The Escape Rate of a Molecule

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Abstract

We show existence and give an implicit formula for the escape rate of the \( n \)-centre problem of celestial mechanics for high energies. Furthermore we give precise computable estimates of this rate. This exponential decay rate plays an important role especially in semiclassical scattering theory of \( n \)-atomic molecules. Our result shows that the diameter of a molecule is measurable in a (classical) high-energy scattering experiment.

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1 Introduction and Statement of Results

The \( n \)-centre problem in three dimensions is given by \( n \) nuclei with charges \( Z_1, \ldots, Z_n \in \mathbb{R} \setminus \{0\} \) fixed at positions \( \vec{q}_1, \ldots, \vec{q}_n \in \mathbb{R}^3 \). We assume that the nuclei are in general position, which means that no three \( \vec{q}_k \) lie on one line. The \( n \)-atomic molecule generates a Coulombic potential on the configuration space \( \hat{M} := \mathbb{R}^3 \setminus \{\vec{q}_1, \ldots, \vec{q}_n\} \):

**Definition 1.1** A smooth potential \( V : \hat{M} \to \mathbb{R} \) is called Coulombic if

1. \( V \) has the form

\[
V(\vec{q}) = \sum_{k=1}^{n} \frac{-Z_k}{||\vec{q} - \vec{q}_k||} + W(\vec{q}) \quad (\vec{q} \in \hat{M})
\]

with \( W : \mathbb{R}^3 \to \mathbb{R} \) smooth.

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2. The potential vanishes at infinity, i.e. \( \lim_{\|\vec{q}\| \to \infty} V(\vec{q}) = 0 \), and its difference to a Coulomb potential is of short range. I.e. there exists \( Z_\infty \in \mathbb{R} \), called the asymptotic charge, \( \varepsilon \in (0, 1] \) and
\[
R_{\min} > 2 \max(\|\vec{q}_1\|, \ldots, \|\vec{q}_n\|)
\]
such that for some \( C_1 > 0 \)
\[
\left\| \nabla V(\vec{q}) - Z_\infty \frac{\vec{q}}{\|\vec{q}\|^2} \right\| < C_1 \frac{R_{\min}}{\|\vec{q}\|^{2+\varepsilon}} \quad (\|\vec{q}\| \geq R_{\min})
\]
and
\[
\|\nabla V(\vec{q}_1) - \nabla V(\vec{q}_2)\| < C_1 \frac{\|\vec{q}_1 - \vec{q}_2\|}{\min(\|\vec{q}_1\|, \|\vec{q}_2\|)^{2+\varepsilon}} \quad (\|\vec{q}_1\|, \|\vec{q}_2\| \geq R_{\min}).
\]

Remark 1.2 1. In [Kna] the high energy dynamics in Coulombic potentials was analyzed, using symbolic dynamics. The results are used here to calculate the escape rate, a quantity measurable in scattering experiments. For semiclassical aspects of the model, see [CJK], for topological methods also applicable to non-singular potentials, see [KK2]. Derezinski and Gerard [DG] is used as a general reference for scattering theory. Narnhofer analyzed time delay for short range potentials in [Nar].

2. In the context of celestial mechanics, \( V \) is sum of the singular Kepler potentials, with \( Z_i > 0 \) interpreted as masses, and \( W = 0 \).

For electrostatic potentials the charges may be positive and negative, i.e. the force can be attractive as well as repulsive. The scattering of a classical electron by a molecule can be well modeled in this setting by positive charges of the nuclei, i.e. \( Z_i > 0 \), and an additional smooth shielding (electronic) potential \( W \), say of Thomas-Fermi type, such that, up to a Coulombic term \( Z_\infty/\|\vec{q}\| \) given by the net charge of the molecule, the resulting potential is of short range, see [CJK].

Note that for \( W = 0 \) we have \( Z_\infty = \sum_{i=1}^n Z_i \).

Both for \( W = 0 \) and in the Thomas-Fermi case one may take \( \varepsilon = 1 \) in Def. 1.1.

The Hamilton function \( \hat{H} : T^* \hat{M} \to \mathbb{R} \) on the phase space \( T^* \hat{M} \simeq \mathbb{R}^3 \times \hat{M} \) is given by
\[
\hat{H}(\vec{p}, \vec{q}) := \frac{1}{2} \|\vec{p}\|^2 + V(\vec{q}). \tag{1.1}
\]

For \( n = 1 \) centres this generalizes the Kepler problem. For large energies no bounded orbits exist, for which reason the time delay is bounded. So we assume \( n \geq 2 \) in the following.

Due to collision orbits for nuclei with positive charge (respectively mass, depending on the interpretation) the Hamiltonian flow generated by (1.1) is incomplete. As we are interested in time-related quantities like time delay and escape rate we use a regularization method which – unlike the so-called Kustaanheimo-Stiefel transform – does not involve a time reparametrization. In Section 5 of [Kna] such a regularization is done by phase space extension of \( T^* \hat{M} \).
After regularization we get a smooth Hamiltonian system \((P, \omega, H)\) with a six-dimensional smooth manifold \(P \supset T^\ast \hat{M}, H \in C^\infty(P, \mathbb{R})\) with \(H|_{T^\ast \hat{M}} = \hat{H}\) and a symplectic two-form \(\omega \in \Omega^2(P)\) such that \(\omega|_{T^\ast \hat{M}} = \omega_0\), with \(\omega_0 = \sum_{i=1}^3 dq_i \wedge dp_i\), the canonical symplectic form on \(T^\ast \hat{M}\).

This Hamiltonian system generates a smooth complete Hamilton flow \(\Phi : \mathbb{R} \times P \to P\). Although for collisions the momentum \(\vec{p}\) diverges, for simplicity we write the flow in the forms

\[
(\vec{p}(t,x), \vec{q}(t,x)) := \Phi_t(x) := \Phi(t,x) \quad (x \in P, \ t \in \mathbb{R}).
\]

### 1.1 Classification of States in Phase Space

We are dealing with Hamiltonian dynamics for which the energy (i.e. the value of the Hamilton function) is conserved. So for a given energy \(E \in H(P)\) the dynamics is confined on the energy surface \(\Sigma_E := H^{-1}(E) \subset P\). For large \(E\) this is a smooth manifold of dimension five.

We now classify the points in the (extended) phase space \(P\) by their asymptotic behaviour:

- states \(b^\pm := \{x \in P : \limsup_{t \to \pm \infty} \|\vec{q}(t,x)\| < \infty\}\), bounded in the future respectively past, and the bounded states \(b := b^+ \cap b^-
- states \(s^\pm := P \setminus b^\pm\), scattered in the future/past and the scattered states \(s := s^+ \cap s^-
- states \(t^\pm := s^\pm \cap b^\pm\), scattered in the future/past and the trapped states \(t := s^+ \Delta s^- = (b^+ \cap s^-) \cup (b^- \cap s^+)\) = \(t^+ \cup t^-\).
- with a subscript \(E\) we denote the corresponding sets restricted to the energy surface \(\Sigma_E\), i.e. \(b_E := b \cap \Sigma_E\).

The assumption that \(V\) is Coulombic gives rise to the virial inequality

\[
\frac{d}{dt} \langle \vec{q}(t), \vec{p}(t) \rangle = 2 \left( E - V(\vec{q}(t)) \right) + \langle \vec{q}(t), \nabla V(\vec{q}(t)) \rangle \geq E > E_{\text{th}} \geq 0. \tag{1.2}
\]

This is valid for \(H(x) = E\) and the trajectory \(t \mapsto \vec{q}(t) \equiv \vec{q}(t,x)\) outside an interaction zone defined by a virial radius \(R_{\text{vir}}\)

\[
\mathcal{I}Z(E) := \{\vec{q} \in \mathbb{R}^3 : \|\vec{q}\| \leq R_{\text{vir}}(E)\} \quad (E > 0). \tag{1.3}
\]

So a trajectory leaving the interaction zone at some time \(t_0\) will move away from the origin for all future times \(t > t_0\), and for any scattered state \(x \in s_E^\pm\) also \(\lim_{t \to \pm \infty} \|\vec{q}(t,x)\| = \infty\).

The function \(E \mapsto R_{\text{vir}}(E)\) can be chosen to be continuous and non-increasing in \(E\), and as we consider high energies, i.e. energies above an energy threshold \(E_{\text{th}} > 0\), we can assume a energy-independent virial radius \(R_{\text{vir}} := R_{\text{vir}}(E_{\text{th}})\) and energy-independent interaction zone \(\mathcal{I}Z := \mathcal{I}Z(E_{\text{th}})\), see [Kna], p. 11 for details. In the course of the article several other lower bounds on the constant \(E_{\text{th}}\) will arise.
We consider the asymptotic behaviour of the flow $\Phi_t : P \to P, x \mapsto (\vec{p}(t, x), \vec{q}(t, x)) \in P$ by defining for $E > 0$ and a point $x \in s^+_E$ the asymptotic velocities, directions and impact parameters

$$
\vec{p}_\pm(x) := \lim_{t \to \pm \infty} \vec{p}(t, x), \quad \hat{p}_\pm(x) := \frac{\vec{p}_\pm(x)}{\sqrt{2E}} \in S^2 \\
\vec{q}_\perp^\pm(x) := \lim_{t \to \pm \infty} \left( \vec{q}(t, x) - \langle \vec{q}(t, x), \hat{p}_\pm(x) \rangle \cdot \hat{p}_\pm(x) \right).
$$

These are $\Phi_t$-invariant and depend continuously on the point $x$, see Theorem 6.5 of [Kna].

Noting that $\hat{p}_\pm(x) \perp \vec{q}_\perp^\pm(x)$, we define the continuous asymptotic maps

$$
A_\pm^E : s^\pm_E \to T^*S^2, \quad x \mapsto (\hat{p}_\pm(x), \vec{q}_\perp^\pm(x)).
$$

(1.4)

We denote the canonical symplectic two-form on the cotangent bundle $T^*S^2$ of the sphere by $\omega_0 \in \Omega^2(T^*S^2)$, and use the volume four-forms

$$
\Omega_E := E \omega_0 \wedge \omega_0 \in \Omega^4(T^*S^2) \quad (E > E_{th}).
$$

The sets $D^+_E := A_+^E(s_E) \subset T^*S^2$ represent the possible asymptotic data in the corresponding time direction, for a given energy $E$.

The asymptotic scattering map of energy $E$

$$
A_{SE} : D_-^E \to D_+^E, \quad AS_E := A_+^E \circ (A_-^E)^{-1}
$$

maps the initial asymptotic data $(\hat{p}^-, \vec{q}_\perp^-) \in D_-^E$ to the final asymptotic data $(\hat{p}^+, \vec{q}_\perp^+) \in D_+^E$.

Remark 1.3 Note that $A_+^E(s_E^+_E) = T^*S^2$ but $T^*S^2 \setminus D_+^E \neq \emptyset$ if the sets $s^+_E \setminus s_E = t^+_E$ of past/future trapped orbits are not empty. The asymptotic completeness of the $n$-centre problem, implies that $D_+^E$ is of full measure with respect to the canonical volume form $\Omega_E$ on $T^*S^2$, see Corollary 6.4 in [Kna].

Since the asymptotic maps $A_+^E$ on $s^+_E$ are $\Phi_t$-invariant, the asymptotic scattering map $AS_E$ carries no information about time-related quantities.

1.2 Møller Transformation

Far from the origin in configuration space, the $n$-centre problem is well approximated by the Kepler problem, given by the phase space $\hat{P}_\infty := T^*(\mathbb{R}^3 \setminus \{0\})$ and Hamilton function

$$
\hat{H}_\infty : \hat{P}_\infty \to \mathbb{R}, \quad \hat{H}_\infty(\vec{p}_\infty, \vec{q}_\infty) := \frac{1}{2} \|\vec{p}_\infty\|^2 - \frac{Z_\infty}{\|\vec{q}_\infty\|}.
$$

Being for $Z_\infty > 0$ a special case of (1.1), it can always be regularized to yield a smooth complete flow

$$
\Phi_\infty : P_\infty \to P_\infty, \quad x_\infty \mapsto (\vec{p}_\infty(t, x_\infty), \vec{q}_\infty(t, x_\infty)).
$$

(1.6)
of the Kepler problem, with the extended Hamilton function $H_\infty \in C^\infty(P_\infty, \mathbb{R})$.

