raison d'être is the following alternative expression for $c(F, \mathcal{F})$:

$$c(F, \mathcal{F}) = \inf_{A \in \mathcal{F}} \sup_A F = \inf_{r \in \mathbb{R}} \{r : M_r(F) \in \mathcal{F}\}, \tag{4-13}$$

where

$$M_r(F) = \{x : F(x) < r\}.$$

Indeed if we write c and $\bar{\alpha}$ for the left and right-hand sides of the second equality in (4-13), then for any $a > c$, we can find $A \in \mathcal{F}$ such that $\sup_A F < a$, which means that $A \subseteq M_a(F)$. This in turn implies that $M_a(F) \in \mathcal{F}$, which leads to $\bar{\alpha} \le c$. In the same fashion, we can verify $c \le \bar{\alpha}$.

It remains to design a family $\mathcal{F}$ such that (1) and (2) hold, and $c(F, \mathcal{F})$ is finite. Once such a family is found, we set $\mathcal{C}(F) = c(F, \mathcal{F})$. In view of (4-13), and property (1), we my choose $\mathcal{F}$ the collection of sets with certain degree of topological complexity, so that $c(F, \mathcal{F})$ is the first r for which the sublevel set $M_r(F)$ reaches such complexity. We now describe the LS strategy. Write $\Omega_k^0(\ell, r_0)$ for the set of $F \in \Omega_k(\ell, r_0)$ such that $F(0) = 0$. Let us consider $F \in \Omega_k^0(\ell, r_0)$, and set $c_0 = r_0\delta(\ell)^{-1}$, $c_1 = r_0c_0$, so that

$$\nabla F(\bar{\alpha}) = 0 \Longrightarrow |\bar{\alpha}| \le c_0 \Longrightarrow |F(\bar{\alpha})| \le c_1,$$

by Proposition 4.17(i). Note that ℓ has a single critical point at the origin. Hence for $a < 0 < b$, the set $M_b(\ell)$ is topologically more complex than $M_a(\ell)$. Since F is a Lipschitz perturbation of ℓ, and all critical values of F are in the interval $[-c_1, c_1]$, we expect $M_{c_1}(F)$ to be topologically more complex than $M_{-c_1}(F)$. We wish to design a collection $\mathcal{F}$ that captures such complexity. *Relative cohomology classes* allow us to measure such complexities.

Definition 4.18. Given two open sets $A \subset B$, we write $\Lambda^j(B, A)$ for the set of closed j forms α in B such that the restriction of α to the set A is exact. We write $\alpha \sim \beta$ for two forms in $\Lambda^j(B, A)$ such that $\beta - \alpha$ is exact in B. We write $H^j(B, A)$ for the set of equivalent classes and $H^*(B, A)$ for the union of $H^j(B, A)$, $j = 0, 1, \ldots$.

For example, for $a < 0 < b$, one can show that $H^*(M_b(\ell), M_a(\ell))$ is the same as $H^*(D, \partial D)$, where D is a disc in $\mathbb{R}^{r^-}$, with r^- denoting the number of the negative eigenvalues of B. In fact the set $M_{-c_1}(F)$ is homeomorphic to $M_{-c_1}(\ell)$, and we may define

$$\mathcal{C}(F) = \inf\{r : H^*(M_r(F), M_{-c_1}(F)) \neq 0\} = \sup\{r : H^*(M_r(F), M_{-c_1}(F)) = 0\}.$$

Remark 4.19. More generally, we may take any $\alpha \in H^*(M_b(\ell), M_a(\ell))$, and set

$$\begin{aligned} \mathcal{C}(F; \alpha) &= \inf\{r : \text{ the restriction of } \alpha \text{ to } M_r(F) \text{ is not exact}\} \\ &= \sup\{r : \text{ the restriction of } \alpha \text{ to } M_r(F) \text{ is exact}\}. \end{aligned}$$

We refer to [5] for more details.

4E. ***Game theory.*** We now offer a way of constructing viscosity solutions via game theory that in spirit is close to our construction of variational solutions in Section 4D When $H(q, p)$ is convex in the momentum variable, then the variational solution is also a viscosity solution and (4-3) offers a control theoretical representation of the solution; see [6] for a thorough discussion on the applications of (4-3). When H is not convex in the momentum, a minimax type variational description does the job.

For our purposes, it is more convenient to solve the final value problem

$$\begin{cases} u_t + H(q, u_q) = 0, & t < T, \\ u(q, T) = g(q). \end{cases} \tag{4-14}$$

We assume that H is of the following form

$$H(q, p) = \inf_{z \in Z} \hat{H}(q, p; z) = \inf_{z \in Z} \sup_{v} (p \cdot v - \hat{L}(q, v; z)),$$

where Z is some measure space, $\hat{H}(q, p; z)$ is convex in p for each $z \in Z$, and we writing $\hat{L}(q, v; z)$ for its Legendre transform in the p-variable. We assume that there exist constants $\eta_0 > 1$, $\delta_0 > 0$, and a_0 such that

$$\begin{aligned} \hat{L}(q, v; z) \geq L_0(v) := \delta_0 |v|^{\eta_0} - a_0, \quad \sup_{|v'| \leq 1} \hat{L}(q, v'; z) \leq a_0, \\ \lim_{\delta \to 0} \sup_{z' \in Z} \sup_{|x| \leq 1} \sup_{|x - x'| \leq \delta} |\hat{H}(x'; z') - \hat{H}(x; z')| = 0, \\ \sup_{z' \in Z} \sup_{q'} \sup_{|p'| \leq \ell} |\hat{H}_p(q', p'; z')| < \infty, \end{aligned} \tag{4-15}$$

for all $q, v \in \mathbb{R}^d$, $z \in Z$, and $\ell > 0$.

