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Compactification of the energy surfaces for n bodies

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Abstract

For n bodies moving in Euclidean d–space under the influence of a homogeneous pair interaction we compactify every center of mass energy surface, obtaining a $(2d(n-1)-1)$–dimensional manifold with corners in the sense of Melrose. After a time change, the flow on this manifold is globally defined and non-trivial on the boundary.

Contents

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1 Introduction and Results

The n–body problem of celestial mechanics is described by the Hamiltonian

$$H(q,p) = K(p) - U(q) \text{ , with } U(q_1,\ldots,q_n) = \sum_{1\le i<j\le n} \frac{Z_{i,j}}{\|q_i - q_j\|^\alpha} \,, \qquad (1.1)$$

kinetic energy $K(p) = \sum_{i=1}^n \frac{\|p_i\|^2}{2m_i}$, $\alpha := 1$ and $Z_{i,j} := Gm_im_j$ with G the gravitational constant. We call U the 'potential' although it is actually the negative of the potential.
We work in the center of mass system. Due to collisions and escape to spatial infinity its energy surfaces $\widehat{\Sigma}_E = H^{-1}(E)$ are non-compact. Our goal here is to compactify the energy surfaces by adding boundary pieces in such a way that the n–body flow extends nontrivially to the added boundaries.

1.1 Theorem

Assume $Z_{i,j} > 0$ and $0 < \alpha < 2$ in the 'potential' U of equation (1.1). *Then the constructions of sections 3 and 4 yield, for each energy E, a compact manifold with corners $\widehat{\Sigma}_E$ whose interior is diffeomorphic to the usual energy level set $\widehat{\Sigma}_E$ away from the Hill boundary $\{U = -E\}$ and on which the usual n–body flow, after a time reparameterization, extends continuously to a non-trivial C^1–flow on the added boundaries.*

For the definition of a manifold with corners and a brief introduction to these spaces see Appendix A.

We prove the theorem by combining two well-established techniques from the n–body world with a technique primarily used in linear PDEs.

The first technique is that of adding sub-manifolds to the standard phase space in order to better understand limiting behaviours. For collisions we add collision manifolds by blow up, following the ideas of McGehee. See [McG1, McG2, ElB, De, LS, Ll] and references cited therein. For widely separated particles with interparticle distances diverging we add a manifold at infinity. See [DMMY].

The second technique, originally developed for the quantum n–body problem, is that of GRAF partitions (see [Gr]). These partitions help us to label the strata of $\widehat{\Sigma}_E$ and understand its topology and combinatorics.

The third technique is Melrose's iterative real blow-up [Me] developed for PDEs. This iterative blow-up provides the appropriate language to get to the final result. In the last section we deduce the topology of the total blow up in Theorem 5.3.

The famous regularizations of binary collisions due to LEVI-CIVITA [LC] or MOSER [Mo] (or any other method) allow us to analytically pass through binary collisions but are only available when $\alpha = 2(1-1/k)$ for $k \in \mathbb{N}$. (See [McG2, Theorem 7.1]). Wanting a unified picture of compactification valid for all values of α, or at least values in the interval $(0,2)$, we have had to treat binary collisions in the same way as we have treated triple or higher collisions: by slowing down the flow and attaching boundaries corresponding to these collisions.

We will work in the center of mass configuration space

$$M = \big\{q = (q_1, \ldots, q_n) \in \mathbb{R}^{nd} \mid \textstyle\sum_{i=1}^n m_i q_i = 0\big\}.$$

The (negative) potential U is defined on $\widehat{M} = M \backslash \Delta$, with collision set

$$\Delta = \{q \in M \mid q_i = q_j \text{ for some } i \neq j\}.$$

In Section 2 the stage is set by introducing the notation necessary to treat the combinatorics encoded in Δ.

The n particle phase space $\widehat{P} = T^*\widehat{M}$ over noncollision configuration space $\widehat{M}$ is non-compact in three ways:

- Total energy $H : \widehat{P} \to \mathbb{R}$ may have any value $E \in \mathbb{R}$.
- There are collisions between the particles, with limits in Δ.
- Particles may escape to spatial infinity.

To compactify phase space the first obvious step[1] is to separately consider motion on the energy surfaces $\widehat{\Sigma}_E$. In Section 3 we compactify configuration space $\widehat{M}$ by

[1] We don't touch upon the question about the limits $E \to \pm\infty$.

adding a sphere $\mathbb{S}$ at infinity to M and by forming the real blow up of the collision set Δ, thus obtaining a *compact* manifold with corners $\widehat{M}$. In Subsection 4.1 we rescale velocities (or momenta) in order to compactify the energy surface $\widehat{\Sigma}_E$. In Subsection 4.2 we rescale time in order to get a well-defined dynamics on the compactified energy surface. We will see that $\widehat{\Sigma}_E = \widehat{M}_E \times \mathbb{S}$ where $\widehat{M}_E \subseteq \widehat{M}$ is the compactified Hill region $\{q : U(q) \geq -E\}$. In particular, points along the traditional Hill boundary have been blown up into spheres. As a result, the original dynamics has been altered at the Hill boundary and some care is required to understand the rescaled dynamics there and recover the original dynamics. By continuity the flow on the boundary mimics the one near the boundary, providing useful information about the original flow (see Remark 4.4).
Finally, in Section 5 the topology of the construction is considered.

1.1 History and Comparisons

An incomplete flow on a noncompact manifold X can always be compactified, but in a useless way. Choose an arbitrary compactification $\bar{X}$ of X. (There are many! [2]) Slow down the flow by rescaling the vector field which defines this flow so that the vector field vanishes on $\bar{X} \setminus X$. Voila! (We thank P. Deligne for this remark.) The real trick is to compactify X and rescale the vector field in such a way that the extended rescaled field **does not vanish** on ∂X and allows you to extract new information about the original flow on X.

McGehee's partial compactification [McG1] succeeds eminently for extracting information about near-total collision motions. Robinson [Ro], McGehee [McG3] and others have "turned McGehee's microscope around to become a telescope" by adding a a manifold at infinity, instead of at collision, this infinity manifold being used to account for escape orbits. Again, they derived non-trivial information about the dynamics by this trick. **In essence, what we do here is systematically implement both of these partial compactifications in order to get our full compactification.**

Ours is the first paper to fully compactify classical n-body problems, $n > 2$, in a *potentially useful way*. (We have yet to establish its utility.)

Two-body problems have been compactified. Moser in particular compactifies the $\alpha = 1$ negative energy 2-body problem in d dimensions, in the center of mass frame. Moser's compactified phase space is the unit sphere bundle of the d-sphere. Like the methods of Levi-Civita [LC], Kuustanheimo-Steifel and a number of others, Moser's method is a 'regularization' rather than a 'blow-up' and as such is quite particular to $\alpha = 1$ and so we will reject it.

Extended versions of regularizations, specific for $\alpha = 1$, were developed

[2] any compact connected N-manifold arises as the compactification of Euclidean N-space

by HEGGIE [He], WALDVOGEL [Wald], LEMAÎTRE, [Le], MOECKEL-MONTGOMERY [MM], and others for improving numerics and deriving partial compactifaction results for n-body problems with $\alpha = 1$.

QIU-DONG WANG [Wa] uses a time and velocity rescaling very similar to ours but for different purposes. In particular, he does not add in collision manifolds or manifolds at infinity. By adding in these manifolds we allow for coherent α and ω limit sets for collections of orbits leaving the honest energy E phase space $\widehat{\Sigma}_E$. These limit sets are actual places for orbits to go to and will afford us, we hope, with an eventual better understanding of the near-collision orbits and of the way in which clusters of particles approach spatial infinity and to what extend the clusters asymptotically become independent. See the Remark 4.4.

GRAF [Gr] constructed what we nowadays call *Graf partitions* in order to prove asymptotic completeness for the quantum n-body problem. VASY, a student of Melrose, used in [Va] essentially these same Graf partitions combined with Melrose style blow-ups into manifolds-with-corners in order to obtain new information about scattering in quantum 3-body and n-body problems.

1.2 Goals

The flows on the boundary strata are simpler than the flow on the bulk $(\widehat{\Sigma}_E)$. For example, the flow on the open part of the locus at infinity is a reparameterization of geodesic flow on the sphere, while the flows on the open strata of the binary collision locus are reparameterized Kepler flows.

Let us agree that we can concatenate two boundary trajectories if the ω-limit of one agrees with the α-limit of the other. Thus, if γ_1 and γ_2 are boundary trajectories for which $\lim_{t\to+\infty}\gamma_1(t) = \lim_{t\to-\infty}\gamma_2(t)$ then we can form the concatenation $\gamma_2 * \gamma_1$ made up of first traversing γ_1 and then traversing γ_2.

We believe that these concatenated boundary trajectories form a kind of skeleton, or support locus which controls the flow in the bulk near the boundary. Specifically, given any such concatenation $c = \gamma_2 * \gamma_1$ we believe that we can prove the existence of sequences c_i of trajectories which lie completely in the bulk and which converge to c in an appropriate sense: $\lim_{i\to\infty} c_i = c$. Establishing the existence of these "shadowing sequences" c_i is work in progress. It would validate various observations and numerical experiments made in [DMMY] and [FKM].