The scattering states of the flow $\Phi^\infty$ with a non-vanishing asymptotic momentum form the set

$$P_{\infty,+} := \{x \in P_\infty : H_\infty(x) > 0\},$$

consisting of $\Phi^\infty$-orbits projecting to Kepler hyperbolae (resp. straight lines for $Z_\infty = 0$) in configuration space.

Scattering theory in general deals with the comparison of two dynamics, in this case the dynamics of $(P, \Phi_t)$ and $(P_\infty, \Phi^\infty_t)$. This is done by the Møller transformations

$$\Omega^\pm : P_{\infty,+} \to s^\pm, \quad \Omega^\pm := \lim_{t \to \pm \infty} \Phi^{-t} \circ \Phi^\infty_t.$$  \hspace{1cm} (1.7)

Here we have omitted the identification of $P$ with $P_\infty$ outside a region near the singularities.

In [Kna], Sect. 6 it was shown that the Møller transformations $\Omega^\pm$ exist point-wisely and are measure-preserving homeomorphisms, and if the partial derivatives of $V$ decay at infinity like

$$\partial_{q}^\beta \left( V(q) + \frac{Z_\infty}{\|q\|} \right) \to O\left( \|q\|^{-|\beta| - 1 - \varepsilon} \right) \quad (\beta \in \mathbb{N}_0^3)$$

for some $0 < \varepsilon \leq 1$, then the Møller transformations are $C^\infty$- symplectomorphisms. Similar statements hold for the asymptotic scattering map, defined in (1.5). Like in Remark 1.2, both for $W = 0$ and in the Thomas-Fermi case one may take $\varepsilon = 1$.

We denote by $\Omega^\pm_* : s^\pm \to P_{\infty,+}$ the inverse of $\Omega^\pm$.

From this follows in particular that $\Omega^\pm(P_{\infty,+}) = s^\pm$, i.e. given a Kepler hyperbola there exists a unique scattered orbit of the $n$-centre problem which is asymptotic to this hyperbola in the time direction described by the sign. Conversely any one-sided scattered orbit is one-sided asymptotic to a unique Kepler hyperbola.

The choice of the Kepler problem as the "comparison dynamics" for defining the Møller transformation is justified by the existence of the limit in (1.7).

### 1.3 Time Delay and Escape Rate

Next we define the time delay $\tau(x)$ for a point $x$ belonging to a scattered orbit by comparison with the Kepler dynamics ($\Theta$ denoting the Heaviside step function):

$$\tau(x) := \lim_{R \to \infty} \int_R^\infty \Theta(R - \|q(t,x)\|) - \frac{1}{2} \left[ \Theta(R - \|q_\infty^+(t, \Omega_+^*(x))\|) + \Theta(R - \|q_\infty^-(t, \Omega_-^*(x))\|) \right] dt.$$  \hspace{1cm} (1.8)

As $\tau$ is $\Phi$-invariant, the time delay $\tau(x)$ only depends on the asymptotic data $(\hat{p}_+, \hat{q}_+^\infty) \in T^*S^2$ (respectively $(\hat{p}_-, \hat{q}_-^\infty) \in T^*S^2$) of $x$. So for $E > 0$ we define $\tau_E := \tau|_{\Sigma_E}$ and the asymptotic time delay

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\[\tau^+_E : T^* S^2 \to \mathbb{R} \cup \{\infty\}, \quad \tau^+_E(\hat{p}, \hat{q}_\perp) := \begin{cases} \tau_E \circ (A^+_E)^{-1}(\hat{p}, \hat{q}_\perp) & \text{if } (\hat{p}, \hat{q}_\perp) \in D^+_E \\ \infty & \text{else} \end{cases}\]  

(remember that \(D^+_E = A^+_E(s_E)\)).

\[\kappa^\infty_E(t) := \int_{T^* S^2} \mathbb{1}_{(\tau^+_E(x) \geq t)} \Omega_E(x) \quad (t > 0)\]  

denotes the \(\Omega_E\)-volume of the set of asymptotic data with a time delay greater or equal than a given time delay \(t > 0\). Clearly \(\kappa^\infty_E(t)\) is monotone decreasing in \(t\).

As the asymptotic scattering map (1.5) is measure-preserving, this quantity would not change if one would use \(A^-_E\) instead of \(A^+_E\) in Def. (1.9).

**Remark 1.4** The passage from the time delay to the asymptotic time delay is motivated by measure theoretical properties of these maps: because of \(\Phi\)-invariance of \(\tau\), for any time interval \(I \subset \mathbb{R}\) the Liouville measure of the set \(\{x \in s_E : \tau_E(x) \in I\}\) of scattered states is either zero or infinite, whereas (1.10) turns out to be finite for \(t > 0\).

Although our main interest lies in the analysis of orbits with large time delay, we also show

1. that the time delay is bounded below on the energy surface,
2. that the volume of orbits with a given positive time delay is bounded,
3. and that complicated dynamics of scattering orbits only occur for large time delay.

More precisely we have the following results:

**Proposition 1.5** There exist constants \(C_1, C_2, C_3 > 0\) such that for all energies \(E > E_{th}\)

1. \(\tau_E > -C_2/E^{1/2}\)
2. with \(\epsilon \in (0, 1]\) from Def. 1.4 we have \(\kappa^\infty_E(t) < C_1 t^{-2/\epsilon} E^{1-3/\epsilon} \quad (t \in (0, C_3/E^{3/2})\)
3. the orbit through \(x\) intersects the interaction zone if \(\tau_E(x) \in [C_3/E^{3/2}, \infty)\).

The proof of Proposition 1.5 is in the Appendix.

For **large time delay** the escape rate \(\beta_E\) is defined as the exponential decay rate of \(\kappa^\infty_E(t)\), i.e.

\[\beta_E := -\lim_{t \to \infty} \frac{1}{t} \ln(\kappa^\infty_E(t)) \quad (E > E_{th})\]  

in the case of existence.

Now we are ready to state our main result. To ease the notation, for real valued functions \(f, g\) we write \(f \asymp g\) (or sloppily \(f(t) \asymp g(t)\)) if there exist constants \(C_1 \geq 1, C_2 > 0\) such that \(C_1^{-1} g(t) \leq f(t) \leq C_1 g(t)\) for all \(t \geq C_2\).
1.4 A Matrix Perron-Frobenius Problem

We now set up a finite matrix problem which we show to approximate the escape rate (1.11) with optimal precision (see Remark 1.6). This then allows to compute the escape rate very precisely, using only a few parameters of the model. Symbolic dynamics will be based on the alphabet

$$\mathcal{A} := \{(i, j) : i, j = 1, \ldots, n \text{ with } i \neq j \}. \quad (1.12)$$

For \((k_0, k_1) = ((i, j), (k, l)) \in \mathcal{A} \times \mathcal{A}\) with \(j = k\) we define the charge \(Z_{k_0, k_1} := Z_j\) and, for distance \(d_{i,j} := \|\vec{q}_i - \vec{q}_j\|\), the mean distance \(\bar{d}_{k_0, k_1} := \frac{1}{2}(d_{i,j} + d_{j,l})\). We set

$$f(k_0, k_1) := \frac{2d_{i,j} \cos^2(\frac{1}{2} \alpha(i, j, l))}{-Z_j}, \quad (1.13)$$

\(\alpha(i, j, l)\) denoting the angle between the vectors \(\vec{q}_i - \vec{q}_j\) and \(\vec{q}_l - \vec{q}_j\). Then, with

$$\tilde{T}_E(k_0, k_1) := \frac{\bar{d}_{k_0, k_1}}{\sqrt{2E}} - \frac{Z_{k_0, k_1} \ln(E)}{(2E)^{3/2}} \quad \text{and} \quad \tilde{F}_E(k_0, k_1) := 2 \ln \left( \frac{2E|f(k_0, k_1)|}{\bar{d}_{k_0}} \right) \quad (1.14)$$

playing the role of approximate Poincaré time respectively unstable Jacobian, we define the weighted transfer matrix (consult Baladi [Bal] for the subject of transfer operators)

$$\begin{aligned}
\left(\mathcal{M}_E(\beta)\right)_{k_0, k_1} := \\
\begin{cases}
\exp \left( -\tilde{F}_E(k_0, k_1) + \beta \tilde{T}_E(k_0, k_1) \right) & \text{if } j = k \\
0 & \text{else}
\end{cases}
\end{aligned} \quad (1.15)$$

Note that the definition of \(\mathcal{M}_E\) only involves the energy \(E\), the positions \(\vec{q}_i\) and the charges \(Z_{i}\) of the \(n\) nuclei and is independent of the potential \(W\).

The Perron-Frobenius eigenvalue \(\lambda_{PF} > 0\) of \(\mathcal{M}_E\) now depends on \(E\) and \(\beta\), and will be shown to have a unique solution \(\tilde{\beta}_E\) of

$$\lambda_{PF}(\beta, E) = 1 \quad (E > E_{th}).$$

By \(d_{\text{max}}\) we denote the maximal mutual distance of the nuclei, that is the diameter of the molecule.

**Main Theorem:** Let \(V\) be a Coulombic \(n\)-centre potential, \(n \geq 2\), and the energy \(E > E_{th}\). Then for the escape rate \(\beta_E\) (defined in Eq. (1.11)) it holds:

(i) \(\beta_E\) exists, even more \(\kappa_E(\infty) \propto e^{-\beta_E t}\).
\(\beta_E\) is given implicitly by a Perron-Frobenius problem.

(ii) The escape rate \(\beta_E\) is asymptotic to \(\frac{2\sqrt{2E} \ln E}{d_{\text{max}}}\). It is approximated by \(\tilde{\beta}_E\), with relative error of order \(O(1/E)\).
Figure 1: Left: Scattering orbit for \( n = 3 \) centres, with symbol sequence 1, 2, 1, 2, 3. Right: Poincaré surfaces projected to the plane in configuration space, containing the three centres

Remark 1.6 As a \( W \)-independent estimate, the \( O(1/E) \) estimate of (ii) is optimal. This can be seen by adding to \( V \) a cut off function \( W \in C^\infty_0(\mathbb{R}^3) \) which equals a constant \( C \) in the interaction zone \( IZ \), see (1.3). Thus the dynamics in \( \Sigma_E \) over \( IZ \) equals the one without \( W \) for energy \( E - C \).

We base our proof on the application of renewal theory, worked out by Lalley in \[Lal\], precisely determining the \( E \)-dependence of all quantities. This is possible by applying a simple symbolic dynamics from \[Kna\], see Figure 1.

2 Proof of the Main Theorem

While our estimates are optimal in their dependence on the energy \( E \), we will be somewhat vague in denoting most energy-independent constants by \( C \), without tracing back their mutual dependence. We hope that this makes the following part more readable. The interested reader, however, may consult \[Kna\] to find in many cases more explicit estimates.

2.1 Proof of Part (i)

Although the escape rate is defined in the realm of scattering theory, the key of showing its existence and determining its value is to study the bounded states. As the escape rate is a limit of large time delay, it is natural that the trapped states play an important role. But in our case for \( E > E_{th} \) the \( \omega \)-limit set of the trapped states equals the bounded states (i.e. \( \omega(t_E) = b_E \)).
2.1.1 Symbolic Dynamics

The set of non-wandering points of the flow $\Phi$ on the energy surface $\Sigma_E$ equals $b_E$, the subset of bounded states. Moreover, for high enough energies $E > E_{th}$, $b_E$ is a hyperbolic set so that the flow $\Phi_t|_{\Sigma_E}$ satisfies Axiom A (see [Kna], Thm. 12.8). This allows, by using Poincaré sections, to model the time-discretized dynamics $\Phi_t|_{b_E}$ with symbolic dynamics given by a two-sided shift space $(X, \sigma)$ of finite type. The left shift $\sigma$ on $X$ in conjugated to the Poincaré map $P_E$, restricted to the bounded states on the Poincaré surfaces.

Lemma 2.1 (Theorem 12.8 of [Kna]) For energies $E > E_{th}$ the flow $\Phi_t|_{b_E}$ of the $n$-centre problem is conjugated to a suspended flow $(X^E, \sigma^E_t)$ by a Hölder continuous homeomorphism $X^E : X^E \rightarrow b_E$.