Definition 4.20. We write $V(t, T)$ for the set of bounded measurable maps $v : [t, T] \to \mathbb{R}^d$, and $Z(t, T)$ for the set of measurable maps $z : [t, T] \to Z$. We write $\Delta(t, T)$ for the set of *strategies*. By a strategy, we mean a map $\alpha : Z(t, T) \to V(t, T)$ such that if $t < s \leq T$, and $z = z'$ on $[t, s]$, then $\alpha[z] = \alpha[z']$ on $[t, s]$.

We are now ready to offer a solution to (4-14). For $t \leq T$, set

$$\begin{aligned} u(q, t) &= \mathcal{S}_t^T(g)(q) \\ &= \sup_{\alpha \in \Delta(t,T)} \inf_{z \in Z(t,T)} \left[g(q(T)) - \int_t^T \hat{L}(q(\theta), \dot{q}(\theta); z(\theta))\, d\theta \right], \end{aligned} \tag{4-16}$$

where $q(\cdot) = q(\cdot\,; t, q, \alpha[z])$ is uniquely specified by the requirements $q(t) = q$, and $\dot{q} = \alpha[z] =: v$. In other words, for $\theta \in [t, T]$,

$$q(\theta) = q + \int_t^\theta \alpha[z](\theta')\, d\theta'.$$

Note that we may write $\dot{q}(\theta) = \hat{H}_p(q(\theta), p(\theta); z(\theta))$, where

$$p(\theta) = \hat{L}_v(q(\theta), \alpha[z](\theta); z(\theta)).$$

In terms of $p(\cdot)$, we have

$$\hat{L}(q(\theta), \dot{q}(\theta); z(\theta)) = p(\theta) \cdot \dot{q}(\theta) - \hat{H}(q(\theta), p(\theta); z(\theta)).$$

When H is not convex in p, the relationship $v = H_p(q, p)$ is no longer invertible in p for a given q. However, if we specify z, then we can invert $p \mapsto \hat{H}_p(q, p; z)$. The role of the path $q(\cdot)$ is the same as the characteristic. The optimal path still solves the Hamiltonian ODE locally, but it is allowed to have corners when we switch from one label z to another.

Theorem 4.21. *The function u as in* (4-16) *is a viscosity solution of* (4-14).

The main ingredient for the proof of Theorem 4.21 is the following *dynamic programming optimality condition*:

Theorem 4.22. *For* $s \in [t, T]$, *we have*

$$\mathcal{S}_t^T(g)(q) = \sup_{\alpha\in\Delta(t,s)} \inf_{z\in Z(t,s)} \left[\mathcal{S}_s^T(g)(q(s)) - \int_t^s \hat{L}(q(\theta), \dot{q}(\theta); z(\theta))\, d\theta \right]. \tag{4-17}$$

Proof. Fix q. We write $u(q,t)$ and $u'(q,t)$ for the left and right hand sides of (4-17) respectively. We carry out the proof in two steps.

First we pick $c < u'(q,t)$ and show that $c < u(q,t)$. Observe that since $c < u'(q,t)$, there exists $\beta \in \Delta[t,s]$ such that for all $y \in Z(t,s)$, we have

$$c < \mathcal{S}_s^T(g)(q(s)) - \int_t^s \hat{L}(q(\theta), \dot{q}(\theta); y(\theta))\, d\theta,$$

with $q(\theta) = q + \int_t^\theta \beta[y](\theta')\, d\theta'$, for $\theta \in [t,s]$. Now given $a = q(s)$, we can find $\gamma_a \in \Delta(s,T)$ such that for every $w \in Z(s,T)$, we have

$$c < g(\rho(T)) - \int_s^T \hat{L}(\rho(\theta), \dot{\rho}(\theta); w(\theta))\, d\theta - \int_t^s \hat{L}(q(\theta), \dot{q}(\theta); y(\theta))\, d\theta, \tag{4-18}$$

where

$$\rho(\theta) = q(s) + \int_s^\theta \gamma_{q(s)}[w](\theta')\, d\theta' = q + \int_t^s \beta[y](\theta')\, d\theta' + \int_s^\theta \gamma_{q(s)}[w](\theta')\, d\theta',$$

for $\theta \in [s,T]$. We now construct $\alpha \in \Delta(t,T)$ as follows: Given $z \in Z(t,T)$, we set

$$\hat{\alpha}[z](\theta) = \begin{cases} \beta[z \restriction_{[t,s]}](\theta), & \theta \in [t,s], \\ \gamma_{\underline{q}(s)}[z \restriction_{[s,T]}](\theta), & \theta \in (s,T], \end{cases}$$

where $\underline{q}(s) = q + \int_t^s \beta[z \restriction_{[t,s]}](\theta)\, d\theta$. More generally, we define $\underline{q}(\,\cdot\,)$, as

$$\underline{q}(\theta) = q + \int_t^\theta \hat{\alpha}[z](\theta')\, d\theta',$$

for $\theta \in [t,T]$. Observe that (4-18) means

$$c < g(\underline{q}(T)) - \int_t^T \hat{L}(\underline{q}(\theta), \dot{\underline{q}}(\theta); z(\theta))\, d\theta \le u(q,t),$$

for every $z \in Z(t,T)$. This completes the proof of $u' \le u$.

We now turn to the proof of $u \le u'$. Pick $c < u(q,t)$, and choose $\hat{\alpha} \in \Delta(t,T)$ such that for every $z \in Z(t,T)$

$$\begin{aligned} c &< g(\underline{q}(T)) - \int_t^T \hat{L}(\underline{q}(\theta), \dot{\underline{q}}(\theta); z(\theta))\, d\theta \\ &= g(\underline{q}(T)) - \int_s^T \hat{L}(\underline{q}(\theta), \dot{\underline{q}}(\theta); z(\theta))\, d\theta - \int_t^s \hat{L}(\underline{q}(\theta), \dot{\underline{q}}(\theta); z(\theta))\, d\theta, \end{aligned}$$