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2 Notation

2.1 Phase flow

Consider n particles of masses $m_i > 0$ moving in d-dimensional Euclidean space $\mathbb{R}^d$. (Take $n > 1$ please!) Introduce a separate copy $M_i := \mathbb{R}^d$ of the Euclidean space for each particle $i \in N := \{1, \ldots, n\}$ so that $q_i \in M_i$. The center of mass zero configuration space is

$$M := \left\{q \in \bigoplus_{i \in N} M_i \mid \sum_{i \in N} m_i q_i = 0\right\}$$

and forms a codimension d linear subspace of the vector space $(\mathbb{R}^d)^n$. We use the mass-inner product $\langle q, q' \rangle_{\mathcal{M}} = \sum_i m_i q_i \cdot q'_i$ on M instead of the standard inner product $\langle q, q' \rangle = \sum_i q_i \cdot q'_i$. The mass matrix $\mathcal{M} : (\mathbb{R}^d)^n \to (\mathbb{R}^d)^n$ defined by $\mathcal{M}(q_1, \ldots, q_n) = (m_1 q_1, m_2 q_2, \ldots, m_n q_n)$ intertwines the two inner products:

$$\langle q, q' \rangle_{\mathcal{M}} := \langle q, \mathcal{M} q' \rangle \ . \tag{2.1}$$

We set $\|q\|_{\mathcal{M}} := \sqrt{\langle q, q \rangle_{\mathcal{M}}}$ omitting the subscript $\mathcal{M}$ whenever possible. We can write the kinetic energy as

$$K(p) := \tfrac{1}{2} \langle p, \mathcal{M}^{-1} p \rangle \ . \tag{2.2}$$

The *collision set* in configuration space is given by

$$\Delta := \{q \in M \mid q_i = q_j \text{ for some } i \neq j \in N\} \,. \tag{2.3}$$

We consider homogeneous potentials on the *noncollision configuration space*

$$\widehat{M} := M \backslash \Delta. \tag{2.4}$$

On the phase space $\widehat{P} := T^* \widehat{M}$ the Hamiltonian function is given by

$$H : \widehat{P} \to \mathbb{R} \quad , \quad H(q, p) = K(p) - U(q) \,, \tag{2.5}$$

with the real-analytic potential $U : \widehat{M} \to \mathbb{R}$ of the form (1.1), with $Z_{i,j} > 0$.

With the Euclidean gradient $\nabla_{(i)}$ on each $M_i = \mathbb{R}^d$ the Hamiltonian equations of (2.5) have the form

$$\dot{q}_i = \frac{p_i}{m_i} \quad , \quad \dot{p}_i = \sum_{j \in N \backslash \{i\}} \nabla_{(i)} U_{i,j}(q_j - q_i) \qquad (i \in N). \tag{2.6}$$

where

$$U_{i,j}(q_j - q_i) = \frac{Z_{i,j}}{\|q_i - q_j\|^\alpha} \tag{2.7}$$

A useful alternative way to write the equations is in terms of velocities:

$$\dot{q} = v \quad , \quad \dot{v} = \nabla U(q) \tag{2.8}$$

where now $q, v \in M$, $q \notin \Delta$ and the gradient ∇ is with respect to the mass metric.

2.1 Remark (other potentials)
The same form for Newton's equations holds for any potential $U(q_1, \ldots, q_n) = \sum_{i<j} U_{i,j}(q_i - q_j)$ which is a sum of pair potentials $U_{i,j} : \mathbb{R}^d \setminus \{0\} \to \mathbb{R}$.
Many of our results leading up to our theorem will also hold for these more general potentials provided their pair potentials have appropriate blow-up and decay conditions mimicking that of the power law potentials. One notable such required condition would be $U_{i,j}(z) \sim Z_{i,j}/\|z\|^\alpha + O(\|z\|^{1-\alpha})$ with $0 < \alpha < 2$ along with corresponding conditions on the derivatives of $U_{i,j}$ as $z \to 0$. It will be important that α does not depend on i, j. $\Diamond$

Using the natural symplectic form ω_0 on $\widehat{P} = T^*\widehat{M}$ we write (2.6) in the form $\dot{x} = X_H(x)$ for the Hamiltonian vector field X_H defined by $\mathbf{i}_{X_H}\omega_0 = dH$.

The flow of this vector field is real-analytic and fixes energy so defines a flow on each of the *energy surfaces*

$$\widehat{\Sigma}_E := \left\{ x \in \widehat{P} \mid H(x) = E \right\} \qquad (E \in \mathbb{R}). \tag{2.9}$$

2.2 Cluster decomposition

Cluster decompositions provide us with the book-keeping we need to index the ways we can end on the collision locus Δ. We borrow the language from combinatorial theory. See AIGNER [Ai].

2.2 Definition

- *A* **partition** *or* **cluster decomposition** *of $N = \{1, 2, \ldots, n\}$ is a collection $\mathcal{C} := \{C_1, \ldots, C_k\}$ of disjoint non-empty subsets of N whose union is N. The elements of $\mathcal{C}$ are called the* **atoms** *or* **clusters** *of the cluster decomposition.*

- *A cluster decomposition $\mathcal{C}$ induces an equivalence relation on N whose equivalence classes are $\mathcal{C}$'s atoms. We write $[i]_\mathcal{C}$ or simply $[i] \in \mathcal{C}$ for the atom containing $i \in N$.*

- *The* **partition lattice** $\mathcal{P}(N)$ *is the set of cluster decompositions* $\mathcal{C}$ *of* N*, partially ordered by* **refinement***, that is*

$$\mathcal{C} = \{C_1, \dots, C_k\} \preccurlyeq \{D_1, \dots, D_\ell\} = \mathcal{D}, \quad \textit{if} \quad C_m \subseteq D_{\pi(m)}$$

  for a suitable surjective relabelling map $\pi : \{1, \dots, k\} \to \{1, \dots, \ell\}$*. Then* $\mathcal{C}$ *is called* **finer** *than* $\mathcal{D}$ *and* $\mathcal{D}$ **coarser** *than* $\mathcal{C}$*.*

- *The* **rank** *of* $\mathcal{C} \in \mathcal{P}(N)$ *is the number* $|\mathcal{C}|$ *of its atoms.*

- *The finest and coarsest elements of* $\mathcal{P}(N)$ *are denoted by*

$$\mathcal{C}_{\min} := \big\{\{1\}, \dots, \{n\}\big\} \quad \textit{and} \quad \mathcal{C}_{\max} := \big\{\{1, \dots, n\}\big\}, \tag{2.10}$$

  and we set

$$\mathcal{P}_\Delta(N) := \mathcal{P}(N) \setminus \{\mathcal{C}_{\min}\} \quad \textit{and} \quad \mathcal{P}_{\mathbb{S}}(N) := \mathcal{P}(N) \setminus \{\mathcal{C}_{\max}\}. \tag{2.11}$$

For a partition $\mathcal{C}$ we define the $\mathcal{C}$*–collision* subspace

$$\Delta^E_{\mathcal{C}} := \{q \in M \mid q_i = q_j \text{ if } [i]_{\mathcal{C}} = [j]_{\mathcal{C}}\}.$$

Note that $\Delta^E_{\mathcal{C}} \subseteq \Delta$ as long as $\mathcal{C} \neq \mathcal{C}_{\min}$. We have that

$$\mathcal{C} \preccurlyeq \mathcal{D} \implies \Delta^E_{\mathcal{D}} \subseteq \Delta^E_{\mathcal{C}}$$

and that

$$\Delta^E_{\mathcal{C}} = \bigcap_{C \in \mathcal{C}} \Delta^E_C$$

where, for a subset $C \subseteq N$ we declare

$$\Delta^E_C := \{q \in M \mid q_i = q_j \text{ for } i, j \in C\}. \tag{2.12}$$

The superscript E refers to the fact that the 'non-frozen' coordinates are *external* to those associated to the atom C of $\mathcal{C}$.

For subsets $C \subseteq N$ we denote the $\mathcal{M}$*–orthogonal* complement to Δ^E_C by

$$\Delta^I_C := (\Delta^E_C)^\perp. \tag{2.13}$$

One computes

$$\Delta^I_C = \mathrm{Ker}\left(\Pi^E_C\right) = \left\{q \in M \mid q_i = 0 \text{ for } i \notin C,\ \textstyle\sum_{i \in C} m_i q_i = 0\right\}. \tag{2.14}$$

In the first equality of (2.14), Π^E_C denotes the orthogonal projection onto Δ^E_C. The superscript I refers to the fact that only coordinates *internal* to the atom

C can vary on this subspace. Thus the orthogonal projection onto Δ^I_C is $\Pi^I_C := \mathbb{1}_M - \Pi^E_C$.