Remark 2.2 Hölder continuity is defined by a choice of Riemannian metric on the Poincaré sections, denoted by $d_{I_E}$ and a metric on the shift space, see (2.5) below.

The roof function is the pull-back $T_E : X \rightarrow \mathbb{R}^+$ of the Poincaré time, see (2.3) below. In particular it is Hölder continuous on the shift space $X$.

From Theorem 19.1.6 and its Corollary 19.1.13 of Katok and Hasselblatt [KH] it follows that the logarithm of the unstable Jacobian, denoted by $F_E$ (see (2.16) below) is also a Hölder continuous function on the intersection of the Poincaré surfaces with the bounded states.

This conjugacy is established by introducing Poincaré surfaces labeled by the alphabet $A$ from (1.12). For $C > 0$ the hypersurfaces in the energy shell $\Sigma_E$, labelled by $(i, j) \in A$

$$I^i_j := \left\{ (\vec{p}, \vec{q}) \in \Sigma_E : \langle \vec{q} - \vec{m}_{i,j}, \hat{q}_{i,j} \rangle = 0, \ |\vec{q} - \vec{m}_{i,j}| < \frac{Cd_{i,j}}{2E}, \langle \vec{p}, \hat{q}_{i,j} \rangle > 0, \ \left| \frac{\vec{p}}{\sqrt{2E}} \times \hat{q}_{i,j} \right| < 2CE^{-1} \right\},$$

(2.1)

are located in configuration space near the midpoint $\vec{m}_{i,j} := \frac{1}{2}(\vec{q}_i + \vec{q}_j)$ between the centre $i$ and $j$, and are perpendicular to the direction $\vec{q}_{i,j} := (\vec{q}_j - \vec{q}_i)/d_{i,j}$ (with $d_{i,j} = ||\vec{q}_i - \vec{q}_j||$), see Figure 1.

For an appropriate constant $C > 0$ these are Poincaré surfaces for all $E > E_{th}$, i.e. they are transversal to the flow $\Phi_t|_{\Sigma_E}$.

We denote the disjoint union of these inner Poincaré surfaces by $I_E := \bigcup_{(i,j) \in A} I^i_j$.

$D_E := \left\{ x = (\vec{p}, \vec{q}) \in \Sigma_E : \|\vec{q}\| \leq R_{vir} \right\}$ denotes the part of the energy surface lying over the interaction zone (1.3). The two submanifolds of the boundary

$$O^\pm_E := \{ (\vec{p}, \vec{q}) \in \Sigma_E : \|\vec{q}\| = R_{vir}, \ \pm(\vec{q}, \vec{p}) > 0 \} \subset \partial D_E;$$

(2.2)

consisting of states leaving resp. entering the interaction zone, are transversal to the flow, too and called outer Poincaré surfaces. We use their disjoint unions

$$O_E := O^+_E \cup O^-_E, \quad H^+_E := I_E \cup O^+_E \quad \text{and} \quad H_E := I_E \cup O_E.$$
The Poincaré map $P_E : H^-_E \to H^+_E$, $P_E(x) := \Phi(T_E(x), x)$ with Poincaré time is given by

$$T_E : H^+_E \to [0, \infty), \quad T_E(x) := \inf\{t > 0 : \Phi_t(x) \in H^+_E\} \quad \text{for} \quad x \in O^+_E$$

$$P_E(x) := \Phi(T_E(x), x) \quad \text{for} \quad x \in H^+_E$$

(2.3)

The Poincaré map $P_E$, restricted to $I_E \cap b_E$, gives rise to the two-sided shift space $(X, \sigma)$

$$X := \{(\ldots, k_{-1}, k_0, k_1, \ldots) \in \mathbb{A}^\mathbb{Z} : (k_{i+1})_1 = (k_i)_2 \forall i \in \mathbb{Z}\}.$$  

(2.4)

Using similar definitions, with $X^+ \subset \mathcal{A}^{\mathbb{N}_0}$ we denote the one-sided shift space and with $X^*$ the set of (unindexed) words in $X^+$ resp. in $X$.

With the metric

$$d([k], [l]) := 2^{-\sup\{i \in \mathbb{N}_0 : k_j = l_j \forall |j| \leq i\}}$$

(2.5)

the space $X$ resp. $X^+$ becomes a metric space. According to Lemma 12.2 of [Kna] we have symbolic dynamics in the following sense: there exists a Hölder continuous homeomorphism

$$F_E : X \to b_E \cap I_E,$$

(2.6)

conjugating the shift on $X$ with the Poincaré map on the bounded orbits. This allows us to consider functions on $b_E \cap I_E$ like Poincaré time $T_E$ as functions on $X$.

For a word $k = (k_0, \ldots, k_m) \in X^*$ of length $m + 1$ we denote the cylinder over $k$ by

$$\lfloor k \rfloor := \{l \in X : l_i = k_i \forall i = 0, \ldots, m\}.$$ 

This corresponds to the open submanifold on the inner Poincaré surface

$$I_E(k) := \{x \in I_E : P_E^i(x) \in I_E^k, \quad i = 0, \ldots, m\}.$$ 

(2.7)

The canonical symplectic form $\omega$ on $\mathcal{P}_E$, restricted to $H_E$ makes this four-dimensional Poincaré surface a symplectic manifold. We denote the restriction of the canonical volume four-form on $H_E$ by $\Omega_E$, like the volume on $T^*S^2$.

Next we define the total inner Poincaré time $\tau_{I_E} : \Sigma_E \to [0, \infty) := [0, \infty) \cup \{+\infty\}$, the time spent in the set $I_E$ of inner Poincaré surfaces, by

$$\tau_{I_E}(x) := \begin{cases} 
\sup\{t \in \mathbb{R} : \Phi_t(x) \in I_E\} - \inf\{t \in \mathbb{R} : \Phi_t(x) \in I_E\} & \text{if } I_E \cap \Phi(\mathbb{R}, x) \neq \emptyset \\
0 & \text{else}
\end{cases}$$

and consider the $\Omega_E$-volume

$$\kappa_{I_E}(t) := \int_{O^+_E \cap \{\tau_{I_E} \geq t\}} \Omega_E \quad \text{of the sets} \quad V_{I_E}^+(t) := \{x \in O^+_E : \tau_{I_E}(x) \geq t\}.$$  

(2.8)

The motivation for studying this function is that it is controllable by symbolic dynamics, and at the same time it is asymptotically near to the function $\kappa_{\infty}^E$ (defined in (1.9)), which gives the escape rate:
Lemma 2.3 $k^\infty_E \lesssim k_{IE}$.

Proof: The $\Phi_t$-invariance of $\tau_{IE}$ permits us to define the asymptotic total inner Poincaré time

$$\tau_{IE}^+: T^*S^2 \to [0, \infty], \quad \tau_{IE}^+(\hat{p}, \hat{q}_\perp) = \begin{cases} \tau_{IE} \circ (A_{IE}^-)^{-1}(\hat{p}, \hat{q}_\perp) & \text{if } (\hat{p}, \hat{q}_\perp) \in D_{IE}^+ \\ \text{else} & \end{cases}$$

By Proposition 9.2 of Kna and Theorem 10.6 of KK (adapted to three dimensions) it follows that there exists an energy dependent constant $C(E) > 0$ such that $|\tau_{IE}(x) - \tau_{IE}(x)| \leq C(E)$ uniformly for all $x \in s_E$. So (setting $\infty - \infty = 0$) we have the uniform estimate

$$|\tau_{IE}^+(x) - \tau_{IE}^+(x)| < C(E) \quad (x \in T^*S^2).$$

Thus for the $\Omega_{IE}$-volume of the set $V_{IE}^\infty(t) := \{x \in T^*S^2 : \tau_{IE}^+(x) \geq t\}$ it holds

$$k^\infty_E(t) \asymp \int_{T^*S^2} 1_{\{\tau_{IE}^+ \geq t\}} \Omega_{IE}.$$ (2.9)

By Remark 1.3 the set of points $x \in T^*S^2$ with $\tau_{IE}^+(x) = \infty$ has measure zero.

The asymptotic maps $A_{IE}^\pm$ map the outer Poincaré surfaces $O_{IE}^\pm$ diffeomorphically to their images $A_{IE}^\pm(O_{IE}^\pm) \subset T^*S^2$. By using the cotangential lift of the polar diffeomorphism $R^3 \setminus \{0\} \to [0, \infty) \times S^2$, see Section 6.3 of Marsden and Ratiu [MR], one can compute that for the pullback with $A_{IE}^\pm$ of the volume forms (which are derived from the symplectic forms) holds $(A_{IE}^\pm)^*\Omega_{IE}|_{O_{IE}^\pm} = \Omega_{IE}|_{O_{IE}^\pm}$. Thus for the $\Omega_{IE}$-volume $k_{IE}(t)$ of the set it holds for $t > C(E)$, see Remark 1.4

$$\int_{V_{IE}^\infty(t)} \Omega_{IE} = \int_{A_{IE}^+(V_{IE}^\infty(t))} \Omega = \int_{A_{IE}^+(V_{IE}^\infty(t))} (A_{IE}^\pm)^*\Omega = \int_{V_{IE}^\infty(t)} \Omega_{IE} = k_{IE}(t).$$

With Eq. (2.9) it follows finally that $k^\infty_E \asymp k_{IE}$. $\square$

In the following we show the estimate $k_{IE}(t) \asymp e^{-\beta_{IE}t}$ for the $\Omega_{IE}$-volume of the sets $V_{IE}^\pm(t) \subset O_{IE}^\pm$. As a first step we define for time $t > 0$ the sets of best fitting words

$$X_{IE} := \{(k_0, \ldots, k_m) \in X^* : \forall \mathbf{k} \in [k] : S_m T_E(\mathbf{k}) \geq t \quad \text{and} \quad \exists \mathbf{k} \in [k] : S_{m-1} T_E(\mathbf{k}) < t\}$$

and

$$X_{IE} := \{(k_0, \ldots, k_m) \in X^* : \exists \mathbf{k} \in [k] : S_m T_E(\mathbf{k}) \geq t \quad \text{and} \quad \forall \mathbf{k} \in [k] : S_{m-1} T_E(\mathbf{k}) < t\}$$
as subsets of words in $X^*$, with the summatory function of $f : X \to \mathbb{C}$

$$S_0 f := 0, \quad S_m f := \sum_{i=0}^{m-1} f \circ \sigma^i \quad (m \in \mathbb{N}).$$
Lemma 2.4 The sets of cylinders $[X_{t,E}] := \{[k] : k \in X_{t,E}\}$ respectively $[X_{t,E}] := \{[k] : k \in \mathcal{X}_{t,E}\}$ constitute partitions of $X$.

Proof: • To show that $[X_{t,E}]$ covers $X$, take some $k \in X$. From Lemma 9.3, Eq. (9.21) in [Kna] it follows $\inf(T_E) > 0$. Thus there is a minimal $m \in \mathbb{N}_0$ such that $S_m T_E(l) \geq t$ for all $l \in ([k_0, \ldots, k_m])$. Then $(k_0, \ldots, k_m) \in X_{t,E}$.
• To show that $[X_{t,E}]$ is a partition of $X$, suppose that $k = (k_1, \ldots, k_m(k)) \in X_{t,E}$ and $l = (l_1, \ldots, l_m(l)) \in \mathcal{X}_{t,E}$ with $[k] \cap [l] \neq \emptyset$. Then w.l.o.g. $[k] \subset [l]$, i.e. $m(k) \geq m(l)$. For all $x \in [l]$ it holds $S_m(l) T_E(x) \geq t$, and there exists an $x \in [k] \subset [l]$ with $S_m(l) T_E(x) < t$. Together this implies that $m(l) \geq m(k)$. So $m(l) = m(k)$ and $k = l$.
• The proof for $[X_{t,E}]$ is analogous. □

With the aid of the 'best fitting words' we approximate $V_{I_E}^-(t)$, defined in (2.8), in the following manner:

Proposition 2.5 There exists a constant $C_\tau(E) > 0$ such that for any $t > 0$ the inclusions

$$\bigcup_{k \in \mathcal{X}_{t+C_\tau,E}} (O_E \cap \mathcal{P}_E^{-1}(I_E([k]))) \subset V_{I_E}^-(t) \subset \bigcup_{k \in \mathcal{X}_{t-C_\tau,E}} (O_E \cap \mathcal{P}_E^{-1}(I_E([k])))$$

(2.10)

hold for the iterated inner Poincaré surfaces $I_E([k])$, defined in (2.7).