where $\underline{q}(\theta) = q + \int_t^\theta \hat{\alpha}[z](\theta')\,d\theta'$, for $\theta \in [t, T]$. We then define $\beta \in \Delta(t, s)$ as follows: for every $y \in Z(t, s)$, we have $\beta[y] = \alpha[y']$, where $y' \in Z(t, T)$, is any extension of y. For this β, we wish to show that for every $y \in Z(t, s)$,

$$c < \mathcal{S}_s^T(g)(q(s)) - \int_t^s \hat{L}(q(\theta), \dot{q}(\theta); z(\theta))\,d\theta,$$

where $q(\theta) = q + \int_t^\theta \beta[y](\theta')\,d\theta'$ for $\theta \in [t, s]$. Given $y \in Z(t, s)$, we need to come up with a family of strategies $\gamma_a \in \Delta(s, T)$ such that for every $w \in Z(s, T)$, we have

$$c < g(\rho(T)) - \int_s^T \hat{L}(\rho(\theta), \dot{\rho}(\theta); w(\theta))\,d\theta - \int_t^s \hat{L}(q(\theta), \dot{q}(\theta); y(\theta))\,d\theta,$$

where

$$\rho(\theta) = q(s) + \int_s^\theta \gamma_{q(s)}[w](\theta')\,d\theta'.$$

This is achieved by setting

$$\gamma_{q(s)}[w] = \alpha[y \oplus w],$$

where

$$(y \oplus w)(\theta) = \begin{cases} y(\theta), & \theta \in [t, s], \\ w(\theta), & \theta \in [s, T]. \end{cases} \qquad \square$$

As our next step we show that we can always restrict α in (4-16) to those with bounded range:

Proposition 4.23. *If $g \in \Lambda_r$, then the supremum in* (4-16) *can be restricted to those α such that*

$$\begin{aligned} M(\alpha) &:= \sup_{z \in Z(t,T)} M(\alpha, z) \\ &:= \sup_{z \in Z(t,T)} \left[\frac{1}{T-t} \int_t^T |\alpha[z](\theta)|^{\eta_0}\,d\theta \right]^{1/\eta_0} \\ &\le C_0, \end{aligned} \tag{4-19}$$

where

$$C_0 = C_0(r, \delta_0, \eta_0, a_0) = 2a_0 + \left(\frac{r+1}{\delta_0} \right)^{1/(\eta_0 - 1)}.$$

Proof. Assume that $g \in \Lambda_r$. Write

$$A(q; \alpha, z(\cdot)) := g(q(T)) - \int_t^T \hat{L}(q(\theta), \dot{q}(\theta); z(\theta))\,d\theta,$$

with $q(\cdot)$ as in (4-16). From $g \in \Lambda_r$, and (4-15),

$$\begin{aligned} A(q;\alpha,z(\cdot)) &\le g(q)+r\left|\int_t^T \alpha[z]\,d\theta\right|+a_0(T-t)-\delta_0(T-t)M(\alpha,z)^{\eta_0} \\ &\le g(q)+r(T-t)M(\alpha,z)+a_0(T-t)-\delta_0(T-t)M(\alpha,z)^{\eta_0}. \end{aligned} \tag{4-20}$$

On the other hand,

$$A(q;0,z(\cdot)) = g(q) - \int_t^T \hat{L}(q,0;z(\theta))\,d\theta \ge g(q) - a_0(T-t),$$

by (4-15). In (4-16), we may ignore those α such that

$$\inf_{z\in Z(t,T)} A(q;\alpha,z(\cdot)) < g(q) - a_0(T-t). \tag{4-21}$$

Using (4-20), the inequality (4-21) would be, if that for some $z(\cdot) \in Z(t,T)$, we have

$$r(T-t)M(\alpha,z) + a_0(T-t) - \delta_0(T-t)M(\alpha,z)^{\eta_0} < -a_0(T-t)$$

Equivalently,

$$\delta_0 M(\alpha,z)^{\eta_0} - rM(\alpha,z) - 2a_0 > 0.$$

This inequality is valid if

$$M(\alpha,z) > C_0 := 2a_0 + \left(\frac{r+1}{\delta_0}\right)^{1/(\eta_0-1)}.$$

In summary, we may ignore those α such that

$$\sup_{z\in Z(t,T)} M(\alpha,z) > C_0.$$

We are done. □

With the aid of (4-19), we can show the regularity of $u = \mathcal{S}_t(g)$.

Theorem 4.24. *Assume that $g \in \Lambda_r$. Then the following statements are true*:

(i) *The value of $u(q,t) = (\mathcal{S}_t^T g)(q)$ depends only on the restriction of g to the set*

$$B_{C_0(T-t)}(q) := \{q' : |q'-q| \le C_0(T-t)\}.$$

(ii) *The value of $u(q,t) = (\mathcal{S}_t^T g)(q)$ depends only on the restriction of $\hat{H}$ to the set*

$$B_{C_0(T-t)}(q) \times \mathbb{R}^d \times Z = \{(q',p,z) \in \mathbb{R}^{2d} \times Z : |q'-q| \le C_0(T-t)\}.$$

(iii) *We have*

$$-a_0(T-t) \le u(q,t) - g(q) \le C_1(T-t), \tag{4-22}$$

where $C_1 = C_1(r) = a_0 + c_1 r^{\eta_1}$, *for constants* $\eta_1 = \eta_0/(\eta_0 - 1)$, *and* $c_1 = c_1(\delta_0, \eta_0)$.

(iv) *Assume that* $s \in [t, T]$. *Then*

$$-a_0(s-t) \le u(q,t) - u(q,s) \le C_1(s-t). \tag{4-23}$$

(v) *For every* $t < T$, *and* $q, q' \in \mathbb{R}^d$, *we have*

$$|u(q',t) - u(q,t)| \le (C_1 + a_0 + r)|q' - q|. \tag{4-24}$$

Proof. (i) The dependence of u on the final data is of the form $g(q(T))$ with

$$|q(T) - q| = \left| \int_t^T \alpha[z] d\theta \right| \le C_0(T-t),$$

by(4-19).