Similarly for a partition $\mathcal{C}$ we define

$$\Delta^I_{\mathcal{C}} := (\Delta^E_{\mathcal{C}})^\perp .$$

Then $\Delta^I_{\mathcal{C}} = \bigoplus_{C\in\mathcal{C}} \Delta^I_C$, since $\Delta^E_{\mathcal{C}} = \bigcap_{C\in\mathcal{C}} \Delta^E_C$. By (2.14)

$$M = \Delta^E_{\mathcal{C}} \oplus \Delta^I_{\mathcal{C}} = \Delta^E_{\mathcal{C}} \oplus \bigoplus_{C\in\mathcal{C}} \Delta^I_C \tag{2.15}$$

is an $\mathcal{M}$–orthogonal decomposition. Associated to the orthogonal decomposition we have the orthogonal projections

$$\Pi^E_{\mathcal{C}} := \prod_{C\in\mathcal{C}} \Pi^E_C \quad \text{, respectively} \quad \Pi^I_{\mathcal{C}} := \mathbb{1}_M - \Pi^E_{\mathcal{C}} = \sum_{C\in\mathcal{C}} \Pi^I_C . \tag{2.16}$$

One easily computes the dimensions

$$\begin{aligned} \dim(\Delta^E_{\mathcal{C}}) &= d\big(n-1-\textstyle\sum_{C\in\mathcal{C}} (|C|-1)\big) = d\,(|\mathcal{C}|-1)\,, \\ \dim(\Delta^I_{\mathcal{C}}) &= \sum_{C\in\mathcal{C}} \dim(\Delta^I_C) = d\sum_{C\in\mathcal{C}} (|C|-1) = d(n-|\mathcal{C}|)\,. \end{aligned} \tag{2.17}$$

To lighten the notation set

$$q^E_{\mathcal{C}} := \Pi^E_{\mathcal{C}}(q) \quad \text{and} \quad q^I_{\mathcal{C}} := \Pi^I_{\mathcal{C}}(q) \qquad (q\in M).$$

We will even omit the subscript $\mathcal{C}$ when the context permits. For a nonempty subset $C \subseteq N$ we define the *cluster mass* and *cluster barycenter* of C by

$$m_C := \sum_{j\in C} m_j \quad \text{and} \quad q_C := \frac{1}{m_C}\sum_{j\in C} m_j q_j .$$

In particular m_N equals the *total mass* of the particle system. Then for the partitions $\mathcal{C} \in \mathcal{P}(N)$ the i–th component of the cluster projection is given by the barycenter

$$\big(q^E_{\mathcal{C}}\big)_i = q_{[i]_{\mathcal{C}}} \qquad (i\in N) \tag{2.18}$$

of its atom. Similarly

$$\big(q^I_{\mathcal{C}}\big)_i = q_i - q_{[i]_{\mathcal{C}}} \qquad (i\in N)$$

is its distance from the barycenter. The *scalar moment of inertia*

$$J : M \to \mathbb{R} \quad , \quad J(q) := \langle q,q\rangle_{\mathcal{M}} \tag{2.19}$$

splits into the *cluster barycenter moment*

$$J^E_{\mathcal{C}} := J \circ \Pi^E_{\mathcal{C}} \quad , \quad J^E_{\mathcal{C}}(q) = \sum_{C \in \mathcal{C}} m_C \langle q_C, q_C \rangle$$

and the *relative moments of inertia* of the clusters $C \in \mathcal{C}$

$$J^I_C := J \circ \Pi^I_C \ , \ J^I_C(q) = \sum_{i \in C} m_i \| \left(q^I_{\mathcal{C}}\right)_i \|^2 = \frac{1}{2m_C} \sum_{i,j \in C} m_i m_j \langle q_i - q_j, q_i - q_j \rangle \, ,$$

that is

$$J = J^E_{\mathcal{C}} + J^I_{\mathcal{C}} \quad \text{for} \quad J^I_{\mathcal{C}}(q) := \sum_{C \in \mathcal{C}} J^I_C(q) = \left\langle q^I_{\mathcal{C}}, q^I_{\mathcal{C}} \right\rangle_{\mathcal{M}} . \tag{2.20}$$

2.3 Example (a binary pair cluster and Jacobi vectors)
For a pair $i \neq j$ of particle labels we can form the cluster decomposition $\mathcal{C}$ of rank $n-1$ whose only non-singleton atom is the cluster $C := \{i, j\}$. These partitions correspond to isolated binary collisions and generate $\mathcal{P}(N)$ under join. For simplicity of notation we will take $n = 3$ and $C = \{1, 2\}$. M has dimension $2d$, $\Delta^E_{(3)} = M$, $\Delta^I_{(3)} = 0$ while $\Delta^E_{(1,2)}$ and $\Delta^I_{(1,2)}$ are both d–dimensional. We have $\Delta^E_{\mathcal{C}} = \Delta^E_{(1,2)}, \Delta^I_{\mathcal{C}} = \Delta^I_{(1,2)}$ and $\Delta^E_{(1,2)} \oplus \Delta^I_{(1,2)} = M$ (orthogonal direct sum). We compute

$$(q^E_{\mathcal{C}})_1 = \frac{m_1 q_1 + m_2 q_2}{m_1 + m_2} = (q^E_{\mathcal{C}})_2 \quad , \quad (q^E_{\mathcal{C}})_3 = q_3$$

while

$$(q^I_{\mathcal{C}})_1 = \frac{m_2}{m_1 + m_2}(q_1 - q_2) \quad , \quad (q^I_{\mathcal{C}})_2 = \frac{m_1}{m_1 + m_2}(q_2 - q_1) \quad , \quad (q^I_{\mathcal{C}})_3 = 0 \, .$$

The vector $q^I_{\mathcal{C}}$ is parameterized by the Jacobi vector $\xi_1 = q_1 - q_2$. The vector $q^E_{\mathcal{C}}$ is parameterized by the other Jacobi vector $\xi_2 = q_3 - \frac{m_1 q_1 + m_2 q_2}{m_1 + m_2}$. (Use $m_1 q_1 + m_2 q_2 + m_3 q_3 = 0$ to show that ξ_2, q_3 and $\frac{m_1 q_1 + m_2 q_2}{m_1 + m_2}$ are all non-zero scalar multiples of each other.) The identity (2.20) becomes the traditional quadratic decomposition

$$\|q\|^2 = \mu_1 \|\xi_1\|^2 + \mu_2 \|\xi_2\|^2 \tag{2.21}$$

with mass coefficients μ_i given by

$$\tfrac{1}{\mu_1} = \tfrac{1}{m_1} + \tfrac{1}{m_2} \quad , \quad \tfrac{1}{\mu_2} = \tfrac{1}{m_1 + m_2} + \tfrac{1}{m_3} \, . \qquad \Diamond$$

2.3 On to phase space

Let M^* denote the dual space of our vector space M. There are natural identifications $TM \cong M \times M$, $T^*M \cong M^* \times M$ of the tangent space resp. phase space of M. These gives rise to the inner products

$$\langle \cdot, \cdot \rangle_{TM} : TM \times TM \to \mathbb{R} \quad , \quad \langle (q,v),(q',v')\rangle_{TM} := \langle q, q'\rangle_{\mathcal{M}} + \langle v, v'\rangle_{\mathcal{M}}$$

and

$$\langle \cdot, \cdot \rangle_{T^*M} : T^*M \times T^*M \to \mathbb{R} \quad , \quad \langle (q,p),(q',p')\rangle_{T^*M} := \langle q, q'\rangle_{\mathcal{M}} + \langle p, p'\rangle_{\mathcal{M}^{-1}} \tag{2.22}$$

$\Big($with $\langle p, p'\rangle_{\mathcal{M}^{-1}} = \sum_{i=1}^n \frac{\langle p_i, p_i'\rangle}{m_i}$ for the *momentum vector* $p = (p_1, \ldots, p_n)\Big)$.

The tangent space TU of any linear subspace $U \subseteq M$ is naturally a linear subspace of TM. Using the inner product, we can also consider T^*U as a subspace of T^*M.

We thus obtain T^*M–orthogonal decompositions

$$T^*M = T^*(\Delta_{\mathcal{C}}^E) \oplus \bigoplus_{C \in \mathcal{C}} T^*(\Delta_C^I) \qquad \big(\mathcal{C} \in \mathcal{P}(N)\big)$$

of phase space. With

$$\widehat{\Pi}_{\mathcal{C}}^I := \mathbb{1}_{T^*M} - \widehat{\Pi}_{\mathcal{C}}^E = \sum_{C \in \mathcal{C}} \widehat{\Pi}_C^I$$

the T^*M–orthogonal projections $\widehat{\Pi}_{\mathcal{C}}^E$, $\widehat{\Pi}_{\mathcal{C}}^I : T^*M \to T^*M$ onto these subspaces are given by the *cluster coordinates*

$$(q^E, p^E) := \widehat{\Pi}_{\mathcal{C}}^E(q,p) \quad \text{with} \quad (q_i^E, p_i^E) = \left(q_{[i]}, \frac{m_i}{m_{[i]}} p_{[i]}\right) \quad (i \in N), \tag{2.23}$$

and *relative coordinates*

$$(q^I, p^I) := \widehat{\Pi}_{\mathcal{C}}^I(q,p) \quad \text{with} \quad (q^I, p_i^I) = (q_i - q_i^E, p_i - p_i^E) \quad (i \in N).$$

Here $p_C := \sum_{i \in C} p_i \in \mathbb{R}^d$ is the *total momentum of the cluster* $C \in \mathcal{C}$. Unlike in (2.18) we omitted the subindex $\mathcal{C}$ in (2.23), but will include it when necessary.

With this notation the equations of motion for particle no. $i \in N$ are

$$\frac{d}{dt} q_i^E = m_i^{-1} p_i^E \quad , \quad \frac{d}{dt} p_i^E = \frac{m_i}{m_C} \sum_{j,k \in N : [j]=[i],\ [k] \neq [i]} \nabla U_{j,k}(q_j - q_k)\,,$$

$\frac{d}{dt} q_i^I = m_i^{-1} p_i^I$ and

$$\frac{d}{dt} p_i^I = \sum_{k \in N \setminus \{i\}} \nabla U_{i,k}(q_i - q_k) - \frac{m_i}{m_C} \sum_{j,k \in N : [j]=[i],\ [k] \neq [i]} \nabla U_{j,k}(q_j - q_k)\,. \tag{2.24}$$

2.4 Lemma *The vector space automorphisms*

$$\left(\widehat{\Pi}^E_{\mathcal{C}}, \widehat{\Pi}^I_{\mathcal{C}}\right) : T^*M \longrightarrow T^*\Delta^E_{\mathcal{C}} \oplus \bigoplus_{C\in\mathcal{C}} T^*(\Delta^I_C) \qquad \left(\mathcal{C} \in \mathcal{P}(N)\right) \tag{2.25}$$

are symplectic w.r.t. the natural symplectic forms on these cotangent bundles.