Proof: • By the hyperbolicity of $\mathcal{P}_E$ on $I_E \cap b_E$, see [Kna], and the Lipschitz-continuity of $T_E$ on $I_E$ it follows that there exists a positive constant $C_\tau = C_\tau(E)$ such that

$$\left| \sum_{i=0}^{m-1} T_E(\mathcal{P}_E^i(x)) - \sum_{i=0}^{m-1} T_E(\mathcal{P}_E^i(y)) \right| < C_\tau$$

for all words $k \in X^*$ and any $x, y \in I_E([k])$, $m + 1$ being the length of $k$.
• To show the first inclusion in (2.10), take some $x \in \mathcal{P}_E^{-1}(I_E([k])) \cap O_E^-$ for some $k = (k_0, \ldots, k_m(k)) \in X_{t+C_\tau,E}$. From $\sum_{i=0}^{m-1} T_E(\mathcal{P}_E^i(y)) \geq t + C_\tau$ for all $y \in I_E([k]) \cap b_E$ it follows that

$$\sum_{i=0}^{m-1} T_E(\mathcal{P}_E^i(y)) \geq t$$

for all $y \in I_E([k])$. $\mathcal{P}_E(x) \in I_E([k])$ together with $\tau_{I_E}(x) = \tau_{I_E}(x)$ imply that $x \in V_{I_E}^-(t)$. This shows the first inclusion.
• To show the second inclusion in (2.10), suppose that $t > 0$ and let $x \in V_{I_E}^-(t)$. Then there exists $m \in \mathbb{N}$ with $\sum_{i=0}^{m-1} T_E(\mathcal{P}_E^i(\mathcal{P}_E(x))) \geq t$ and a word $k = (k_0, \ldots, k_m) \in X^*$ such that $\mathcal{P}_E^{i+1}(x) \in I_E(k_i)$ for $i = 0, \ldots, m$. Since $\mathcal{P}_E(x) \in I_E(k_0, \ldots, k_m)$, it follows that there exists $y \in I_E(k_0, \ldots, k_m) \cap b_E$ such that $\sum_{i=0}^{m-1} T_E(\mathcal{P}_E^i(y)) \geq t - C_\tau$. So after eventually shortening the finite sequence $(k_0, \ldots, k_m)$ to length $m' \leq m$ there exists $k' = (k_0, \ldots, k_m') \in \mathcal{X}_{t-C_\tau,E}$ such that $\mathcal{P}_E(x) \in I_E(k) \subset I_E(k')$ and so $x \in \mathcal{P}_E^{-1}(I_E(k')) \cap O_E^-$ for some $k' \in \mathcal{X}_{t-C_\tau,E}$ showing the second inclusion.
• The fact that these unions are disjoint follows from Lemma 2.4 and completes the proof. □
2.1.2 Measure-Theoretical Estimates

In order to estimate \( V_{IE}(t) \) using \((2.10)\), we now approximate the \( \Omega_E \)-volume of \( O^{-E}(I_E) \) for the words \( k \in X^* \).

In [Kna] local coordinates \((\vec{y}, \vec{z}) = (y_1, y_2, z_1, z_2)\) on the inner Poincaré surfaces \( I_{E}^{i,j} \) were introduced, with \( \vec{z} \) affine in the position \( \vec{q} \), \( \vec{y} \) affine in the momentum \( \vec{p} \), and the volume form
\[
dy_1 \wedge dy_2 \wedge dz_1 \wedge dz_2 = \frac{2d^2_{i,j}}{E} \Omega_E |_{I_{E}^{i,j}}. \tag{2.11}\]

By using the Euclidean metric on \( \mathbb{R}^4 \), these coordinates serve also for defining a metric \( d_{IE} \) on \( I_E \). In these coordinates the Poincaré surfaces defined in \( (2.1) \) take the form \( I_{E}^{i,j} = B_y \times B_z \), \( B_y \) and \( B_z \) being two-dimensional disks whose radii are proportional to \( 1/E \).

With \( f \) from \((1.13)\), the linearized Poincaré map equals
\[
T_xP_E = f(k_0, k_1)E \left( \begin{smallmatrix} 1 & 0 \\ 0 & \frac{1}{E} \end{smallmatrix} \right) + \mathcal{O}(E^0) \quad (x \in I_E(k_0, k_1)), \tag{2.12}\]
see Prop. 11.2 of [Kna]. In order to use symbolic dynamics, we compare these maps with the ones along the bounded orbits. Since \( I_E \cap b_E \) is a hyperbolic set for \( P_E \), the tangent space has the \( TP_E \)-invariant splitting
\[
T_xI_E = T_x^u \oplus T_x^s \quad (x \in I_E \cap b_E) \tag{2.13}\]
into the unstable and stable Lagrangian subspace.

In \((\vec{y}, \vec{z})\)-coordinates, the cone field \( C_E^+ \equiv C_E \) on \( I_E \) is defined by
\[
C_E(x) := \left\{ (\delta\vec{y}, \delta\vec{z}) \in T_{(\vec{y}, \vec{z})}I_E : |\delta\vec{y} - \delta\vec{z}| \leq \frac{C}{E} |\delta\vec{y} + \delta\vec{z}| \right\}, \tag{2.14}\]
and \( C_E^- \) denotes the image of \( C_E^+ \) under time reversal. So their aperture is of order \( \mathcal{O}(1/E) \).

Furthermore, by estimate \((2.12)\), for an appropriately chosen constant \( C > 0 \), for all \( E > E_{th} \), the cone field \((2.14)\) is strictly \( P_E \)-invariant on \( I_E \cap P_{E}^{-1}(I_E) \).

The logarithmic Jacobian of a subbundle \( U \) of \( T(I_E \cap P_{E}^{-1}(I_E)) \) is generally defined by
\[
F_{E,U} : I_E \cap P_{E}^{-1}(I_E) \to \mathbb{R} \ , \ F_{E,U}(x) = \ln \left( \det \left( T_xP_E |_{U_x} \right) \right), \tag{2.15}\]
with the determinant depending on the choice of the Riemannian metric \( d_{IE} \). For the two-dimensional Lagrangian unstable bundle in \((2.13)\) the logarithmic unstable Jacobian is given by
\[
F_E : I_E \cap b_E \to \mathbb{R}^+, \ F_E := F_{E,T^u}. \tag{2.16}\]

Let \( \tilde{U}, \tilde{V} \) be two transversal Lagrangian subbundles on \( I_E \). Then any tangent vector \( w \in T_xI_E \) has a unique decomposition \( w = u + v \) with \( u \in \tilde{U} \) and \( v \in \tilde{V} \).
This decomposition gives rise to the quadratic form \( Q_E(w) := 2\omega(u, v) \) and defines the sector
\[
S_E := \bigcup_{x \in I_E} \{ w \in T_x I_E : Q_E(w) \geq 0 \},
\]
both depending on the pair \( \tilde{U}, \tilde{V} \).

There exist two Lagrangian subbundles \( \tilde{U}, \tilde{V} \) such that for their sector it holds: \( C_E \subset S_E \) (for example, one can choose \( \tilde{V} \) to be tangential to the kernel of the cotangent bundle projection \( T^* M \to \hat{M} \) and \( \tilde{U} \) to be horizontal w.r.t. the Euclidean metric, see Sect. 11 of [Kna]). In the following we denote with \( S_E \) the sector defined by such a pair of transversal Lagrangian subbundles.

**Lemma 2.6** For any \( E > E_{th} \) the tangent map of the Poincaré map \( P_E \) is strictly monotone with respect to the sector \( S_E \), i.e. \( T_x P_E(S_{E,x} \setminus \{0\}) \subset \text{int}S_{E,x} \) for any \( x \in I_E \cap P_{E}^{-1}(I_E) \).

**Proof:** Let \( v \in S_{E,x} \setminus \{0\} \) for some point \( x \in I_E \cap P_{E}^{-1}(I_E) \). Since \( T^u I_E \subset C_{E,y} \subset S_{E,y} \) and the logarithmic unstable Jacobian of \( T_y P_E \) is of order \( E \) for \( y \in I_E \cap b_E \) the claim follows by a compactum argument. \( \square \)

Following Liverani and Wojtkowski [LV], we denote for \( x \in I_E \) by
\[
L_{E,x} := \{ \text{Lagrangian subspace } U \subset T_x I_E : \forall u \in U \setminus \{0\} : Q_{E,x}(u) > 0 \}
\]
the set of *positive* Lagrangian subspaces. With \( L_E \) we denote the set of positive Lagrangian subbundles of \( T\hat{I}_E \). For two subspaces \( U, V \in L_{E,x} \) the distance
\[
s_{E,x}(U, V) := \sup_{u \in U \setminus \{0\}, v \in V \setminus \{0\}} \left| \text{Asinh} \left( \frac{\omega_x(u, v)}{\sqrt{Q_{E,x}(v)\sqrt{Q_{E,x}(w)}}} \right) \right|
\]
gives a complete metric on \( L_{E,x} \), see [LV].

By Theorem 1 of [LV] and the strict monotonicity of the Poincaré map \( P_E \) it follows that \( Q_E(T_x P_E(v)) > Q_E(v) \) for any \( v \in C_{E,x}, v \neq 0 \) and thus
\[
\gamma_E := \sup_{x \in I_E \cap P_{E}^{-1}(I_E)} \sup_{v \in S_{E,x} : ||v||_{I_E} = 1} \frac{Q_E(v)}{Q_E(T_x P_E(v))} < 1
\]
by a compactness argument. Thus for any \( u, v \in \text{int}S_{E,x} \) it holds (note that \( P_E \) is a symplectomorphism) that
\[
\text{Asinh} \left( \frac{\omega(T_x P_E^m(u), T_x P_E^m(v))}{\sqrt{Q_E(T_x P_E^m(u))}Q_E(T_x P_E^m(v))} \right) \leq \text{Asinh} \left( \frac{\omega(u, v)}{\sqrt{Q(u)Q(v)}} \gamma_E^m \right) \xrightarrow{m \to \infty} 0
\]
implying \( \lim_{m \to \infty} s_{E,P_E^m}(x)(T_xP_E^m(U),T_xP_E^m(V)) = 0 \) for any positive Lagrangian subspaces \( U,V \in \mathcal{L}_{E,x} \subset T_x\mathcal{L}_E \) and \( x \in \mathcal{I}_E \cap b_E \).

Since the set of positive Lagrangian subspaces lying in the cone \( C_{E,x} \) is compact, it follows that there exists a constant \( C_{s,E} > 0 \) such that

\[
s(T_xP_E^m(U),T_xP_E^m(V)) \leq C_{s,E} \cdot \gamma_E^m \quad (x \in \cap_{i=0}^m \mathcal{P}^{-i}_{E,i}(\mathcal{I}_E)). \tag{2.17}
\]

Given a two-dimensional subspace \( U_x \subset T_x\mathcal{I}_E \) we denote with \( F_{E,U_x}(x) \) the logarithm of the Jacobian of \( T_xP_E \) restricted to \( U_x \) with respect to the metric \( d_{E,x} \).

For a two-dimensional subbundle \( U \) of \( T\mathcal{I}_E \) and \( m \geq 1 \) we have

\[
S_m F_{E,U}(x) := \sum_{i=0}^{m-1} F_{E,T_xP_E^{i}(U_x)}(P_E^i(x)) \quad (x \in \cap_{i=0}^{m-1} \mathcal{P}^{-i}_{E,i}(\mathcal{I}_E)). \tag{2.18}
\]

Note that \( S_m F_{E,U}(x) \) is the logarithm of the Jacobian of \( P_E^m \) restricted to \( U_x \subset T_x\mathcal{I}_E, x \in \cap_{i=0}^m \mathcal{P}^{-i}_{E,i}(\mathcal{I}_E) \).