(ii) The spatial dependence of $\hat{L}$ is $q(\theta)$ with $\theta \in [t, T]$. We are done because $|q(\theta) - q| \le C_0(T-t)$ by (4-19).

(iii) By choosing the strategy $\alpha = 0$ in the definition of u, and using (4-15) we get

$$u(q,t) \ge g(q) - a_0(T-t).$$

On the other hand, by $g \in \Lambda_r$ and (4-15),

$$\begin{aligned}
u(q,t) &\le g(q) + \sup_{\alpha \in \Delta(t,T)} \inf_{z \in Z(t,T)} \left[r|q(T) - q| - \int_t^T L_0(\dot{q}(\theta))\, d\theta \right] \\
&\le g(q) + \sup_{\alpha \in \Delta(t,T)} \inf_{z \in Z(t,T)} \left[r|q(T) - q| - (T-t) L_0\left(\frac{q(T) - q(t)}{T-t} \right) \right] \\
&= g(q) + \sup_Q \left[r|Q - q| - (T-t) L_0\left(\frac{Q - q}{T-t} \right) \right] \\
&= g(q) + (T-t) \sup_{a \ge 0} [ra - \delta_0 a^{\eta_0} + a_0] \\
&= g(q) + (T-t)[a_0 + c_1 r^{\eta_1}],
\end{aligned}$$

as desired.

(iv) Set $\delta = s - t$. From (4-17) and since $\hat{L}$ does not depend on time,

$$u(q,t) = (\mathcal{S}_{s-\delta}^T g)(q) = (\mathcal{S}_{s-\delta}^{T-\delta}(\mathcal{S}_{T-\delta}^T g))(q) = (\mathcal{S}_s^T(\mathcal{S}_{T-\delta}^T g))(q).$$

From this, $u(q,s) = \mathcal{S}_s^T g(q)$, and the contraction of the operator $\mathcal{S}_s^T$,

$$\inf(\mathcal{S}_{T-\delta}^T g - g) \le u(q,t) - u(q,s) \le \sup(\mathcal{S}_{T-\delta}^T g - g).$$

This and (4-22) yield (4-23).

(v) First we assume that $|q - q'| \ge T - t$. We then use (4-22) to write

$$\begin{aligned} u(q',t) - u(q,t) &\le (C_1 + a_0)(T-t) + g(q') - g(q) \\ &\le (C_1 + a_0)(T-t) + r|q'-q| \\ &\le (C_1 + a_0 + r)|q'-q|. \end{aligned}$$

Hence

$$|q'-q| \ge T - t \Longrightarrow |u(q',t) - u(q,t)| \le (C_1 + a_0 + r)|q'-q|. \tag{4-25}$$

On the other hand, when $\rho := |q - q'| < T - t$, we use (4-17) and (4-21) to write

$$\begin{aligned} &u(q,t) \\ &\quad = \sup_{\alpha\in\Delta(t,t+\rho)} \inf_{z\in Z(t,t+\rho)} \left[u(q(t+\rho), t+\rho) - \int_t^{t+\rho} \hat{L}(q(\theta), \dot{q}(\theta); z(\theta))\, d\theta \right] \\ &\quad \ge \sup_{\alpha\in\Delta(t,t+\rho)} \inf_{z\in Z(t,t+\rho)} \left[u(q(t+\rho), t) - \int_t^{t+\rho} \hat{L}(q(\theta), \dot{q}(\theta); z(\theta))\, d\theta \right] - C_1\rho. \end{aligned}$$

Pick a vector e and choose the constant strategy $\alpha[z] = e$ to assert

$$\begin{aligned} u(q,t) &\ge \inf_{z\in Z(t,t+\rho)} \left[u(q+\rho e, t) - \int_t^{t+\rho} \hat{L}(q+\theta e, e; z(\theta))\, d\theta \right] - C_1\rho \\ &\ge u(q+\rho e, t) - (C_1 + a_0)\rho. \end{aligned}$$

We now choose $e = (q'-q)/|q'-q|$ to conclude

$$u(q,t) - u(q',t) \ge -(C_1 + a_0)\rho,$$

which yields

$$|q'-q| \le T - t \Longrightarrow |u(q',t) - u(q,t)| \le (C_1 + a_0)|q'-q|.$$

This and (4-25) yield (4-24). □

Proof of Theorem 4.21. Fix (q_0, t_0), and assume that $\phi \in C^1$ with

$$u(q_0,t_0) = \phi(q_0,t_0), \quad u \le \phi, \quad p_0 = \phi_q(q_0,t_0), \quad r_0 = \phi_t(q_0,t_0). \tag{4-26}$$

Pick $\delta > 0$, and write $\Delta'(t_0, t_0+\delta)$ for the set of $\alpha \in \Delta(t_0, t_0+\delta)$ such that

$$M(\alpha) := \sup_{z\in Z(t_0,t_0+\delta)} \left[\delta^{-1} \int_{t_0}^{t_0+\delta} |\alpha[z](\theta)|^{\eta_0}\, d\theta \right]^{1/\eta_0} \le C_0.$$

By Theorem 4.22, and (4-19),

$$u(q_0,t_0) \\ = \sup_{\alpha\in\Delta'(t_0,t_0+\delta)} \inf_{z\in Z(t_0,t_0+\delta)} \left[u(q(t_0+\delta),t_0+\delta) - \int_{t_0}^{t_0+\delta} \hat{L}(q(\theta),\dot{q}(\theta);z(\theta))\,d\theta \right],$$

where $q(\theta)=q_0+\int_{t_0}^{\theta}\alpha[z](\theta)\,d\theta$. To ease the notation, we write Δ'_δ and Z_δ for $\Delta'(t_0,t_0+\delta)$ and $Z(t_0,t_0+\delta)$. From this and our assumption (4-26) we deduce