Proof. This follows from $T^*\left(\Delta^E_{\mathcal{C}} \oplus \bigoplus_{C\in\mathcal{C}} \Delta^I_C\right) = T^*\Delta^E_{\mathcal{C}} \oplus \bigoplus_{C\in\mathcal{C}} T^*(\Delta^I_C)$. □

The *total kinetic energy*

$$K : T^*M \to \mathbb{R} \quad , \quad K(q,p) \equiv K(p) = \tfrac{1}{2}\left\langle p,p\right\rangle_{M^*} = \textstyle\sum_{i=1}^n \frac{\langle p_i, p_i\rangle}{2m_i}$$

splits into the external or *barycentric* kinetic energy

$$K^E_{\mathcal{C}} \;:=\; K \circ \widehat{\Pi}^E_{\mathcal{C}} \quad , \quad K^E_{\mathcal{C}}(q,p) = \textstyle\sum_{C\in\mathcal{C}} \frac{\langle p_C, p_C\rangle}{2m_C}$$

and internal or *relative* kinetic energy associated to each cluster $C \in \mathcal{C}$

$$K^I_C \;:=\; K \circ \widehat{\Pi}^I_C \quad , \quad K^I_C(q,p) = \textstyle\sum_{i\in C} \frac{\left\langle p^I_i, p^I_i\right\rangle}{2m_i}\,.$$

That is,

$$K = K^E_{\mathcal{C}} + K^I_{\mathcal{C}} \quad \text{with} \quad K^I_{\mathcal{C}} := \sum_{C\in\mathcal{C}} K^I_C\,.$$

The *internal* and *external cluster potentials* and *Hamiltonians* are given by

$$U^I_{\mathcal{C}}(q) := \sum_{C\in\mathcal{C}} U^I_C(q) \quad \text{with} \quad U^I_C(q) := \sum_{i<j\in C} U_{i,j}(q_i - q_j), \tag{2.26}$$

$$H^I_{\mathcal{C}}(p,q) := K^I_{\mathcal{C}}(p) - U^I_{\mathcal{C}}(q) = \sum_{C\in\mathcal{C}} H^I_C(p,q) \quad \text{with} \quad H^I_C(p,q) := K^I_C(p) - U^I_C(q) \tag{2.27}$$

and

$$U^E_{\mathcal{C}}(q) := \sum_{i<j\in N:\,[i]_{\mathcal{C}}\neq[j]_{\mathcal{C}}} U_{i,j}(q_i - q_j) \quad , \quad H^E_{\mathcal{C}}(p,q) := K^E_{\mathcal{C}}(p) - U^E_{\mathcal{C}}(q). \tag{2.28}$$

We have for all $\mathcal{C} \in \mathcal{P}(N)$

$$U = U^I_{\mathcal{C}} + U^E_{\mathcal{C}} \quad \text{and} \quad H = H^I_{\mathcal{C}} + H^E_{\mathcal{C}}. \tag{2.29}$$

(Unlike the kinetic energies, the cluster potentials cannot be written as $U \circ \Pi^I_{\mathcal{C}}$ etc).

2.5 Remark (partition of configuration space)
The linear subspaces $\Delta_{\mathcal{C}}^E$ generate a stratification [3] of M with strata

$$\Xi_{\mathcal{C}} \equiv \Xi_{\mathcal{C}}^{(0)} := \Delta_{\mathcal{C}}^E \Big\backslash \bigcup_{\mathcal{D} \succneqq \mathcal{C}} \Delta_{\mathcal{D}}^E \qquad \big(\mathcal{C} \in \mathcal{P}(N)\big). \tag{2.30}$$

The upper index (0) is generalized in (5.1) but omitted if there is no danger of confusion. $\Xi_{\mathcal{C}}$ consists of those collisions where only those particles whose particle indices belonging to the same $C_\ell \subseteq N$ of $\mathcal{C} = \{C_1, \ldots, C_k\}$ coincide. As $\Xi_{\mathcal{C}}$ is open in the vector space $\Delta_{\mathcal{C}}^E$, by (2.17) it is a manifold with dimension $\dim(\Xi_{\mathcal{C}}) = d\,(|\mathcal{C}| - 1)$. $\Diamond$

3 Blowing up the configuration space

The center of mass configuration space M, being a finite-dimensional real vector space, is diffeomorphic to its open unit ball $B \subseteq M$. For diffeomorphism we can take

$$\Phi : M \to B \quad , \quad \Phi(0) = 0 \ , \ \Phi(q) = \tanh(\|q\|) \tfrac{q}{\|q\|} \quad (q \in M \backslash \{0\}) \, .$$

B is compactified by attaching its boundary $\mathbb{S} := \partial B$, the unit sphere of dimension $d(n-1)-1$ which corresponds to letting $\|q\| \to \infty$ in the expression for Φ. Abusing notation, we set $\partial M := \mathbb{S}$, and

$$\overline{M} := M \sqcup \mathbb{S} \, , \tag{3.1}$$

a manifold with boundary. In this sense the topological boundary of the open configuration manifold $\widehat{M} = M \backslash \Delta$ is $\Delta \sqcup \mathbb{S}$.

The partial compactifications $\widehat{M_{\widehat{\mathbb{S}}}}$ of $\widehat{M} \sqcup \widehat{\mathbb{S}}$ along $\widehat{\mathbb{S}} := \mathbb{S} \backslash \Delta$ (Subsection 3.2) and $\widehat{M_\Delta}$ of $\widehat{M}$ along Δ (Subsection 3.3) are of independent interest. The first is relevant for the dynamics of the n particles as their mutual distances go to infinity and was treated in [DMMY]. The second corresponds to collisions and leads to a generalisation of the blow-up of the total collisions for the case $n = 3$ as first treated by McGehee in [McG1].

The full compactification $\widehat{M}$ in Subsection 3.4 gives rise to an additional aspect, because it includes the points of the sphere $\mathbb{S}$ at infinity corresponding to non-trivial clusters. This will, we hope (work in progress) lead us to a positive solution of the problem of asymptotic completeness[4] in the three-body problem,

[3] A stratification of a manifold is a locally finite partition into smooth submanifolds. See for example [Wall, p. 83].

[4] See Dereziński and Gérard [DG, Section 5.10].

thus asymptotically relating the joint motion of the particles and the pure two-body dynamics in the non-trivial cluster.[5]

3.1 Real blow up, generally

We will be repeatedly implementing the real blow-up construction as described in Melrose [Me, Sect. 5.3]. Our constructions will be concrete and essentially linear-algebraic so the general construction is not needed here. However, it may be useful to get a rough understanding of it, if for no other reason than to familiarize ourselves with the notation.

The general construction proceeds as follows. Given an embedded submanifold Y of a manifold X the real blow-up $[X : Y]$ is formed by deleting Y from X and replacing it with the space S^+NY of rays in the normal bundle NY to Y. This space S^+NY is a sphere bundle over Y with the spheres having one less than the codimension of Y. The resulting $[X : Y]$ is a manifold with boundary, that boundary being the sphere bundle. The manifold comes with a smooth blow-down map $[X : Y] \to Y$ which takes the sphere bundle onto Y by the bundle projection and is a diffeomorphism away from the sphere bundle. The manifold structure is obtained by invoking the tubular neighborhood theorem. This is commonly done by using an auxiliary Riemannian structure which allows us to use geodesics normal to Y to form a diffeomorphism between a neighborhood of Y and a neighborhood of the zero section of the normal bundle of Y. When one looks at things in local Gaussian-cylindrical coordinates about Y the whole construction boils down to using polar coordinates normal to Y.

The construction works if X has a boundary and Y is transverse to the boundary, intersecting it in its own boundary. In that case $[X : Y]$ is a manifold with codimension two corners. The construction can be iterated upon choosing a finite collection $Y_a, a \in I$ of embedded submanifolds, provided certain conditions are verified concerning the intersections of the closures of the Y_a with each other, and with corners arising in previous steps, yielding manifolds with deeper and deeper corners.

3.2 Blowing up configuration space at infinity

Although we do not blow up the entire configuration vector space M, diffeomorphic to the open ball $B \subseteq \mathbb{R}^k$ of radius one, it is instructive to notice that this

[5] In the case of smooth *bounded* pair potentials that are α-homogeneous for large distances, a positive solution of the asymptotic completeness problem for arbitrary number n of particles is expected, too. In the present setting, however, the motion is not asymptotically complete for $n > 3$ because of the existence of non-collision singularities.

would just reproduce the closed ball $\overline{B} = B \sqcup \mathbb{S}$ from (3.1). In other words,

$$[\,\overline{M} : \mathbb{S}\,] \;\cong\; \overline{M}\,.$$

The reason is the following one:

3.1 Example (blowing up configuration space M)
As $\mathbb{S}$ is the boundary of the configuration manifold M, its blow up is based on the general definition given in MELROSE [Me, Sect. 5.3]. As $\overline{M}\backslash\mathbb{S} = M$, we thus set

$$[\overline{M} : \mathbb{S}] := M \sqcup (S^+N\,\mathbb{S})\,,$$

with $S^+N\,\mathbb{S}$ being the *inward pointing part* of the normal sphere bundle of $\mathbb{S} \subseteq \overline{M}$. Since $\mathbb{S} \subseteq \overline{M}$ is of codimension one, $S^+N\,\mathbb{S}$ is diffeomorphic to $\mathbb{S}$, so that we get a simple result of that blow up: $[\overline{M} : \mathbb{S}] \cong \overline{M}$, the closed unit ball. $\Diamond$

With the open subset $\widehat{\mathbb{S}} := \mathbb{S}\backslash\Delta$ of the sphere we similarly obtain the disjoint union

$$\widehat{M_{\widehat{\mathbb{S}}}} := [\widehat{M} \sqcup \widehat{\mathbb{S}} : \widehat{\mathbb{S}}] \cong \widehat{M} \sqcup \widehat{\mathbb{S}}\,, \tag{3.2}$$

which is a manifold with boundary.