In order to estimate the volumes in (2.10), in the proof of Prop. 2.8 we control \( S_m F_{E,U} \) for a concrete positive Lagrangian subbundle \( U \in \mathcal{L}_E \). The following lemma relates this to \( S_m F_E \), defined on the much smaller set \( \mathcal{I}_E \cap b_E \).

**Lemma 2.7** There exists a constant \( C_{F_E} \) such that for any \( x,y \in \mathcal{I}_E(k) \), \( x \in b_E \) with \( k = (k_0,\ldots,k_m) \in X^* \) and any smooth positive Lagrangian subbundle \( V \in \mathcal{L}_E \subset C_E \) it holds:

\[
|S_m F_{E,V}(y) - S_m F_E(x)| < C_{F_E}.
\]

**Proof:** Let \( x,y \in \mathcal{I}_E(k), x \in b_E \) with \( k = (k_0,\ldots,k_m) \in X^* \). Then we have

\[
|S_m F_E(x) - S_m F_{E,V}(y)| \leq |S_m F_E(x) - S_m F_{E,V}(x)| + |S_m F_{E,V}(x) - S_m F_{E,V}(y)|. \tag{2.19}
\]

Since for any \( x \in \mathcal{I}_E \cap \mathcal{P}_{E}^{-1}(\mathcal{I}_E) \) the set \( (\mathcal{L}_{E,x},s_E) \) of positive Lagrangian subspaces in the cone \( C_{E,x} \) is a compact metric space and since the topology defined by this metric coincides with the standard topology, see Corollary on p. 8 of [LW], the map \( \mathcal{L}_{E,x} \to \mathbb{R}, U \mapsto F_{E,U}(x) \) is continuously differentiable. Thus it holds by a compactness argument that this map is Lipschitz continuous, i.e.

\[
|F_{E,U}(x) - F_{E,V}(x)| \leq C \cdot s_E(U_x,V_x)
\]

for an appropriate constant \( C > 0 \). Hence by Eq. (2.17)

\[
|S_m F_E(x) - S_m F_{E,V}(x)| \leq \sum_{i=0}^{m-1} \left| F_{E,T_xP_E^{i}(U_x)}(P_E^i(x)) - F_{E,T_xP_E^{i}(V_x)}(P_E^i(x)) \right|
\]

\[
\leq C \sum_{i=0}^{m-1} s_E(T_xP_E^i(V_x),T_xP_E^i(T_xP_E)(U_x)) \leq C \cdot C_{s,E} \sum_{i=0}^{m-1} \gamma_E^i \leq \frac{C \cdot C_{s,E}}{1 - \gamma_E},
\]

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The iterated Poincaré maps related by $\Omega$.

**Proof:**
By the chain rule of differentials

$$F_{E,U}: I \mapsto \Omega^\ell$$

is smooth on $I_E \cap P_E^{-1}(I_E)$, and thus also Lipschitz-continuous on $I_E \cap P_E^{-1}(I_E)$ by a compactness argument.

Note that by the chain rule of differentials $S_m F_E(x) = \sum_{i=0}^{m-1} F_E(P_k^i(x))$ is the logarithm of the unstable Jacobian of $P_E^m(x)$ for $x \in I_E \cap b_E$.

**Proposition 2.8**
With $F_E : I_E \cap b_E \to \mathbb{R}^+$ the logarithm of the unstable Jacobian it holds:

There exists a constant $C > 1$ such that for all $E > E_{th}$

$$C^{-1} \exp\left(-\frac{S_m F_E(x)}{E^3}\right) \leq \Omega_E(I_E(k)) \leq C \exp\left(-\frac{S_m F_E(x)}{E^3}\right)$$

(2.20)

uniformly for any $k = (k_0, \ldots, k_m) \in X^*$ and $x \in I_E(k) \cap b_E$.

**Proof:**
For the word $k \in X^*$ and $\ell = 0, \ldots, m$ we denote by $(\bar{y}, \bar{z})$ the local $(\bar{y}, \bar{z})$–coordinates on $I_E(k_\ell)$. By (2.11) the canonical volume form $\Omega_E$ appearing in (2.20) and the standard coordinate area forms $\Omega_y := dy_1 \wedge dy_2$ on the disk $B_y$, $\Omega_z := dz_1 \wedge dz_2$ on $B_z$ are related by $\Omega_E|_{I_E(k_\ell)} = \frac{E}{2d_{k_\ell}} \Omega_y \wedge \Omega_z$.

For all points $\bar{z}_0 \in B_z$ the set $B_{y_0}(\bar{z}_0, k) := \{ x = (\bar{y}, \bar{z}) \in I_E(k) : \bar{z} = \bar{z}_0 \}$ is a two-disk, and is identified with its image in $B_y$. Then

$$\int_{I_E(k)} \Omega_E = \frac{E}{2d_{k_0}} \int_{B_z} \left( \int_{B_{y_0}(\bar{z}_0, k)} \Omega_{y_0} \right) \Omega_{z_0}. \tag{2.21}$$

We restrict the iterated Poincaré maps $P_E^m$ to the two-disks $B_{y_0}(\bar{z}_0, k) \subset I_E(k_0)$ ($\bar{z}_0 \in B_{z_0}$), and denote by $\pi_{\bar{z}_0} : P_E^m(B_{y_0}(\bar{z}_0, k)) \to B_{z_m}$ the projections of their images to the $z_m$–coordinate plane. By Prop. 11.5 (1) of [Kna] the composition of these maps gives rise to the diffeomorphisms

$$Z_{\bar{z}_0, k} := \pi_{\bar{z}_0} \circ P_E^m|_{B_{y_0}(\bar{z}_0, k)} : B_{y_0}(\bar{z}_0, k) \to B_{z_m} \quad (\bar{z}_0 \in B_{z_0}). \tag{2.22}$$

In the inner integral on the right hand side of (2.21) we apply the transformation rule of integration

$$\int_{B_{y_0}(\bar{z}_0, k)} \Omega_{y_0} = \int_{Z_{\bar{z}_0, k}^{-1}(B_{z_m})} \Omega_{y_0} = \int_{B_{z_m}} Z_{\bar{z}_0, k}^* \Omega_{y_0} \tag{2.23}$$

• We denote by $\mathcal{V}_E$ the vertical bundle whose form in $(\bar{y}, \bar{z})$–coordinates is

$$\mathcal{V}_{E,x} := \{ (\delta \bar{y}, \delta \bar{z}) \in T_x I_E : \delta \bar{z} = 0 \} \quad (x \in I_E \cap P_E^{-1}(I_E)).$$
To combine them note that the sets appearing in Prop. 2.5 can be written as tangent vectors are contained in the local cone at that

\[ \Omega \]

Since \( \Omega \) is \( J \)-invariant, this trivially implies the upper bound in

\[ \frac{1}{2}\Omega_E(I_E(k)) \leq \Omega_E(\mathcal{O}_E \cap \mathcal{P}_E^{-1}(I_E(k))) \leq \Omega_E(I_E(k)) \quad (E > E_{\text{th}}, k \in X^*) \]  

(2.28)

The volume of the r.h.s. in (2.28) equals \( \Omega_E(I_E(k)) - \Omega_E(\mathcal{P}_E^{-1}(I_E(k)) \cap I_E) \).

Propositions 2.5 respectively 2.8 concern subsets of the outer resp. inner Poincaré surfaces. To combine them note that the sets appearing in Prop. 2.5 can be written as

\[ \mathcal{O}_E \cap \mathcal{P}_E^{-1}(I_E(k)) = \mathcal{P}_E^{-1}(I_E(k)) \setminus I_E. \]  

(2.27)

Since \( \Omega_E \) is \( \mathcal{P}_E \)-invariant, this trivially implies the upper bound in

\[ 1 \quad \Omega_E(I_E(k)) \]

(2.24) in (2.23), estimating its constituents.

**That Jacobian in (2.24) is estimated uniformly in the parameter \( \tilde{z}_0 \in B_{z_0} \) by**

\[ J_{z_0} = \frac{1}{2} + \mathcal{O}(1/E). \]  

(2.25)

To show this we choose an orthonormal basis \( w^{(1)}, w^{(2)} \) of \( T_\alpha S \) at \( a := \mathcal{P}_E(x) \). Then the tangent vectors are contained in the local cone at \( a \). Writing \( w^{(1)} = (\delta y^{(1)}, \delta z^{(1)}) \), this implies that \( ||\delta y^{(i)}||^2 - \frac{1}{2} \leq ||\delta z^{(i)}||^2 - \frac{1}{2} \leq C/E \), with \( C \) from (2.14). On the other hand

\[ \langle \delta y^{(1)}, \delta y^{(2)} \rangle = - \langle \delta z^{(1)}, \delta z^{(2)} \rangle \]

by orthogonality of \( w^{(1)} \) and \( w^{(2)} \). With (2.14) this implies \( ||\delta z^{(1)}||^2 - \delta z^{(2)} ||^2 \) \( = \mathcal{O}(1/E) \). As \( J_{z_0} = \sqrt{||\delta z^{(1)}||^2 ||\delta z^{(2)}||^2 - \langle \delta z^{(1)}, \delta z^{(2)} \rangle^2} \), we have proven (2.25).

**Note that both the unstable bundle \( T^u(I_E \cap b_E) \) and the iterates of the vertical bundle \( V \) are contained in the cone \( C_E \). Furthermore the smoothness of the map \( x \mapsto F_E V E \) \( x \) for \( V \in L_E \) a positive Lagrangian subbundle together with compactum argument and Lemma 2.7 shows the existence of a constant \( C \) such that the first factor on the right hand side of (2.24) is estimated by**

\[ C^{-1} \exp \left( - S_m F_E(x_0) \right) \leq \exp \left( - S_m F_E(x_0) \right) \leq C \exp \left( - S_m F_E(x_0) \right) \]  

(2.26)

uniformly in \( E > E_{\text{th}} \) and for any \( x \in I_E(k), x_0 \in I_E(k) \cap b_E \).

**Insertion of (2.25) and (2.26) in (2.24) completes the proof, taking into regard the fact that \( \Omega_E(B_y) \approx 1/E^2 \) and \( \Omega(z_m(B_y)) \approx 1/E^2 \).**

Using the notation (2.18), the push-forward of the two-form \( \Omega y_0 \) with the diffeomorphism (2.22) equals for \( x \in B_{y_0}(\tilde{z}_0, k) \)

\[ \Omega y_0 \left( Z_{\tilde{z}_0,k}(x) \right) = \exp \left( - S_m F_{E,V} (x) \right) \left( J_{\pi_{z_0}} \mathcal{P}_E^{-1} (x) \right)^{-1} \Omega_{z_m} \left( Z_{\tilde{z}_0,k}(x) \right), \]  

(2.24)

with \( J_{\pi_{z_0}} \) the Jacobian of the projection \( \pi_{z_0} \), of the surface \( S := \mathcal{P}_E(B_{z_0}(\tilde{z}_0, k)) \). We insert (2.24) in (2.23), estimating its constituents.

\[ \left( \mathcal{O}_E \cap \mathcal{P}_E^{-1}(I_E(k)) \right) \left( \mathcal{O}_E \cap \mathcal{P}_E^{-1}(I_E(k)) \right) \left( \mathcal{O}_E \cap \mathcal{P}_E^{-1}(I_E(k)) \right) \left( \mathcal{O}_E \cap \mathcal{P}_E^{-1}(I_E(k)) \right) \]  

(2.27)
The explicit formula (2.12) for the differential $T_P^E$ shows that the unstable Jacobian diverges (like $E^2$) as $E \to \infty$ and so does its logarithm $F_E$.

So the lower bound in (2.28) (even with any constant smaller than one instead of $1/2$) also follows for large enough threshold energy $E_{th}$ from (2.27) and the estimate of Proposition 2.8 in terms of scaling factors $F_E$.

Thus for an appropriate constant $C > 1$ we obtain the estimate

$$C^{-1} \sum_{k \in X_t + C, E} \exp \left( - S_{m(k)} F_E(x_k) \right) \leq \kappa_{I_E}(t) \leq C \sum_{k \in X_{t-C}, E} \exp \left( - S_{m(k)} F_E(x_k) \right)$$

(2.29)

valid for all $E > E_{th}$ and arbitrary representatives $x_k \in [k] \subset X$.