$$\begin{aligned} 0 &\le \sup_{\alpha\in\Delta'_\delta}\inf_{z\in Z_\delta}\left[\phi(q(t_0+\delta),t_0+\delta)-\phi(q_0,t_0)-\int_{t_0}^{t_0+\delta}\hat{L}(q(\theta),\dot{q}(\theta);z(\theta))\,d\theta\right] \\ &= \sup_{\alpha\in\Delta'_\delta}\inf_{z\in Z_\delta}\left[\int_{t_0}^{t_0+\delta}(\phi_t(q(\theta),\theta)+\dot{q}(\theta)\cdot\phi_q(q(\theta),\theta)-\hat{L}(q(\theta),\dot{q}(\theta);z(\theta)))\,d\theta\right] \\ &\le \sup_{\alpha\in\Delta'_\delta}\inf_{z\in Z_\delta}\left[\int_{t_0}^{t_0+\delta}(\phi_t(q(\theta),\theta)+\hat{H}(q(\theta),\phi_q(q(\theta),\theta);z(\theta)))\,d\theta\right] \\ &\le \sup_{\alpha\in\Delta'_\delta}\inf_{z\in Z}\left[2\int_{t_0}^{t_0+\delta}(\phi_t(q(\theta),\theta)+\hat{H}(q(\theta),\phi_q(q(\theta),\theta);z))\,d\theta\right], \end{aligned} \tag{4-27}$$

where, for the last inequality, we take the infimum over constant paths in $Z(t_0,t_0+\delta)$. On the other hand, since $M(\alpha)\le C_0$, for $\theta\in[t_0,t_0+\delta]$,

$$|q(\theta)-q_0| \le \int_{t_0}^{\theta}|\alpha[z](\theta')|\,d\theta' \le \int_{t_0}^{t_0+\delta}|\alpha[z](\theta)|\,d\theta \le \delta M(\alpha) \le C_0\delta, \tag{4-28}$$

where we used the Hölder's inequality for the third inequality.

From this and the continuity of $\hat{H}$ as in (4-15),

$$\phi_t(q(\theta),\theta)+\hat{H}(q(\theta),\phi_q(q(\theta),\theta);z)\le\phi_t(q_0,t_0)+\hat{H}(q_0,\phi_q(q_0,t_0);z)+c_1(\delta),$$

for a constant $c_1(\delta)$ such that $c_1(\delta)\to 0$ as $\delta\to 0$. This and (4-27) imply

$$\begin{aligned} 0 &\le \delta \sup_{\alpha\in\Delta'_\delta}\inf_{z\in Z}[\phi_t(q_0,t_0)+\hat{H}(q_0,\phi_q(q_0,t_0);z)+c_1(\delta)] \\ &= \delta\inf_{z\in Z}[r_0+\hat{H}(q_0,p_0;z)+c_1(\delta)] \\ &= \delta[r_0+H(q_0,p_0)+c_1(\delta)]. \end{aligned}$$

We divide both sides by δ and send $\delta\to 0$ to arrive at $0\le r_0+H(q_0,p_0)$, as desired. (Note that since we are solving a backward HJE, this is the correct inequality.)

We next assume that $\phi\in C^1$ is Lipschitz with

$$u(q_0,t_0)=\phi(q_0,t_0),\quad u\ge\phi,\quad p_0=\phi_q(q_0,t_0),\quad r_0=\phi_t(q_0,t_0).$$

After a repetition of what we did above, we now have

$$0 \geq \sup_{\alpha \in \Delta'_\delta} \inf_{z \in Z_\delta} \left[\int_{t_0}^{t_0+\delta} \big(\phi_t(q(\theta), \theta) + \dot{q}(\theta) \cdot \phi_q(q(\theta), \theta) - \hat{L}(q(\theta), \dot{q}(\theta); z(\theta)) \big) \, d\theta \right]. \tag{4-29}$$

We now make a selection for α. In principle, we wish to solve the ODE

$$\dot{q}(\theta) = v(q(\theta), \theta; z(\theta)) := \hat{H}_p(q(\theta), \phi_q(q(\theta), \theta); z(\theta)), \quad q(t) = q,$$

for a given $z(\cdot) \in Z(t, T)$, and use the solution to define

$$\alpha[z](\theta) = v(q(\theta), \theta; z(\theta)).$$

Choosing such a strategy in (4-29) allows us to deduce

$$\begin{aligned} 0 &\geq \inf_{z \in Z_\delta} \left[\int_{t_0}^{t_0+\delta} \big(\phi_t(q(\theta), \theta) + \hat{H}(q(\theta), \phi_q(q(\theta), \theta); z(\theta)) \big) \, d\theta \right] \\ &\geq \int_{t_0}^{t_0+\delta} \big(\phi_t(q(\theta), \theta) + H(q(\theta), \phi_q(q(\theta), \theta)) \big) \, d\theta. \end{aligned}$$

Again using (4-15) and (4-28) we know

$$\phi_t(q(\theta), \theta) + H(q(\theta), \phi_q(q(\theta), \theta)) \geq r_0 + H(q_0, p_0) - c_1(\delta),$$

for some constant $c_1(\delta)$ satisfying $c_1(\delta) \to 0$ if $\delta \to 0$. As a result,

$$0 \geq \delta[r_0 + H(q_0, p_0) + c_1(\delta)].$$

We divide both sides by δ and send $\delta \to 0$ to arrive at $0 \geq r_0 + H(q_0, p_0)$, as desired. □

Remark 4.25. Theorem 4.21 was established by Evans and Souganidis [9] for more general games. For our presentation we have chosen a game that is more in line with our definition of variational solutions. In fact, [9] assumes that the analog of the set Z is bounded. Under such an assumption the bound on $M(\alpha)$ becomes trivial and Proposition 4.23 is no longer needed. Though, the results of [9] are applicable only for bounded Hamiltonian functions.