3.3 Blowing up configuration space at collisions

Next we blow up the configuration space $\widehat{M} = M\backslash\Delta$ along the thick diagonal

$$\Delta = \bigcup_{\mathcal{C}\in\mathcal{P}_\Delta(N)} \Delta^E_{\mathcal{C}}\,,$$

using the family (2.15) of $\mathcal{M}$-orthogonal decompositions $M = \Delta^E_{\mathcal{C}} \oplus \Delta^I_{\mathcal{C}}$ (Recall that $\mathcal{P}_\Delta(N)$ denotes $\mathcal{P}(N) \setminus \{\mathcal{C}_{\min}\}$.) With the definition (2.20) of $J^I_{\mathcal{C}}$, we write the coordinate $q^I_{\mathcal{C}}$ in the form

$$q^I_{\mathcal{C}} = r\,Q^I_{\mathcal{C}} \quad \text{with } J^I_{\mathcal{C}}(Q^I_{\mathcal{C}}) = 1 \text{ and } r := \big(J^I_{\mathcal{C}}(q^I_{\mathcal{C}})\big)^{1/2} \qquad \big(\mathcal{C} \in \mathcal{P}_\Delta(N)\big). \tag{3.3}$$

For $q^I_{\mathcal{C}} \neq 0$ this polar decomposition is unique and

$$\widehat{\Delta}^I_{\mathcal{C}} := \Delta^I_{\mathcal{C}} \setminus \{0\} \cong (0,\infty) \times S^I_{\mathcal{C}} \quad \text{, with the sphere } S^I_{\mathcal{C}} := \big(J^I_{\mathcal{C}}\big)^{-1}(1)\,. \tag{3.4}$$

Somewhat loosely speaking, we call the $Q^I_{\mathcal{C}}$ of equation (3.3) the *coordinates* on $S^I_{\mathcal{C}}$.
We consider $M \cong \mathbb{R}^{(n-1)d}$ as the vector bundle $M \cong \Delta^E_{\mathcal{C}} \oplus \Delta^I_{\mathcal{C}} \to \Delta^E_{\mathcal{C}}$ and

follow MELROSE [Me, Sect. 5.2] in defining the blow-up of M along the zero section $\Delta_{\mathcal{C}}^E \times \{0\} \cong \Delta_{\mathcal{C}}^E$ as the manifold with boundary

$$[M : \Delta_{\mathcal{C}}^E] := \Delta_{\mathcal{C}}^E \times \widehat{\Delta}_{\mathcal{C}}^I \quad \text{with} \quad \widehat{\Delta}_{\mathcal{C}}^I := [0,\infty) \times S_{\mathcal{C}}^I \,.$$

The diagonal map

$$\hat{I}_\Delta : \widehat{M} \longrightarrow \prod_{\mathcal{C}\in\mathcal{P}_\Delta(N)} [M : \Delta_{\mathcal{C}}^E] \quad , \quad q \longmapsto (q)_{\mathcal{C}\in\mathcal{P}_\Delta(N)} \tag{3.5}$$

smoothly imbeds $\widehat{M}$ as a submanifold of the manifold $\prod_{\mathcal{C}\in\mathcal{P}_\Delta(N)} \Delta_{\mathcal{C}}^E \times \widehat{\Delta}_{\mathcal{C}}^I$.

On $\widehat{\Delta}_{\mathcal{C}}^I = [0,\infty) \times S_{\mathcal{C}}^I$ the 'coordinates' $(r_{\mathcal{C}}^I, Q_{\mathcal{C}}^I)$ are used. With definitions contained in Appendix A we get the so-called *graph blow up*, see [AMN, Eq. 8]:

3.2 Lemma

1. *The graph blow up of $M \cong \mathbb{R}^{(n-1)d}$ by the family $\{\Delta_{\mathcal{C}}^E \mid \mathcal{C} \in \mathcal{P}_\Delta(N)\}$ is the topological space*
$$\widehat{M}_\Delta := \mathrm{closure}\big(\hat{I}_\Delta(\widehat{M})\big) \,. \tag{3.6}$$
It is an $(n-1)d$–dimensional manifold with corners, see Figure 3.1).

2. *The blow-down map $\beta : \widehat{M}_\Delta \to M$ is proper, and for binary collisions*
$$\beta^{-1}(\Xi_{\mathcal{C}}) \;\cong\; \Xi_{\mathcal{C}} \times S_{\mathcal{C}}^I \qquad (\mathcal{C} \in \mathcal{P}_\Delta(N), |\mathcal{C}| = n-1).$$

Proof:

1. The family $\{\Delta_{\mathcal{C}}^E \mid \mathcal{C} \in \mathcal{P}_\Delta(N)\}$ is a finite semilattice of linear subspaces of $M = \Delta_{\mathcal{C}_{\min}}^E$, that is, closed p–submanifolds in the sense of Def. A.3. As they are linear subspaces, they form a cleanly intersecting family in the sense of [AMN, Def. 5.4]. Then it follows from [AMN, Theorem 5.12] that the graph blow-up $\widehat{M}_\Delta$ is a weak submanifold. Since a weak submanifold of a manifold with corners is the image of an injective immersion of a manifold with corners, the first statement follows.

2. As applied to the present problem, the main statement of [AMN, Theorem 5.12] is that the graph blow-up $\widehat{M}_\Delta$ is diffeomorphic (in the sense of Definition A.1) to the iterated blow-up. Thus properness of the blow-down map β follows from iteration of [AMN, Cor. 3.7]. Moreover, as the $\Xi_{\mathcal{C}} \subseteq \Delta_{\mathcal{C}}^E$ are the relatively open complements (2.30), the blow-up of $\Xi_{\mathcal{C}} \times \widehat{\Delta}_{\mathcal{C}}^I$ at $\Xi_{\mathcal{C}} \times \{0\}$ coincides with $\Xi_{\mathcal{C}} \times \widehat{\Delta}_{\mathcal{C}}^I$. □

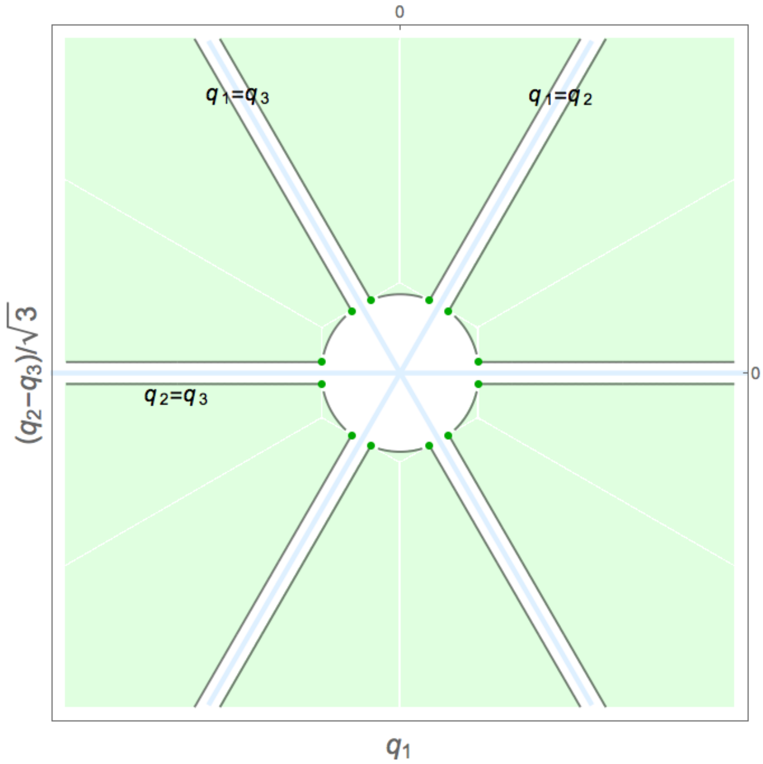

Figure 3.1: Schematic view of the manifold with corners $\widehat{M}_\Delta$ (light green) arising by blowing up configuration space $M \cong \mathbb{R}^{(n-1)d}$, for $n=3$ particles in $d=1$ dimension. The thick diagonal Δ is light blue. Boundary points of $\widehat{M}_\Delta$ are black, except for those of depth two (shown in dark green).

It follows from [AMN, Theorem 5.12] that the graph blow up $\widehat{M}_\Delta$ is diffeomorphic to the so-called *total boundary blow-up*, see also [Me, Sect. 5.13].

We identify $\widehat{M}_\Delta \setminus \partial\widehat{M}_\Delta$ with $\widehat{M}$.