The hyperbolicity of $b_E$ assures that also the logarithm of the unstable Jacobian $F_E$ is Hölder continuous on $I_E \cap b_E$ resp. on $X$, see Thm. 19.1.6 and its Corollary 19.1.13 in [KH].

Like for $T_E$ from (2.3) we will, using the homeomorphism (2.6), consider $F_E : b_E \cap I_E \to \mathbb{R}^+$ (see (2.16)) also as an element of $\mathcal{F}_\alpha(X^+, \mathbb{R})$.

Since the following approach depends on the cohomology classes of the functions $T_E$ and $F_E$ only, we can assume that $T_E$ and $F_E$ are Hölder continuous functions on $X$ only depending on the future, and by a natural identification that $T_E$ and $F_E$ are Hölder continuous functions on the one-sided shift $X^+$. See Bowen [Bow], Sect. 6 for more details.

Next we define, using the one-sided shift $(X^+, \sigma)$, for $x \in X^+$ the function

$$\kappa_{I_E}^x : \mathbb{R} \to \mathbb{R}^+ , \quad \kappa_{I_E}^x := \sum_{m=0}^{\infty} \sum_{y \in \sigma^{-m}(x)} \exp \left( - S_m F_E(y) \right) \mathbb{1}_{\left(-\infty, S_m T_E(y)\right]}$$

(2.30)

This quantity models $\kappa_{I_E}$, defined in (2.8), but is only based on data of bounded orbits. We start with a rough upper estimate, needed later on for renewal theory.

**Lemma 2.9** For a suitable energy threshold $E_{th} > 0$ and $C > 0$ for all energies $E > E_{th}$ the sum $\kappa_{I_E}^x(t)$ converges for any $t \in \mathbb{R}$ and any choice $x \in X^+$. Furthermore

$$0 < \kappa_{I_E}^x(t) \leq C \exp \left( - \omega^-(E) \max(t, 0) \right)$$

with

$$0 < \omega^-(E) := \frac{\inf(F_E) - h_{top}(X^+, \sigma)}{\sup(T_E)} \leq \omega^+(E) := \frac{\sup(F_E) - h_{top}(X^+, \sigma)}{\inf(T_E)} ,$$

(2.31)

$h_{top}(X^+, \sigma) \geq 0$ being the ($E$-independent) topological entropy of the shift space $(X^+, \sigma)$.

**Proof:** For all $n \geq 2$ there exists a constant $C_h \geq 1$ such that

$$C_h^{-1} \cdot e^{n h_{top}(X^+, \sigma)} \leq |\sigma^{-m}(x)| \leq C_h \cdot e^{n h_{top}(X^+, \sigma)} \quad (n \in \mathbb{N}, x \in X^+).$$
For $n = 2$ this follows since the topological entropy $h_{\text{top}}(X^+, \sigma) = 0$ and $|\sigma^{-m}(x)| = 1$. For $n \geq 3$ the estimate follows since then the shift is topological mixing.

- We already remarked that the logarithmic unstable Jacobian $F_E$ diverges as $E \to \infty$. Thus for $E_{\text{th}} \geq 1$ large enough we have

$$F_E - h_{\text{top}}(X^+, \sigma) \geq \ln(2) \quad (E > E_{\text{th}}),$$

which in particular vindicates the first inequality in (2.31).

- With the constant $C > 0$ from Prop. 2.8 and for $m_0 := \lfloor \max(t, 0) / \sup(T_E) \rfloor$

$$\kappa_{T_E}^c(t) \leq \frac{C C_h}{E^3} \sum_{m=m_0}^{\infty} e^{\inf(h_{\text{top}}(X^+, \sigma))} e^{-m \inf(F_E)} \leq \tilde{C}(E) \exp(-\omega^-(E) \max(t, 0)) < \infty,$$

with $\tilde{C}(E) := \frac{2 C C_h}{E^3} e^{F_E - h_{\text{top}}(X^+, \sigma)} = O(\frac{1}{E})$, using (2.32) in estimating the geometric series. \(\Box\)

The following lemma shows the asymptotic equivalence of the functions $\kappa_{T_E}$ and $\kappa_{T_E}^c$.

**Lemma 2.10** For any energy $E > E_{\text{th}}$ it holds uniformly in $x \in X^+$ that

$$\kappa_{T_E}^c(t) \approx \kappa_{T_E}(t).$$

**Proof:** We show the existence of a constant $C > 1$ such that for all $E > E_{\text{th}}$, and $x \in X^+$

$$C^{-1} \kappa_{T_E}^c(t) \leq E^3 \kappa_{T_E}(t) \leq C \kappa_{T_E}^c(t) \quad (t > 0).$$

We start with the first inequality in (2.34).

Since by Lemma 2.4 the cylinders over the set $\mathcal{X}_{t+C_{rE}, E} \subset [X^+]$ of best fitting words constitute a partition of the shift space $X^+$, it holds:

$$\kappa_{T_E}^c(t) = \sum_{k \in \mathcal{X}_{t+C_{rE}, E}} \left( \sum_{m=0}^{\infty} \sum_{y \in \sigma^{-m}(k)} e^{-S_{mF_E(y)}(\Pi_{(-\infty, S_mT_E(y)]}(t))} \cdot \Pi_{[k]}(y) \right).$$

By Eq. (2.20) and the fact that $S_{m(k)}(T_E) \Pi_{[k]} < t$ it follows that for an appropriate $C_1 > 1$ and any best fitting word $k \in \mathcal{X}_{t+C_{rE}, E}$ the corresponding term in (2.35) is dominated by

$$\sum_{m=0}^{\infty} \sum_{y \in \sigma^{-m}(k)} e^{-S_{mF_E(y)}(\Pi_{(-\infty, S_mT_E(y)]}(t))} \cdot \Pi_{[k]}(y) \leq \sum_{m=m(k)}^{\infty} \sum_{y \in \sigma^{-m}(k)} e^{-S_{mF_E(y)}(\Pi_{[k]}(y))}$$

$$= \sum_{m'=0}^{\infty} \sum_{y \in \sigma^{-(m'+m(k))}(k)} \exp \left[ - S_{m(k)}(F_E) \Pi_{[k]}(y) - S_{m'}(F_E(\sigma^{m(k)}(y))) \right] \Pi_{[k]}(y)$$

$$\leq C_1 E^3 \Omega_E(T_E(k)) \sum_{m'=0}^{\infty} \sum_{y \in \sigma^{-m'}(k)} e^{-m' \inf(F_E)}.$$

(2.36)
Note that $|\sigma^{-m}(x)| \asymp e^{h_{\text{top}}(X,\sigma)m}$ uniformly in $x \in X^+$. Thus since the unstable Jacobian diverges as $E \to \infty$, the double sum in (2.35) converges (if $E_{\text{th}}$ is chosen large enough) for all $E > E_{\text{th}}$ and $x$, with upper bound 2. So the first estimate in (2.34) follows by using (2.29). With analogous arguments we get

\[
\kappa_{\overline{x}_E}(t) \geq C_1^{-1} E^3 \Omega_E(I_E(k)) \sum_{m'=0}^{\infty} \sum_{y \in \sigma^{-m'}(x)} e^{-m' \max\{F_E\}},
\]

showing (after an adaptation on the constant $C$ if necessary) the second estimate in (2.34). □

The key-feature of the function $t \mapsto \kappa_{\overline{x}_E}(t)$ which allows for a precise study of its asymptotic behaviour is the following:

**Lemma 2.11** The function $\kappa_{\overline{x}_E}: \mathbb{R} \to \mathbb{R}$ satisfies the renewal equation

\[
\kappa_{\overline{x}_E}(t) = \mathbb{1}_{\{t \leq 0\}} + \sum_{z \in \sigma^{-1}(x)} e^{-F_E(z)} \kappa_{\overline{x}_E}(t - T_E(z)).
\]

**Proof:** Noting that the sums $S_0 T_E = 0$, we decompose (2.30) into

\[
\kappa_{\overline{x}_E}(t) = \mathbb{1}_{\{t \leq 0\}} + \sum_{l=1}^{\infty} \sum_{y \in \sigma^{-l}(x)} \exp(-S_l F_E(y)) \cdot \mathbb{1}_{\{S_l T_E(y) \geq t\}}
\]

\[
= \mathbb{1}_{\{t \leq 0\}} + \sum_{z \in \sigma^{-1}(x)} e^{-F_E(z)} \sum_{m=0}^{\infty} \sum_{y \in \sigma^{-m}(z)} \exp(-S_m F_E(y)) \cdot \mathbb{1}_{\{S_{m+1} T_E(y) \geq t\}}
\]

\[
= \mathbb{1}_{\{t \leq 0\}} + \sum_{z \in \sigma^{-1}(x)} e^{-F_E(z)} \kappa_{\overline{x}_E}(t - T_E(z)),
\]

that is, the renewal equation. □

For any $E > E_{\text{th}}$ and $\omega \in \mathbb{C}$ the function $\omega T_E - F_E$ is Hölder continuous. The associated Ruelle transfer operator

\[
\mathcal{L}_{\omega,E}: C(X^+, \mathbb{R}) \to C(X^+, \mathbb{R}), \quad \mathcal{L}_{\omega,E} f(k) := \sum_{l \in \sigma^{-1}(k)} e^{\omega T_E(l) - F_E(l)} f(l)
\]

is a Perron-Frobenius (PF) operator if $\omega \in \mathbb{R}$. We denote with $\lambda_{\omega,E}$, $h_{\omega,E}$ and $\nu_{\omega,E}$ its PF eigenvalue, its normalized positive PF eigenfunction and its adjoint Borel PF probability measure respectively, i.e. (omitting the index $E$)

\[
\mathcal{L}_{\omega} h_{\omega} = \lambda_{\omega} h_{\omega}, \quad \mathcal{L}_{\omega}^* \nu_{\omega} = \lambda_{\omega} \nu_{\omega} \quad \text{and} \quad \int_{X^+} h_{\omega} \, d\nu_{\omega} = 1.
\]

The solution $\omega_0(E)$ of the implicit equation $\lambda_{\omega,E} = 1$ turns out to be the escape rate.
Lemma 2.12 For all $E > E_{\text{th}}$ there exists a unique solution $\omega_0(E) \in \mathbb{R}^+$ of the equation $\lambda_{\omega,E} = 1$, and $\omega_0(E) \in [\omega^-(E), \omega^+(E)]$ with $\omega^\pm$ from (2.31).

Proof: • The fact that $\omega \mapsto \lambda_\omega$ is continuously differentiable with
\[
\frac{d\lambda_\omega}{d\omega} = \frac{d}{d\omega} \int_X L_\omega h_\omega \, d\nu_\omega = \lambda_\omega \int_{X^+} T_E h_\omega \, d\nu_\omega > 0, \tag{2.40}
\]
using the normalizations (2.39), shows uniqueness of the solution.

• For existence and localization first notice that for $\omega \leq \omega^-(E) = \frac{\inf(F_E) - h_{\text{top}}(X^+, \sigma)}{\sup(T_E)}$ and independent of $k \in X^+$
\[
\lambda_{\omega,E} = \lim_{m \to \infty} \left( \frac{\sum_{l \in \sigma_{m}^{-1}(k)} \exp \left(S_m(\omega T - F_E)(l)\right) h_\omega(l)}{h_\omega(k)} \right)^{1/m} \leq \lim_{m \to \infty} \left( \frac{C_h \sup(h_\omega)}{\inf(h_\omega)} \exp \left(m(\omega - \omega^+(E)) \sup(T_E)\right) \right)^{1/m} \leq 1,
\]
since for $E > E_{\text{th}}$ we have $h_{\text{top}}(X^+, \sigma) < F_E$, see (2.31).