5. Homogenization

In Section 1G, we discussed the homogenization phenomenon and its connection to weak KAM theory. In this section we explore the question of homogenization more closely. Several approaches have been developed to establish the homogenization for HJEs and their viscous variants that we now review:

(1) The earliest homogenization for HJE was carried out in Lions, Papanicolaou and Varadhan [17] when the Hamiltonian function is periodic in position variable. This is achieved by solving (1-6) for w^P, for every $P \in \mathbb{R}^d$. Regarding the graph of a solution to HJE as an evolving interface separating different phases, the graph of $P + \nabla w^P$, is a realization of an invariant measure associated with the inclination P. Fathi [10] extends [17] from $\mathbb{T}^d \times \mathbb{R}^d$ to the cotangent bundles of compact manifolds provided that the Hamiltonian function is Tonelli.

(2) The homogenization for the variational solutions in the periodic setting (i.e., when $M = \mathbb{T}^d \times \mathbb{R}^d$) has been established by Viterbo [31]. The *homogenized Hamiltonian function* $\overline{H}$ (see (1-12)) that Viterbo obtains for the variational solutions differs from what Lions et al. [17] obtains in the viscosity setting. Viterbo uses his homogenized Hamiltonian function to address questions in symplectic geometry.

(3) For Tonelli Hamiltonians, Lax–Oleinik formula (4-3) allowed Souganidis [29] and Rezakhanlou and Tarver [26] to establish the homogenization when the Hamiltonian function is selected according to a shift invariant probability measure. The evolution of the interface (which is the graph of a random *height function*) is a classical example of a stochastic growth model; see, for example, [25]. The homogenization in this case (as many other stochastic growth models) can be shown with the aid of the *subadditive ergodic theorem*; see [29] and [26].

(4) Homogenization for a viscous HJE with $H(x, p) = |p|^2 + V(q)$ for a potential function V is equivalent to the large deviation principle (LDP) for a Brownian motion with killing; see for example Sznitman [30]. This suggests using LDP ideas (see for example [23]) to establish homogenization; see [15].

(5) A probability measure on the space Hamiltonians yields a probability measure on the set of semigroup associated with the corresponding HJEs. Homogenization question can be formulated as a dynamical system problem for a group of transformations that are defined on the set of HJ semigroups. This approach was initiated in [22].

For the rest of this section, we explain the approaches (3) and (4) for the Frenkel–Kontorova (FK) model of Section 3A (for the part of our presentation, we follow [18]).

Let us write $\mathcal{L}$ for the set of maps $S : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ such that the map $L(q, v) = S(q, q + v)$ satisfies Assumption 3.1. We equip $\mathcal{L}$ with the topology of L^∞_{loc} that is metrizable. For the question of homogenization, we define an operator that turns a microscopic height function $g : \mathbb{R}^d \to \mathbb{R}$ to a macroscopic height function. Its inverse does the opposite:

$$(\Gamma_n g)(q) = n^{-1} g(nq), \quad (\Gamma_n^{-1} g)(q) = (\Gamma_{n^{-1}} g)(q) = n g(n^{-1} q).$$

We think of g as an initial macroscopic height function. Its growth is governed microscopically by the operators $\mathcal{T}$ or $\widehat{\mathcal{T}}$ of (3-3). The macroscopic height function after one macroscopic time step (which is n microscopic time steps) is given by $u_n = u_n^S := \widetilde{\mathcal{T}}_n^S g$, where the operator $\widetilde{\mathcal{T}}_n^S$ is defined as

$$\widetilde{\mathcal{T}}_n^S := \Gamma_n \circ (\widehat{\mathcal{T}}_S)^n \circ \Gamma_n^{-1}.$$

A *homogenization* occurs if the limit

$$\overline{\mathcal{T}}(g) := \lim_{n\to\infty} u_n^S, \tag{5-1}$$

exists for every Lipschitz function g. In the stochastic setting, we wish to establish the homogenization for almost all choices of S with respect to a probability measure that is defined on the set $\mathcal{L}$. This probability measure is assumed to be translation invariant and ergodic with respect to a natural notion of translation that will be defined shortly.

We may write

$$\begin{aligned} u_n^S(q) &= \sup_{q_1,\dots,q_n} [g(n^{-1}q_n) - n^{-1}(S(nq, q_1) + S(q_1, q_2) + \cdots + S(q_{n-1}, q_n))] \\ &= \sup_Q [g(Q) - n^{-1} S_n(nq, nQ)], \end{aligned} \tag{5-2}$$

where

$$S_n(q, Q) = \inf_{q_1,\dots,q_{n-1}} (S(q, q_1) + S(q_1, q_2) + \cdots + S(q_{n-1}, Q)).$$

To display the dependence of S_n on the generating function S, let us write $S_n(q, Q; S)$ for $S_n(q, Q)$. We also define the translations (in position variable q) as

$$\tau_a S(q, Q) = S(q + a, Q + a) = L(q + a, Q - q), \quad \tau_a g(q) = g(q + a).$$

Observe

$$\widetilde{\mathcal{T}}_n^{\tau_a S} = \tau_a \circ \widetilde{\mathcal{T}}_n^S \circ \tau_{-a} \quad \text{or} \quad \tau_a(\widetilde{\mathcal{T}}_n^S g) = \widetilde{\mathcal{T}}_n^{\tau_a S}(\tau_a g). \tag{5-3}$$

We are now ready to formulate our stochastic homogenization question.

Homogenization problem. Let $\mathbb{P}$ be a probability measure on the set $\mathcal{L}$ that is invariant with respect to the translation group $\{\tau_a : a \in \mathbb{R}^d\}$. Show that the limit (5-1) exists almost surely with respect $\mathbb{P}$. Study the properties of the limit $\overline{\mathcal{T}}$ in terms of the underlying measure $\mathbb{P}$.

Recall that our probability measure $\mathbb{P}$ is concentrated on the set of $S(q, Q) = L(q, Q - q)$ with L satisfying (3-1). This brings us two useful properties for the sequence u_n

$$u_n^S(q) = \sup_{|Q-q|\le \ell(r)} [g(Q) - n^{-1} S_n(nq, nQ)], \tag{5-4}$$

$$\lim_{\delta\to 0} \sup_{S\in\mathcal{L}} \sup_{|q|\le c} \sup_n |u_n^S(q+\delta) - u_n^S(q; S)| = 0, \tag{5-5}$$

for every $c > 0$. The proofs of these properties are similar to the proofs of Theorem 4.24(i) and(v), and are omitted. From (5-5) we can readily deduce the compactness of the sequence u_n is L^∞_{loc}. For the rest of this section, we describe two strategies that can be employed to prove the existence of a pointwise limit for the sequence u_n^S.