For some $\alpha \in (0,2)$ we henceforth consider $(-\alpha)$–homogeneous potentials $U : \widehat{M} \to \mathbb{R}$ that are of the form (1.1) with $Z_{i,j} > 0$ in the two-body potentials

$$U_{i,j}(q) = Z_{i,j}\, \|q\|^{-\alpha} \quad \big(q \in \mathbb{R}^d \setminus \{0\}\big).$$

In extending the Hamiltonian flow of (2.6) to the collision manifold, the function $U^{-1/\alpha}$ will appear in the differential equations (4.5). Extended by zero on $\Delta = M \backslash \widehat{M}$, this is a function $f : M \to \mathbb{R}$ on $M \cong \mathbb{R}^{(n-1)d}$ that is Lipschitz continuous but not continuously differentiable. Instead, when lifting it to the graph blow up $\widehat{M}_\Delta$, it is in the Hölder space $C^{(1+\alpha)}(\widehat{M}_\Delta, \mathbb{R})$.[6] This (together

[6]We set $C^{(\alpha)} := C^{k,\alpha'}$ with $k := \lceil \alpha \rceil - 1 \in \mathbb{N}_0$ and $\alpha' := \alpha - k$ for $\alpha \in (0,\infty)$.

with a similar property of F defined in (4.5)) will imply differentiability of the flow.

Before treating the general case, we will give a simple example.

3.3 Example (boundary defining function) Consider for $\alpha > 0$ the function

$$f : \mathbb{R}^2 \to \mathbb{R} \quad , \quad f(x) = \begin{cases} \left(1/|x_1|^\alpha + 1/|x_2|^\alpha\right)^{-1/\alpha} & , x \in \widehat{X} \\ 0 & , x \in \mathbb{R}^2 \setminus \widehat{X} \end{cases} , \tag{3.7}$$

with $\widehat{X} := \{x = (x_1, x_2) \in \mathbb{R}^2 \mid x_1 \neq 0 \neq x_2\}$. We think of f as the extension of $U^{-1/\alpha}$, with the potential of two independent pairs of masses on a line

$$U \in C^\infty(\widehat{X}, \mathbb{R}) \quad , \quad U(x_1, x_2) = |x_1|^{-\alpha} + |x_2|^{-\alpha} .$$

f is 1–homogeneous and Lipschitz continuous ($f \in C^{0,1}(\mathbb{R}^2, \mathbb{R})$), but $f \notin C^1(\mathbb{R}^2, \mathbb{R})$, see Figure 3.2.

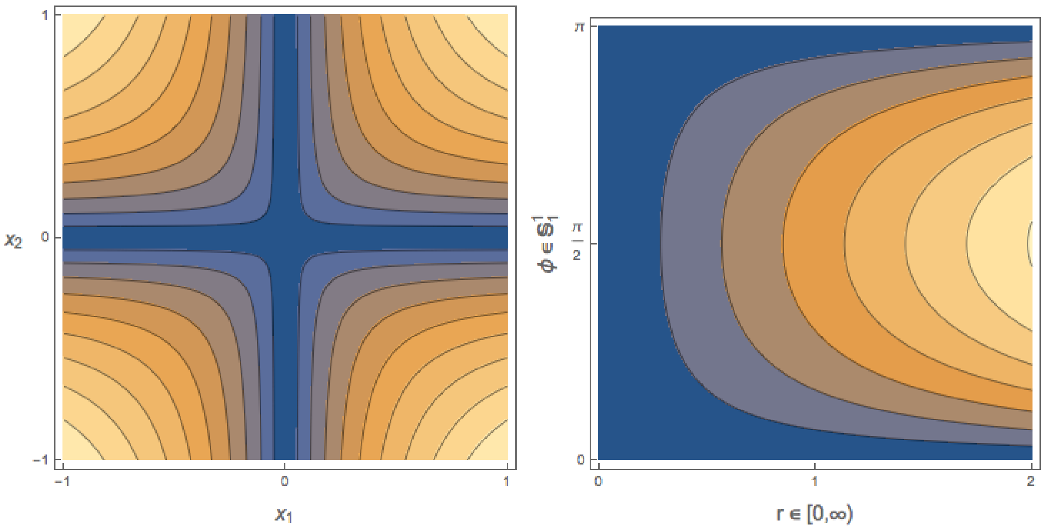

Figure 3.2: Example 3.3 for $\alpha = 1$: The Lipschitz function (3.7) on $\mathbb{R}^2$ (left) and its lift $\rho \in C^\infty(\widehat{X}, \mathbb{R})$, for the blow-up $S_1^1 \times [0, \infty)$ of one quadrant (right)

However, if we continuously extend $U^{-1/\alpha}$ by zero to $\rho : \widehat{X} \to \mathbb{R}$ on the total boundary blow-up $\widehat{X} \supseteq \widehat{X}$, then we claim that ρ is in the Hölder space $C^{(1+\alpha)}(\widehat{X}, \mathbb{R})$. For the gravitational case $\alpha = 1$ we even have $\rho \in C^\infty(\widehat{X}, \mathbb{R})$, and ρ is a boundary defining function in the sense of Melrose.[7] Here $\widehat{X}$ is

[7]**Definition** (Melrose [Me, Lemma 1.6.2])**:** A **boundary defining function** on a manifold with corners X is a function $\rho \in C^\infty(X, \mathbb{R})$ with $\rho|_{\partial X} = 0$, $\rho|_{X \setminus \partial X} > 0$ and in local coordinates at $p \in \partial_k X$, $\rho(x) = a(x) x_1 \cdot \ldots \cdot x_k$ with $a(p) > 0$ and a smooth.

diffeomorphic to the disjoint union of four copies of the manifold with corners

$$S^1_1\times[0,\infty)\cong[0,\pi]\times[0,\infty)\quad\text{, with}\quad S^m_k:=S^m\cap\mathbb{R}^{m+1}_k$$

and half-angle polar coordinates $x_1=r\cos(\phi/2)$, $x_2=r\sin(\phi/2)$, $r=\|x\|$. Compare with [AMN, Lemma 5.10] for such pair blow-ups. Then

$$\rho(\phi,r)=f(x)=\frac{r}{(1/\cos^\alpha(\phi/2)+1/\sin^\alpha(\phi/2))^{1/\alpha}}=\frac{r\sin(\phi/2)}{(1+\tan^\alpha(\phi/2))^{1/\alpha}}\,.$$

So $\rho\in C^{(1+\alpha)}(\widehat{X},\mathbb{R})$. For $\alpha=1$, $\rho(\phi,r)=\frac{r\sin(\phi)}{\sqrt{8}\sin(\phi/2+\pi/4)}$, proving the claim. $\Diamond$

Example 3.3 generalizes as follows:

3.4 Lemma (boundary defining function)
The function on the total boundary blow-up, defined for $\alpha>0$ by

$$\rho:\widehat{M}_\Delta\to\mathbb{R}\quad,\quad\rho|_{\widehat{M}}:=U^{-1/\alpha}\ \text{and}\ \rho|_{\partial\widehat{M}_\Delta}:=0\,,\tag{3.8}$$

is in the Hölder space $C^{(1+\alpha)}(\widehat{M}_\Delta,\mathbb{R})$.
For the case $\alpha=1$ of celestial mechanics ρ is a boundary defining function.

Proof: Note that by our assumption $Z_{i,j}>0$, $U>0$ diverges to $+\infty$ at Δ. It is immediate that $\rho|_{\widehat{M}}>0$ is smooth. The behaviour of ρ at the boundary of $\widehat{M}_\Delta$ is given by iterated Taylor expansion with respect to a chain for a *size order* of the $\Delta^E_{\mathcal{C}}$, see [AMN, Section 5.2]. For $\mathcal{C}\in\mathcal{P}_\Delta(N)$ and $q^E_{\mathcal{C}}\in\Xi_{\mathcal{C}}$ so that $q^E_C\neq q^E_D$ for $C\neq D\in\mathcal{C}$ we write $q^I_{\mathcal{C}}=rQ^I_{\mathcal{C}}$ with the notation from (3.3). Then we expand

$$\rho(q)=r\left(\sum_{C\in\mathcal{C}}\sum_{i<j\in C}\frac{Z_{i,j}}{\|Q^I_{\mathcal{C},i}-Q^I_{\mathcal{C},j}\|^\alpha}+r^\alpha\sum_{C\neq D\in\mathcal{C}}\sum_{i\in C,j\in D}\frac{Z_{i,j}}{\|q^E_C-q^E_D+r(Q^I_{\mathcal{C},i}-Q^I_{\mathcal{C},j})\|^\alpha}\right)^{-1/\alpha}$$

with respect to r, obtaining a (local) Hölder $C^{(1+\alpha)}$ dependence.
For $\alpha=1$ smoothness at the boundary of $\widehat{M}_\Delta$ reduces to Lemma 5.13.3 of [Me]. $\Box$

3.4 Compactifying configuration space

We begin by compactifying the subspaces $\Delta^E_{\mathcal{C}}\subseteq M$ in $\overline{M}=M\sqcup\mathbb{S}$, resulting in closed disks $\overline{\Delta}^E_{\mathcal{C}}$ whose boundary $\mathbb{S}\cap\overline{\Delta}^E_{\mathcal{C}}$ is a subsphere of $\mathbb{S}$.
With $\mathcal{P}_{\mathbb{S}}(N)=\mathcal{P}(N)\backslash\{\mathcal{C}_{\max}\}$ from (2.11), modifying (3.5), we use the map

$$\hat{I}:\widehat{M}\longrightarrow\prod_{\mathcal{C}\in\mathcal{P}_\Delta(N)}\left[\overline{M}:\overline{\Delta}^E_{\mathcal{C}}\right]\times\prod_{\mathcal{C}\in\mathcal{P}_{\mathbb{S}}(N)}\left[\overline{M}:(\mathbb{S}\cap\overline{\Delta}^E_{\mathcal{C}})\right]\,,\quad q\longmapsto(q)_{\mathcal{C}\in\mathcal{P}_\Delta(N)\sqcup\mathcal{P}_{\mathbb{S}}(N)},$$

which smoothly imbeds $\widehat{M}$ as a submanifold. We omitted $\mathcal{C}_{\max}$ in the second product, since $\mathbb{S} \cap \overline{\Delta}^E_{\mathcal{C}_{\max}} = \mathbb{S} \cap \{0\} = \emptyset$.