• Similarly for $\omega \geq \omega^+(E) = \frac{\sup(F_E) - h_{\text{top}}(X^+, \sigma)}{\inf(T_E)}$ independent of $k \in X^+$
\[
\lambda_{\omega,E} = \lim_{m \to \infty} \left( \frac{\sum_{l \in \sigma_{m}^{-1}(k)} \exp \left(S_m(\omega T - F_E)(l)\right) h_\omega(l)}{h_\omega(k)} \right)^{1/m} \geq \lim_{m \to \infty} \left( \frac{C_h^{-1} \inf(h_\omega)}{\sup(h_\omega)} \exp \left(m(\omega - \omega^+(E)) \inf(T_E)\right) \right)^{1/m} \geq 1,
\]
together showing existence of a solution $\omega_0(E) \in [\omega^-(E), \omega^+(E)]$. \qed

Proposition 2.13 With $\kappa_{F,E}$ from (2.30) and $\omega_0(E)$ from Lemma 2.12 there exists a constant $C \geq 1$ such that
\[
C^{-1} K_E(x) \exp \left(-\omega_0(E)t\right) \leq \kappa_{F,E}(x) \exp \left(-\omega_0(E)t\right) \leq C K_E(x) \exp \left(-\omega_0(E)t\right) \quad (t \in \mathbb{R}^+, x \in X^+),
\]
\[
K_E \in C(X^+, \mathbb{R}^+) \quad , \quad K_E(x) := \frac{h_\omega(x)}{\omega_0(1 - e^{-\omega_0}) \int_{X^+} T_E h_\omega \, d\nu_\omega}
\]
being defined with the help of (2.39).
Proof: • We first suppose that $T_E$ is integer-valued, but the image $T_E(X^+)$ is not contained in a proper subgroup $n\mathbb{Z}$, $n > 1$ of $\mathbb{Z}$. Then the piecewise constant map $t \mapsto \kappa_{T_E}^x(t)$ has jumps only at $t \in \mathbb{Z}$. We claim that even
\[
\kappa_{T_E}^x(t) \sim K_E(x)e^{-\omega_0|t|} \quad (t \to \infty),
\]
and it is sufficient to check (2.41) for $t \in \mathbb{N}$. By Lemma 2.9 the Fourier-Laplace transform
\[
\hat{\kappa}_{T_E}^x(\omega) := \sum_{t \in \mathbb{Z}} \kappa_{T_E}^x(t)e^{\omega t} \quad (x \in X^+)
\]
of $\kappa_{T_E}^x$ converges absolutely in a strip $\text{Re}(\omega) \in (0, \omega^-(E))$ of the complex plane, with $\omega^-(E) > 0$ defined in (2.31). Namely for these $\omega$ one has, with $C > 0$ from Lemma 2.9
\[
\sum_{t \in \mathbb{Z}\setminus \mathbb{N}} \kappa_{T_E}^x(t)e^{\omega t} = \kappa_{T_E}^x(0) \frac{1}{1-e^{-\omega}} \quad \text{and} \quad \sum_{t \in \mathbb{N}} \left| \kappa_{T_E}^x(t)e^{\omega t} \right| \leq \frac{C}{1-\exp\left(\text{Re}(\omega) - \omega^-(E)\right)}.
\]
The Fourier-Laplace transform of the renewal equation (2.37) is given by
\[
\hat{\kappa}_{T_E}^x(\omega) = \frac{1}{1-e^{-\omega}} + \sum_{y \in \sigma^{-1}(x)} \exp\left(\omega T_E(y) - F_E(y)\right) \kappa_{T_E}^y(\omega) \quad (x \in X^+).
\]
In terms of the Ruelle transfer operator (2.38) this leads to the formula
\[
\hat{\kappa}_{T_E}^x(\omega) = (1 - e^{-\omega})^{-1}(1 - \mathcal{L}_{\omega})^{-1}1(x) \quad (x \in X^+).
\]
The right hand side of Eq. (2.42) is real-analytic in the extended strip $\text{Re}(\omega) \in (0, \omega_0)$, with $\lambda_{\omega_0} = 1$ from Lemma 2.12.

Similar as in Prop. 7.2 of Lalley [Lal] one decomposes the PF-operator in the form
\[
\mathcal{L}_{\omega} = \lambda_{\omega} \nu_{\omega}(\cdot)h_{\omega} + \mathcal{L}_{\omega}''
\]
such that (with (2.39)) $\mathcal{L}_{\omega}''$ maps $C(X^+, \mathbb{C})$ to the subspace $\{g \in C(X^+, \mathbb{C}) : \nu_{k}(g) = 0\}$. Thus
\[
\sum_{m=0}^{\infty} \mathcal{L}_{\omega}^m = \left( \sum_{m=0}^{\infty} \lambda_{\omega}^m \right) \nu_{\omega}(\cdot)h_{\omega} + \sum_{m=0}^{\infty} (\mathcal{L}_{\omega}''^m)
\]
and we obtain in some punctured neighbourhood of $\omega_0$
\[
(1 - \mathcal{L}_{\omega})^{-1} = (1 - \lambda_{\omega})^{-1} \nu_{\omega}(\cdot)h_{\omega} + (1 - \mathcal{L}_{\omega}''^{-1})^{-1},
\]
the second term of the right hand side being holomorphic. Combining Equations (2.42), (2.43) and (2.40) and using $\lambda_{\omega_0} = 1$ we see that the residue of $\omega \mapsto \hat{\kappa}_{T_E}^x(\omega)$ at $\omega = \omega_0$ equals
\[
(1 - e^{-\omega_0})^{-1} \left( \frac{d\lambda_{\omega_0}}{d\omega}(\omega_0) \right)^{-1} h_{\omega_0}(x) = -(1 - e^{-\omega_0})^{-1} \frac{h_{\omega_0}(x)}{\nu_{\omega_0}(T_Eh_{\omega_0})} = -K_E(x).
\]
To show (2.41) we introduce, similar to the proof of Thm. 2 of [La], the function
\[ F(z, x) := \sum_{m=0}^{\infty} z^m (e^{m\omega_0} \kappa_{\mathbb{Z}}^x(m) - K_E(x)) \quad (x \in X^+). \]

By Lemma 2.9 the function \( z \mapsto F(z, x) \) is holomorphic in an open disk around 0 of radius \( \exp(\omega^-(E) - \omega_0) \leq 1 \) (see Lemma 2.12). For \( z \) in the open annulus \( e^{-\omega_0} < |z| < e^{\omega^-(E) - \omega_0} \) we rewrite
\[ F(z, x) = \hat{\kappa}_{\mathbb{Z}}^x (\ln z + \omega_0) + \frac{K_E(x)}{z - 1} - \sum_{\ell=1}^{\infty} z^{-\ell} e^{-\ell \omega_0} \kappa_{\mathbb{Z}}^x(-\ell). \]

By Lemma 2.9 the last term is analytic in \( z \) for \( |z| > e^{-\omega_0} \), whereas the residue of the sum of the first and second term vanishes by (2.44). Thus one can analytically extend as in [La] the function \( z \mapsto F(z, x) \) to an open disk \( |z| < 1 + 2\varepsilon(E) \) for some \( \varepsilon(E) > 0 \).

Then Cauchy’s integral formula gives
\[ e^{m\omega_0} \kappa_{\mathbb{Z}}^x(m) - K_E(x) = (2\pi i)^{-1} \int_{|z|=1+\varepsilon(E)} F(z, x) z^{-m-1} \, dz = O((1 + \varepsilon(E))^{-m}) \]
and thus \( \kappa_{\mathbb{Z}}^x(m) \sim e^{-m\omega_0} K_E(x) \) for non-negative integer \( m \). This shows the claim for the case when \( T_E \) is integer-valued and not contained in a proper subgroup of \( \mathbb{Z} \).

- The general lattice case, i.e. the image \( T_E(X^+) \) generates the discrete subgroup \( c\mathbb{Z}, c > 0 \) of \( \mathbb{R} \) is treated by a multiplication of \( T_E \) by the factor \( 1/c \).

- The non-lattice case follows by appropriate modification of the proof of Thm. 1 in [La], as the above lattice case followed by modifying the proof of Thm. 2 in [La].

The Lemmata 2.3 and 2.10, together with this proposition imply Part (i) of the Main Theorem:
\[ \kappa_{\mathbb{Z}}^x(t) \asymp \kappa_{\mathbb{Z}}(t) \asymp \kappa_{\mathbb{Z}}(t) \asymp \exp(-\omega_0(E)t) \quad (E > E_{th}). \]

### 2.2 Proof of Part (ii)

The escape rate \( \beta_E \) from (1.11) has been shown to equal the solution \( \omega_0(E) \) of the implicit eigenvalue formula \( \lambda_{PF}(\mathcal{L}_{\omega,E}) = 1 \) of the transfer operator \( \mathcal{L}_{\omega,E} \) defined in (2.33).

To obtain a finite-dimensional approximation of \( \mathcal{L}_{\omega,E} \), we approximate the functions \( F_E, T_E \), originally defined in (2.3) and (2.16) and later considered as elements of \( \mathcal{F}_h(X^+, \mathbb{R}) \), using the homeomorphism (2.6), by the matrices \( \tilde{T}_E \) and \( \tilde{F}_E \) from (1.14), depending only on two symbols \((k_0, k_1)\), but also considered as (locally constant) functions in \( \mathcal{F}_h(X^+, \mathbb{R}) \).

It follows from (2.12) and Lemma 10.6 of [Kna] that that there exists a \( C > 0 \), so that with \( \delta_T(E) := C E^{-3/2} \) and \( \delta_F(E) := C E^{-1} \) for all \( E > E_{th} \)
\[ \tilde{T}_E - \delta_T(E) \leq T_E \leq \tilde{T}_E + \delta_T(E) =: \tilde{T}_E^+ \quad \text{and} \]
\[ \tilde{F}_E := \tilde{F}_E + 2 \ln(1 - \delta_F(E)) \leq F_E \leq \tilde{F}_E + 2 \ln(1 + \delta_F(E)) =: \tilde{F}_E^+. \]
Next we define for $\vec{\delta} = (\delta_1, \delta_2) \in \mathbb{R}^2$ and $\mathcal{M}_E$ from (2.15) the weighted transfer matrices

$$\mathcal{M}_E(\beta, \vec{\delta}) \in \mathbb{R}^{4 \times A}, \quad \mathcal{M}_E(\beta, \vec{\delta})_{k_0, k_1} := \exp(\beta \delta_1 + \delta_2) \mathcal{M}_E(\beta)_{k_0, k_1}.$$  

Note that $\mathcal{M}_E^2(\beta, \vec{\delta})$ has strictly positive entries, i.e. $\mathcal{M}_E(\beta, \vec{\delta})$ is a Perron-Frobenius matrix.

With $\lambda_{PF}(\mathcal{M}_E(\beta, \vec{\delta}))$ we denote the Perron-Frobenius eigenvalue of the matrix $\mathcal{M}_E(\beta, \vec{\delta})$. The approximate escape rate $\tilde{\beta}_E$ and its bounds $\tilde{\beta}_E^\pm$ are defined implicitly by

$$\lambda_{PF}(\mathcal{M}_E(\tilde{\beta}_E)) = 1 \quad \text{and} \quad \lambda_{PF}(\mathcal{M}_E(\tilde{\beta}_E^\pm, (\pm \delta F(E), \mp \delta T(E)))) = 1. \quad (2.47)$$

The following lemma tells that $\tilde{\beta}_E$ and $\tilde{\beta}_E^\pm$ are well defined for large enough energies $E$:

**Lemma 2.14** For all $\vec{\delta} \in \mathbb{R}^2$ the map $\beta \mapsto \lambda_{PF}(\mathcal{M}_E(\beta, \vec{\delta}))$ is continuous. If $\delta_2 > -\inf(\tilde{T}_E)$, it is strictly monotone increasing.

**Proof:** It is well known that $\lambda_{PF}$ is related to the topological pressure by

$$\ln(\lambda_{PF}(\mathcal{M}_E(\beta, \vec{\delta}))) = P_{top}(X, \sigma, -\tilde{F}_E + \delta_1 + \beta(\tilde{T}_E + \delta_2)).$$

Continuity of $\beta \mapsto \ln(\lambda_{PF}(\mathcal{M}_E(\beta, \vec{\delta})))$ follows from Theorem 9.7 of [Wal]. By using the variational principle for the topological pressure and the fact that $\tilde{T}_E + \delta_2 > 0$ one gets

$$\frac{\ln(\lambda_{PF}(\mathcal{M}_E(\beta_2, \vec{\delta}))) - \ln(\lambda_{PF}(\mathcal{M}_E(\beta_1, \vec{\delta})))}{\beta_2 - \beta_1} \geq \inf(\tilde{T}_E) + \delta_2 \quad (\beta_2 > \beta_1).$$

2.2.1 High Energy-Limit of the Approximate Escape Rate

With $d_{max}$ being the maximum of the distances of the $n$ centres, we denote the approximation to the escape rate, appearing in Part (ii) of the Main Theorem, by $\beta_E^\infty := \frac{2\sqrt{2E} \ln E}{d_{max}}$.