If we set $K_n(Q; S) = S_n(0, Q; S)$, we then have

$$S_n(q, Q; S) = K_n(Q - q; \tau_q S),$$

and the following subadditivity of K_n:

$$K_{m+n}(Q + Q'; S) \le K_m(Q; S) + K_n(Q'; \tau_Q S).$$

As a consequence

$$K_{m+n}((m+n)Q; S) \le K_m(mQ; S) + K_n(nQ; \tau_{mQ} S).$$

This subadditivity can be used to establish the homogenization with the aid of the subadditive ergodic theorem; we refer to [29; 26] for more details. More precisely, the subadditive ergodic theorem can guarantee the large n limit of $n^{-1} K_n(nQ; S)$ exists almost surely. The disadvantage of this approach is that it does not offer much information about the limit.

We now turn to approach (4) This approach is based on the following intuition that we partially discussed in Section 3: If for some C^1 Lipschitz function U, and a constant c, we have $\widehat{\mathcal{T}}(U) = U + c$, then $\Phi(q, \nabla U(q)) = (Q, \nabla U(Q))$, for the corresponding symplectic map Φ. Relationship between q and $Q = F(q)$ is that Q is a critical point of $A(Q; q) = U(Q) - S(q, Q)$. So, $F(q)$ is implicitly given by

$$\nabla U(F(q)) = S_Q(q, F(q)). \tag{5-6}$$

For such a function U, the set $\mathrm{Gr}(U)$ is invariant for Φ. Moreover, the q-component of the flow associated with the restriction of Φ to the set $\mathrm{Gr}(U)$ can be fully determined in terms of the function $F : \mathbb{R}^d \to \mathbb{R}^d$. In fact in approach (1), we show that such solutions U exist. If we can show that for each $P \in \mathbb{R}^d$, there exists a solution $U = U^P$ such that $U(q) = P \cdot q + o(|q|)$, as $|q| \to \infty$, then we are in a position to establish our homogenization as in [17]. However, in general a solution U^P may not exist for every P in the stochastic setting. Nonetheless the intuition behind such (equilibrium-like) solutions would allow us to design a strategy that consists of three steps; this should be compared with ideas coming from LDP [23].

Step 1 (*lower bound*) To simplify our presentation, we first assume that the function $L(q, v) = S(q, q + v)$ is 1-periodic in q. Motivated by (5-6), we pick any continuous function $f : \mathbb{T}^d \to \mathbb{T}^d$, and write $F : \mathbb{R}^d \to \mathbb{R}^d$ for its lift. In particular, we can write $F(q) = q + G(q)$, with G a periodic function. We select $q_i = F^i(q_0)$ with $q_0 = a$ in (5-1). Note

$$n^{-1} q_n = n^{-1} \sum_{i=0}^{n-1} G(F^i(q_0)), \qquad \sum_{i=0}^{n-1} S(q_i, q_{i+1}) = \sum_{i=0}^{n-1} S^F(F^i(q_0)),$$

where $S^F(q) = S(q, F(q)) = L(q, G(q)) =: L^G(q)$, which is also periodic. Recall that we only need to study $w_n(S) = u_n(0)$. As a result $u_n(0)$ is close to $u_n(n^{-1}a)$. We certainly have

$$u_n(n^{-1}a) \geq g\left(n^{-1}a + n^{-1} \sum_{i=0}^{n-1} G(F^i(a))\right) - n^{-1} \sum_{i=0}^{n-1} S^G(F^i(a)). \tag{5-7}$$

We wish to find the limit of the right-hand side of (5-7). Since both G and S^F are periodic, we may regard them as functions that are defined on the torus; with a slight abuse of notation, we write $G, S^F : \mathbb{T}^d \to \mathbb{R}$, so that we can write $G \circ F^i = G \circ f^i$, and $S^F \circ F^i = S^F \circ f^i$. Now if we pick any ergodic invariant measure for f, then we have

$$\begin{aligned} \lim_{n\to\infty} n^{-1} \sum_{i=0}^{n-1} G(F^i(a)) &= \int G \, d\mu, \\ \lim_{n\to\infty} n^{-1} \sum_{i=0}^{n-1} S^F(F^i(a)) &= \int L^G \, d\mu, \end{aligned} \tag{5-8}$$

for μ almost all choices of a. From this we obtain

$$\liminf_{n\to\infty} u_n(0) = \liminf_{n\to\infty} u_n(n^{-1}a) \geq g\left(\int G \, d\mu\right) - \int L^G \, d\mu.$$

This being true for any such pair (F, μ), we deduce

$$\liminf_{n\to\infty} u_n(0) \geq \sup_{(F,\mu)\in\mathcal{M}} \left[g\left(\int G \, d\mu\right) - \int S^F \, d\mu \right] = \sup_v [g(v) - \hat{L}(v)],$$

where $\mathcal{M}$ is the set of pairs (F, μ) such that μ is an ergodic invariant measure for the corresponding map f, and

$$\hat{L}(v) = \inf_{(F,\mu)\in\mathcal{M}} \left\{ \int S(q, F(q)) \mu(dq) : \int (F(q) - q) \, \mu(dq) = v \right\}. \tag{5-9}$$

Using (5-2), it is not hard to replace 0 with any $q \in \mathbb{R}^d$ to obtain

$$\liminf_{n\to\infty} u_n(q) \geq \sup_{(F,\mu)\in\mathcal{M}} \left[g\left(\int G\, d\mu \right) - \int S^F\, d\mu \right] \\ = \sup_v [g(q+v) - \hat{L}(v)]. \tag{5-10}$$