Note that the $\overline{\Delta}^E_{\mathcal{C}}$ intersect the boundary $\mathbb{S}$ of $\overline{M}$ neatly (see, *e.g.* HIRSCH [Hi, Section 1.4]), and are p–submanifolds of $\overline{M}$ in the sense of [Me, Definition 1.7.4]. So like in Lemma 3.2 the graph blow up

$$\widehat{\overline{M}} := \operatorname{closure}\bigl(\hat{I}(\widehat{M})\bigr) \tag{3.9}$$

of the compact ball $\overline{M}$ has the structure of an $(n-1)d$–dimensional manifold with corners. The new feature is that, unlike $\widehat{M}_\Delta \subseteq \widehat{M}$ defined in (3.6) and $\widehat{M} \sqcup \widehat{\mathbb{S}} \subseteq \widehat{\overline{M}}$ from (3.2), $\widehat{\overline{M}}$ is compact.

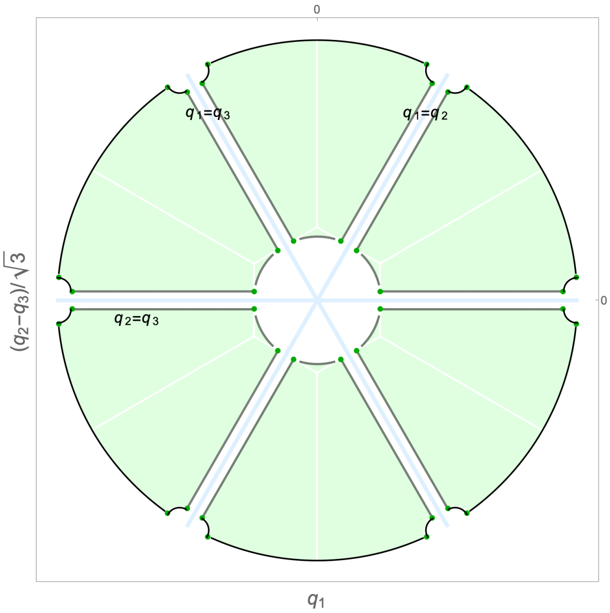

Figure 3.3: Schematic view of the blown-up configuration space $\widehat{\overline{M}}$ (light green) arising by blowing up configuration space $M \cong \mathbb{R}^2$ for $n = 3$ particles in $d = 1$ dimension. The thick diagonal Δ is light blue. Boundary points of $\widehat{\overline{M}}$ are black, except for those of depth two (shown in dark green).

4 Blowing up the energy surfaces

We will use Section 3 to blow up and compactify the energy surfaces $\widehat{\Sigma}_E = H^{-1}(E)$. The resulting compact manifolds with corners, denoted $\widehat{\overline{\Sigma}}_E$, are easy to define and understand via their projection to $\widehat{\overline{M}}$. See equation (4.2).

Analysing the dynamics induced on the flow-invariant boundary components takes some work. After the introductory example of two bodies in Subsection 4.3, we separately consider the dynamics on the pieces of the energy surfaces over the boundary blow-ups $\widehat{M}_{\widehat{\mathbb{S}}}$, $\widehat{M}_{\Delta}$ and finally over the entire compact total blow-up $\widehat{M}$ of configuration space $\widehat{M} := M \setminus \Delta$.

4.1 Rescaling velocities

We prefer to work with velocities

$$v = \mathcal{M}^{-1}\, p$$

rather than momenta. Then the energy is given by

$$E = \tfrac{1}{2}\|v\|^2_{\mathcal{M}} - U(q)$$

Make the position dependent rescaling of velocities

$$w := G_E(q)v \quad \text{with } G_E := \big(2(E+U)\big)^{-\frac{1}{2}}\,, \tag{4.1}$$

so that the energy becomes

$$E = \big(E + U(q)\big)\|w\|^2 - U(q)\,.$$

Solving, we see that the energy in the (q,w)–variables is E iff $\|w\| = 1$.

The substitution (4.1) requires that $E + U \geq 0$ (we don't want imaginary w's!) which means that q must lie in the Hill region

$$\widehat{M}_E := \big\{q \in \widehat{M} \mid U(q) \geq -E\big\}\,.$$

If $E \geq 0$ this is no restriction since our U is positive everywhere and so $\widehat{M}_E = \widehat{M}$. In this case the energy level set $\widehat{\Sigma}_E$ is equal to $\widehat{M} \times \mathbb{S}$ where $\mathbb{S} = \mathbb{S}^{(n-1)d-1}$ is the unit sphere in the w–variables. We can now simply take closures by letting $q \to \partial\widehat{M}$ and realizing our spheres are staying constant. So for $E \geq 0$ we arrive at

$$\widehat{\Sigma}_E = \widehat{M} \times \mathbb{S}\,.$$

When $E < 0$ we must pay attention to the behaviour of velocities as we approach the Hill boundary $\{U = -E\}$. In the interior of the Hill boundary the fibers of the original velocity projection $(q,v) \mapsto q$ restricted to $\widehat{\Sigma}_E$ are spheres whose radius shrinks so that they degenerate to points when we reach the Hill boundary. In our new w–variables the spheres are all the same size, so as we approach the boundary they remain the same. In going to the w–variables we thus replace the original smooth $\widehat{\Sigma}_E$ by $\widehat{M_E} \times \mathbb{S}$. The extraneous directions along the boundary will not cause problems with the dynamics, but will require a bit of analysis in order to make sense of brake orbits – orbits hitting the Hill boundary. This is done in Subsection 4.4 . Letting q tend to boundary points of $\widehat{M}$ while remaining in $\widehat{M_E}$ we see that again the w–spheres do not change size: we just have $w \in S$, the fixed unit sphere. Thus regardless of the energy E we get

$$\widehat{\Sigma}_E \cong \widehat{M_E} \times \mathbb{S} \tag{4.2}$$

where $\widehat{M_E}$ denotes the closure of the smooth manifold with boundary $\widehat{M_E}$ within $\widehat{M}$.

4.1 Remarks

1. **Rescaling of velocities:** Our rescaling of velocities is half of our globalization of the construction first devised by McGehee in [McG1], and developed further by Devaney [De] and many others. See in particular Lacomba and Ibort [LI]. The other half comes with the next section when we rescale time.
2. **Critical points:** For our choice of U the function U has no critical values and hence the Hill boundary is smooth regardless of the choice of energy E.
3. **Tangent space:** Note here that the tangent space TX of a manifold with corners X like $\widehat{M_E}$ is well-defined, since X is contained in a smooth manifold $\widetilde{X}$ of the same dimension. TX can then be defined invariantly by the restriction of the bundle $T\widetilde{X} \to \widetilde{X}$ to X, see [AMN, Remark 2.7]. $\Diamond$

4.2 Rescaling time

To extend the differential equations to $\widehat{\Sigma}_E$, we introduce a new time parameter τ along orbits with

$$\tfrac{dt}{d\tau} = \widetilde{G}_E(q)\, G_E(q) \quad \text{for } \widetilde{G}_E := \tfrac{E+U}{1+U} U^{-1/\alpha} \tag{4.3}$$

and denote $\frac{d}{d\tau}$ by $'$. If we set

$$F(q) := \frac{\mathcal{M}^{-1}\nabla U(q)}{2(1+U(q))\, U(q)^{\frac{1}{\alpha}}}\,, \tag{4.4}$$

the Hamiltonian equations (2.6) on $\widehat{P}$ acquire the form

$$q' = \widetilde{G}_E(q)\, w \quad , \quad w' = F(q) - \langle F(q), w\rangle\, w \tag{4.5}$$

leaving the energy surfaces $\widehat{\Sigma}_E$ invariant. As $q \to 0$, the force term $F(q)$ is asymptotically homogeneous of degree zero. It is bounded, since the terms

$$\frac{\nabla_q U_{i,j}(q)}{U_{i,j}(q)^{1+\frac{1}{\alpha}}} = -\alpha Z_{i,j}^{-\frac{1}{\alpha}} \frac{q}{\|q\|} \qquad \big(q \in \mathbb{R}^d \setminus \{0\}\big) \tag{4.6}$$

are bounded and since $U_{i,j} > 0$.

4.2 Remarks (scalings)

1. **Change of speed:** To normalize it to one is just a convenient choice.

2. **Time change:** The factor $U^{-1/\alpha}$ in the choice (4.3) of the time change is motivated by the desire that the velocity q' should vanish asymptotically linearly in the distance from the boundary. Looking at the first equation in (4.5), this is more or less obvious for boundary points in Δ. As we shall see, this is also true for boundary points in the sphere $\mathbb{S}$ at infinity.

3. **Alternatives:** One drawback of our choice is that $\|w\| = 1$ also at the boundary $\partial\widehat{M}_E$ of Hill's region.
   Therefore in our companion paper [KM] we use scalings for speed and time change that depend on total energy E. $\Diamond$

Before looking carefully at the different aspects of the compactification, we present the simplest example.