**Lemma 2.15** $\tilde{\beta}_E$ from (2.47) satisfies $\lim_{E \to \infty} \frac{\tilde{\beta}_E}{\beta_E^\infty} = 1$.

**Proof:** First note that the estimate $\max_{i \in A} \sum_{j \in A} (\mathcal{M}_E(\tilde{\beta}_E))_{i,j} \geq \lambda_{PF}(\mathcal{M}_E(\tilde{\beta}_E)) = 1$ implies that not all entries of the PF-matrix $\mathcal{M}_E(\tilde{\beta}_E)$ can tend to zero for $E \to \infty$. This, together with the asymptotic formula

$$(\mathcal{M}_E(\tilde{\beta}_E))_{k_0, k_1} \sim f^{-2}(k_0, k_1) \exp \left( -2 \ln E + \tilde{\beta}_E \left( \frac{d_{k_0, k_1}}{\sqrt{2E}} + \frac{Z_{k_0, k_1} \ln E}{(2E)^{3/2}} \right) \right) \quad (k_0, k_1 \in A)$$

for the non-zero entries of $\mathcal{M}_E(\tilde{\beta}_E)$, implies

$$\liminf_{E \to \infty} \frac{\tilde{\beta}_E}{\beta_E^\infty} \geq 1.$$
Next assume that
\[ \limsup_{E \to \infty} \frac{\tilde{\beta}_E}{\beta^\infty} > 1 \]
such that at least one entry of \( M_E(\tilde{\beta}) \) is unbounded for \( E \to \infty \). The symmetry
\[ (M_E)_{(i,j),(j,i)} = (M_E)_{(k,j),(j,k)} \]
implies that for two centres \( i_0, j_0 \in \{1, \ldots, n\} \) of maximal distance \( d_{i_0,j_0} = d_{\text{max}} \) the entry
\[ (M_E)_{k_0,k_0} = (M_E)_{i_0,j_0} \to \infty \text{ for } E \to \infty, \]
\( k_0 = (i_0, j_0) \in A \) and \( k'_0 = (j_0, i_0) \in A \). Then the \( k_0 \)-th diagonal element of \((M_E(\tilde{\beta}))^2 \) is unbounded as \( E \to \infty \), since
\[ (M^2_E)_{k_0,k_0} = \sum_{\ell \in A} (M_E)_{k_0,\ell} (M_E)_{\ell,k_0} \geq (M_E)_{k_0,k'_0} \cdot (M_E)_{k'_0,k_0} = (M^2_E)_{k_0,k'_0}. \]
This is a contradiction to the fact that for the matrix \( M^2_E \) the diagonal elements has to be bounded above by one, as \((M_E(\tilde{\beta}))^2 \) is a PF-matrix whose PF-eigenvalue equals one.
Thus it follows \( \lim_{E \to \infty} \tilde{\beta}^\infty_E = 1 \). \( \square \)

### 2.2.2 Quality of the Approximation

We will now estimate the quality of the approximation of \( \beta_E \) by \( \tilde{\beta}_E \). Recall that the escape rate \( \beta_E \) was defined by \( \lambda_{PF}(L_{F_E+\beta_ET_E}) = 1 \). The estimates \((2.45)\) and \((2.46)\) for the functions \( \tilde{T}^E_\pm \) and \( \tilde{F}^E_\pm \) with the original functions \( F_E \) and \( T_E \) together with the monotonicity of topological pressure show that \( \tilde{\beta}^-_E \leq \beta_E \leq \tilde{\beta}^+_E \).

Together with our last lemma this completes the proof of the Main Theorem, Part (ii).

**Lemma 2.16** \( \tilde{\beta}^\pm_E = \tilde{\beta}_E (1 + O(1/E)) \).

**Proof:** We are now going to express the bounds \( \tilde{\beta}^\pm_E \) for the escape rate \( \beta_E \) in terms of the approximate escape rate \( \beta_E \). For this consider the Taylor expansion
\[ \beta(\delta) = \beta(0) \left< d\beta(0), \delta \right> + O(\|\delta\|^2) \]
of \( \beta(\delta) \), implicitly defined by \( 1 = \lambda_{PF}(M_E(\beta(\delta), \delta)) =: \lambda_{PF}(\beta(\delta), \delta) \).

This implicit definition of \( \beta \) gives
\[ 0 = d\beta \lambda_{PF}(\beta(\delta), \delta) = \left< \partial_\beta \lambda_{PF}(\beta, \delta), d\beta(\delta) \right> + \partial_\delta \lambda_{PF}(\beta(\delta), \delta) . \]

By taking the derivative of the formula
\[ \lambda_{PF}(M_E(\beta, \delta)) = \left< v^l_{PF}(\beta, \delta), M_E(\beta, \delta) v^r_{PF}(\beta, \delta) \right> \]
with \( \left< v^l_{PF}(\beta, \delta), v^r_{PF}(\beta, \delta) \right> = 1 \).
it follows
\[
\frac{\partial_{\delta_1} \beta}{\partial \lambda_{PF} (\beta, \tilde{\delta})} = -\frac{\partial_{\delta_2} \lambda_{PF} (\beta, \tilde{\delta})}{\partial \lambda_{PF} (\beta, \tilde{\delta})} = -\frac{\langle v_{PF} (\beta, \tilde{\delta}) \rangle}{\partial_{\delta_1} \lambda_{PF} (\beta, \tilde{\delta})} \frac{\partial_{\delta_2} M_E (\beta, \tilde{\delta})}{\partial \lambda_{PF} (\beta, \tilde{\delta})} (v_{PF} (\beta, \tilde{\delta})) (i = 1, 2).
\]

With the \( A \times A \) matrix \( \tilde{T}_E \) from (1.14) we get, * denoting the pointwise product,
\[
\frac{\partial_{\delta_1} M_E (\beta, \tilde{\delta})}{\partial \beta (0, 0)} = \tilde{T}_E \ast M_E (\beta (0)) ,
\]
\[
\frac{\partial_{\delta_1} M_E (\beta, \tilde{\delta})}{\partial \beta (0, 0)} = M_E (\beta (0)) \text{ and } \frac{\partial_{\delta_2} M_E (\beta, \tilde{\delta})}{\partial \beta (0, 0)} = 0, M_E (\beta (0)).
\]

Setting \( \tau_E := \langle v_{PF} (\beta (0), 0) \rangle (\tilde{T}_E \ast M_E (\beta (0))) v_{PF} (\beta (0), 0) \rangle \) one gets
\[
\frac{\partial_{\delta_1} \beta (0)}{\partial \beta (0, 0)} = -1/\tau_E , \frac{\partial_{\delta_2} \beta (\tilde{\delta})}{\partial \beta (0, 0)} = -\beta (0)/\tau_E
\]
and finally \( \beta (\tilde{\delta}) = \beta (0) - \frac{1}{\tau_E} (\delta_1 + \beta (0) \delta_2) + O(\|\tilde{\delta}\|^2\). \)

As the non-zero entries of \( \tilde{T}_E \) are bounded below by \( C/\sqrt{E} \), we get \( \tau_E^{-1} \in O(E^{1/2}) \). From \( \delta_E (E) \in O(E^{-1}) \) and \( \delta_T (E) \in O(E^{-3/2}) \) (see (2.45) and (2.46)) and \( \beta (0) = \beta_E \times 2 \sqrt{2E \ln (E)/d_{\max}} \) we get the approximation \( \beta_E = \beta_E (1 + O(1/E)) \).

\[\square\]

### A Proof of Proposition 1.5

We use the following estimate from [Kna], Thm. 6.5: If \( E > E_{th} \) and \( (\vec{p}_0, \vec{q}_0) \equiv x_0 \in \Sigma_E \) with \( q_0 := \|\vec{q}_0\| \geq R_{vir} (E) \) and \( \pm \langle \vec{q}_0, \vec{p}_0 \rangle \geq 0 \), then (with the symbol \( O \) meaning existence of a bound for \( x_\infty := (\vec{p}_\infty, \vec{q}_\infty) := \Omega^E (\vec{p}_0, \vec{q}_0) \)
\[
\vec{p}_\infty - \vec{p}_0 = O \left( q_0^{-1-\varepsilon} E^{-2} \right) , \quad \vec{q}_\infty - \vec{q}_0 = O \left( q_0^{-\varepsilon} E^{-1} \right) . \tag{A.1}
\]

From (A.1) and \( \vec{p}_\infty = O(\sqrt{E}) \) we conclude that in the case \( \langle \vec{q}_0, \vec{p}_0 \rangle = 0 \)
\[
\langle \vec{q}_\infty, \vec{p}_\infty \rangle = \langle \vec{q}_\infty - \vec{q}_0, \vec{p}_\infty \rangle + \langle \vec{q}_\infty, \vec{p}_\infty - \vec{p}_0 \rangle = O \left( q_0^{-\varepsilon} E^{-2} \right) . \tag{A.2}
\]

For the Kepler flow (1.6), on the other hand we use the Lagrange-Jacobi equation, followed by an inequality valid for all \( Z_\infty \in \mathbb{R} \):
\[
\frac{d}{dt} \langle \vec{q}_\infty (t), \vec{p}_\infty (t) \rangle = 2E + Z_\infty \frac{Z_\infty}{\langle \vec{q}_\infty (t) \rangle} \geq E > E_{th} \geq 0. \tag{A.3}
\]

The time \( t_0 \) needed to reach the pericentre of the Kepler flow is thus uniquely defined by \( \langle \vec{q}_\infty (t_0), \vec{p}_\infty (t_0) \rangle = 0 \). Together with (A.2) this shows that \( t_0 \) is estimated by
\[
|t_0| \leq \frac{\langle \vec{q}_\infty, \vec{p}_\infty \rangle}{E} = O \left( q_0^{-\varepsilon} E^{-3/2} \right) . \tag{A.4}
\]
1. \((A.4)\) implies Assertion 1.:

If the \(\Phi\)-scattering orbit has a pericentre, whose distance from the origin is larger than \(R_{\text{vir}}\), then by the virial inequality \((1.2)\) that pericentre is unique, and the total time delay is smaller than \(2|t_0|\), with \(t_0\) from \((A.4)\).

Otherwise it enters the interaction zone at a unique time, which we assume to equal zero w.l.o.g.. At that moment \(q_0 = R_{\text{vir}}\) and \(\langle \vec{q}_0, \vec{p}_0 \rangle \leq 0\) and so by \((A.1)\)

\[
\vec{q}_\infty \leq R_{\text{vir}} \pm \mathcal{O}\left(R_{\text{vir}}^{-\epsilon}E^{-1}\right) \leq 2R_{\text{vir}}
\]

for \(E_{\text{th}}\) large enough. With \((A.3)\) we get that the time spent by the Kepler orbit inside the interaction zone is smaller than \(2R_{\text{vir}}/\sqrt{E}\).

2. If \(\tau_E(x) \geq t\) for \(t \in (0, C_3/E_{3/2})\), then by \((A.4)\) the \(\Phi\)-orbit through \(x\) cannot have a pericentre \((\vec{p}_0, \vec{q}_0)\) with \(q_0 > C(t^{E_{3/2}})^{-1/\epsilon}\) (here \(C_3 := (C/R_{\text{vir}})^{\epsilon}\) is chosen so that \(q_0 \geq R_{\text{vir}}\)). This implies Assertion 2, since the total symplectic volume of the Poincaré surface \(\{(\vec{p}, \vec{q}) \in \Sigma_E : \|\vec{q}\| = q_0, \langle \vec{q}, \vec{p} \rangle < 0\}\) is of order \(q_0^2E\).

3. By our choice of \(C_3\) in Assertion 2, \(q_0 \leq C (\tau_E(x)E_{3/2})^{-1/\epsilon} \leq C C_3^{-1/\epsilon} = R_{\text{vir}}\). \(\square\)

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