In the stochastic setting, we have a probability measure $\mathbb{P}$ on $\mathcal{L}$ that is τ invariant and ergodic. Here we equip $\mathcal{L}$ with the topology of local uniform convergence and $\mathcal{P}$ is a Radon measure with respect to this topology. We take any bounded continuous function $G : cL \to \mathbb{R}^d$. Out of this, we define a map $F(\,\cdot\,; S) : \mathbb{R}^d \to \mathbb{R}^d$, by

$$F(q; S) = q + G(\tau_q S).$$

We then use the sequence $q_n = F^n(a)$, to obtain a lower bound. Indeed, if we set

$$T = T_G : cL \to \mathcal{L}, \quad T(S) = \tau_{G(S)} S, \quad L^G(S) = S(0, G(S)),$$

then

$$q_n = F^n(a) = \sum_{i=0}^{n-1} G(T^i(\tau_a S)), \quad \sum_{i=0}^{n-1} S(q_i, q_{i+1}) = \sum_{i=0}^{n-1} L^G(T^i(\tau_a S)),$$

To apply the ergodic theorem, we pick any T-invariant ergodic measure μ so that (5-8) is true. Moreover, if μ is absolutely continuous with respect to $\mathbb{P}$, then we also have (5-10), provided that the supremum is taken over pairs (G, μ) such that μ is T_G ergodic and invariant, and $\mu \ll \mathbb{P}$.

Step 2 (*upper bound*) Let us assume that the initial condition is of the form $g_p(q) = q \cdot p$ for some $p \in \mathbb{R}^d$. Let us write $\mathcal{U}$ for the set of continuous functions $w : \mathbb{R}^d \to \mathbb{R}$, such that

$$\lim_{|q|\to\infty} |q|^{-1} w(q) = 0.$$

We then define

$$\overline{H}(p; w) = \sup_{q,Q} (w(Q) - w(q) + p \cdot (Q - q) - S(q, Q)).$$

For any $w \in \mathcal{U}$, we use (5-4) to produce an upper bound for the large n limit of u_n as follows:

$$u_n(q) = \mathcal{T}_n^S g_p(q) \\ \leq \sup_{|Q-q|\leq \ell(|p|)} [g_p(Q) - (Q-q)\cdot p - n^{-1}(w(nQ) - w(nq))] + H(p; w) \\ = q \cdot p + H(p; w).$$

As a result,

$$\limsup_{n\to\infty} u_n(q) \le q\cdot p + \inf_{w\in\mathcal{U}} \overline{H}(p;w) =: q\cdot p + \overline{H}(p) = \sup_v [g_p(q+v) - L(v)],$$

where $\bar{\alpha}$ is the Legendre transform of $\overline{H}$.

When H is periodic in q, we have a candidate for what the minimizing $w\in\mathcal{U}$ is namely, the solution $w=w^p$ of (1-6). Writing $\mathcal{U}_0$ for the set of continuous 1-periodic functions, we may write

$$\overline{H}(p) = \inf_{w\in\mathcal{U}_0} \overline{H}(p;w).$$

The point is that a more restrictive infimum in the definition of $\overline{H}$ makes it easier when we try to match our upper bound with our lower bound in step 1. We can also be more selective in the stochastic setting by choosing the type of w that have τ-stationary gradient; for example see [15] for more details.

Step 3 ($\hat{L}=\bar{\alpha}$) To establish homogenization, it remains to show that the upper and lower limits of Steps 1 and 2 coincide. This may be achieved by an introduction of a *Lagrange multiplier*, and an application of *minimax principle*. We explain this in the periodic case. Also, we simplify our presentation by replacing the set $\mathcal{M}$ with a larger set $\mathcal{M}'$. The set $\mathcal{M}'$ is the set of pairs (F,μ) such that μ is an invariant measure for the corresponding map f (we dropped the ergodicity requirement so that our choice of Lagrange multiplier simplifies). We also set

$$\hat{L}'(v) = \inf_{(F,\mu)\in\mathcal{M}'} \left\{ \int S(q,F(q))\mu(dq) : \int (F(q)-q)\,\mu(dq) = v \right\},$$

which is what we get as we replace $\mathcal{M}$ with $\mathcal{M}'$ in (5-9). If we write $\hat{H}'$ for the Legendre transform of $\hat{L}'$;

$$\hat{H}(p) := \sup_v (p\cdot v - \hat{L}(v)),$$

then we can show that $\hat{H}' = \overline{H}$:

$$\begin{aligned}
\hat{H}'(p) &= \sup_{(F,\mu)\in\mathcal{M}'} \left(\int \big((F(q)-q)\cdot p - S(q,F(q))\big)\,\mu(dq) \right)\\
&= \sup_F \sup_\mu \inf_{w\in\mathcal{U}_0} \left(\int \big((F(q)-q)\cdot p - S(q,F(q))\big)\,\mu(dq) \right.\\
&\qquad\qquad\qquad\qquad \left. + \int \big(w(F(q)) - w(q)\big)\,\mu(dq) \right)\\
&= \inf_{w\in\mathcal{U}_0} \sup_F \sup_\mu \left(\int \big((F(q)-q)\cdot p - S(q,F(q))\big)\,\mu(dq) \right.\\
&\qquad\qquad\qquad\qquad \left. + \int (w(F(q)) - w(q))\,\mu(dq) \right)
\end{aligned}$$

$$
\begin{aligned}
&= \inf_{w\in\mathcal{U}_0} \sup_F \sup_q \big((F(q)-q)\cdot p - S(q, F(q)) + w(F(q)) - w(q)\big)\\
&= \inf_{w\in\mathcal{U}_0} \sup_Q \sup_q \big((Q-q)\cdot p - S(q, Q) + w(Q) - w(q)\big)\\
&= \overline{H}(p).
\end{aligned}
$$

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rezakhan@math.berkeley.edu *Department of Mathematics, University of California, Berkeley, CA, United States*