4.3 The example of two bodies

The simplest case is the reduced system with Hamiltonian $\|p\|^2/2 - U(q)$ and $U(q) = \|q\|^{-\alpha}$ where $q \in \mathbb{R}^d$ stands for $q_1 - q_2$. Hamiltonian equations are

$$\dot{q} = p \quad , \quad \dot{p} = \nabla U(q) \tag{4.7}$$

with $\nabla U(q) = -\alpha\, Q/\|q\|^{\alpha+1}$ for $Q := q/\|q\|$, so that our force term (4.4) equals

$$F(q) = -\tfrac{\alpha}{2}\tfrac{Q}{1+\|q\|^\alpha}\,.$$

The scaling functions (4.1) for velocity and (4.3) for time have the form

$$G(q) = \big(2(E + \|q\|^{-\alpha})\big)^{-1/2} \quad , \quad \widetilde{G}_E(q) = \tfrac{E+\|q\|^{-\alpha}}{1+\|q\|^{-\alpha}}\|q\|\,.$$

For total energy $E \in \mathbb{R}$ the differential equation (4.5) extends to the boundary of the energy surface $\widehat{\Sigma}_E = \widehat{M}_E \times \mathbb{S}^{d-1}$ over compactified configuration space

$$\widehat{M}_E := \begin{cases} [0,\infty] \times \mathbb{S}^{d-1} & , \quad E \geq 0 \\ \big[0, |E|^{-1/\alpha}\big] \times \mathbb{S}^{d-1} & , \quad E < 0 \end{cases} .$$

The boundary of $\widehat{\Sigma}_E$ has two components, one with $r = 0$ and the other with either $r = \infty$ or $r = |E|^{-1/\alpha}$ where $r = \|q\|$.

Using $Q = q/r$ one gets

$$r' = r\tfrac{1+Er^\alpha}{1+r^\alpha}\langle Q, w\rangle \ , \ Q' = \tfrac{1+Er^\alpha}{1+r^\alpha}\big(w - \langle Q, w\rangle Q\big) \ , \ w' = \tfrac{-1}{1+r^\alpha}\tfrac{\alpha}{2}\big(Q - \langle w, Q\rangle w\big) \, . \tag{4.8}$$

As $\mathrm{span}(Q, w)$ is invariant, it suffices to consider dimension $d = 2$. So we use polar coordinates for the q and w variables, assumed to be complex-valued:

$$q = r\exp(\imath\,\theta) \quad , \quad w = \exp(\imath\, w_\theta)\, .$$

Setting

$$\psi = w_\theta - \theta$$

the differential equation takes the form

$$r' = r\tfrac{1+Er^\alpha}{1+r^\alpha}\cos(\psi) \quad , \quad \theta' = \tfrac{1+Er^\alpha}{1+r^\alpha}\sin(\psi) \quad , \quad w_\theta' = \tfrac{\alpha}{2}\tfrac{1}{1+r^\alpha}\sin(\psi)\, . \tag{4.9}$$

The r equation shows that the two boundary components are invariant. They are tori coordinatized by (θ, w_θ). On these tori the circles $\{\theta = w_\theta\}$ and $\{\theta = w_\theta + \pi\}$ consist of rest points (see Figure 4.1).

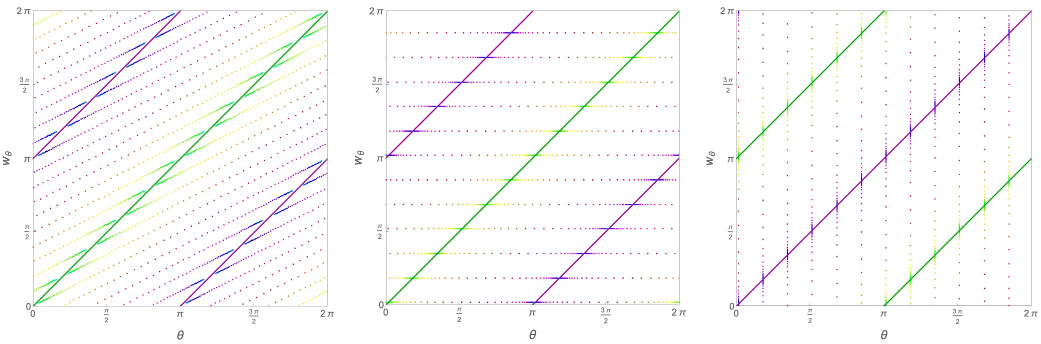

Figure 4.1: Flows on invariant boundary tori, for the gravitational case $\alpha = 1$. Left: At collision. Middle: At infinity, for energy $E = 1$. Right: At the boundary of Hill's region, for energy $E = -1$. The unstable rest points are coloured in magenta, the stable ones in green. The flow lines are coloured by time τ.

- **Collision:**
  At the flow invariant boundary component of $\widehat{\Sigma}_E$ with $q = 0$ the o.d.e. (4.9) equals
  $$\theta' = \sin(w_\theta - \theta) \quad , \quad w_\theta' = \tfrac{\alpha}{2}\sin(w_\theta - \theta)\, .$$

So the differential equation $\psi' = -(1-\frac{\alpha}{2})\sin(\psi)$ or $\psi := w_\theta - \theta$ is solved for initial conditions with $w_\theta(0) = \theta(0) \pm \pi/2$ by $\psi(\tau) = \pm 2\cot^{-1}\left(e^{(1-\frac{\alpha}{2})\tau}\right)$, whereas $w_\theta - \frac{\alpha}{2}\theta = (1-\frac{\alpha}{2})\theta(0) \pm \pi/2$ is a constant of the motion. We obtain

$$\theta(\tau) = \theta(0) \pm \frac{\frac{\pi}{2} - 2\cot^{-1}(e^{(1-\frac{\alpha}{2})\tau})}{1-\frac{\alpha}{2}} \quad , \quad w_\theta(\tau) = \theta(0) \pm \frac{\pi/2 - \alpha\cot^{-1}\left(e^{(1-\frac{\alpha}{2})\tau}\right)}{1-\frac{\alpha}{2}} \,.$$

The total angle covered is

$$\lim_{\tau \nearrow \infty} \big(\theta(\tau) - \theta(-\tau)\big) = \pm \frac{\pi}{1-\frac{\alpha}{2}} \,.$$

This agrees, as it should, with the range of 'Rutherford' type scattering for homogeneous central forces as calculated in [KK, Section 4]. The limit points

$$\lim_{\tau \to +\infty} \big(\theta(\tau), w(\tau)\big) = \big(\theta(0) \pm \tfrac{\pi}{2-\alpha}\,,\, \theta(0) \pm \tfrac{\pi}{2-\alpha}\big)\,,$$
$$\lim_{\tau \to -\infty} \big(\theta(\tau), w(\tau)\big) = \big(\theta(0) \mp \tfrac{\pi}{2-\alpha}\,,\, \theta(0) \mp (\tfrac{\pi}{2-\alpha} - \pi)\big)$$

are stable respectively unstable rest points. So the two unstable orbits of a rest point converge to the *same* stable rest point exactly in the cases

$$\alpha = 2(1 - 1/m) \qquad \big(m \in \mathbb{N} \backslash \{1\}\big).$$

Only then we can uniquely regularize the original o.d.e. (4.7) at collision. The cases m odd then correspond to motion in the forward direction, whereas m even (including the gravitational case $\alpha = 1$) corresponds to backscattering.

- **Spatial infinity:**
  Similarly, for $E \geq 0$ the boundary component at $r = \infty$ is invariant under the flow, as one sees by considering the o.d.e. $\rho' = -\rho\frac{E+\rho^\alpha}{1+\rho^\alpha}\langle Q, w\rangle Q$ for $\rho := 1/r$. Thus at spatial infinity (4.9) takes the form

  $$\theta' = E\sin(w_\theta - \theta) \quad , \quad w_\theta' = 0\,,$$

  with the solutions for $w_\theta(0) = \theta(0) \pm \pi/2$

  $$\theta(\tau) = \theta(0) \pm \left(\tfrac{\pi}{2} - 2\tan^{-1}\left(\exp(-E\tau)\right)\right) \quad , \quad w_\theta(\tau) = w_\theta(0)\,.$$

  They converge to the rest points $\big(\theta(0) \pm \pi/2, w_\theta(0)\big)$ as $\tau \nearrow \infty$ and $\big(\theta(0) \mp \pi/2, w_\theta(0)\big)$ as $\tau \searrow -\infty$. So the stable manifold of a rest point (θ, θ) equals the unstable manifold of $(\theta + \pi, \theta)$, see Figure 4.1, middle.
  For energy $E = 0$ the whole boundary $\mathbb{S}^1 \times \mathbb{S}^1$ at infinity consists of rest points.
  All energy E solutions of (4.8) (except those colliding) thus have the property that they go to a stable fixed point as $\tau \nearrow \infty$.

- **Boundary of Hill's region:**
For energy $E < 0$ the boundary $\partial\widehat{M}_E = \{q \in \mathbb{R}^2 \mid \|q\| = |E|^{-1/\alpha}\}$ of Hill's region is invariant under the flow, too. Then (4.9) becomes

$$\theta' = 0 \quad , \quad w'_\theta = \tfrac{\alpha}{2}\tfrac{1}{1+1/|E|}\sin(w_\theta - \theta)\,,$$

with the solutions for $w_\theta(0) = \theta(0) \pm \pi/2$ and $c := \tfrac{\alpha}{2}\tfrac{1}{1+1/|E|}$

$$\theta(\tau) = \theta(0) \quad , \quad w_\theta(\tau) = w_\theta(0) \pm \left(\tfrac{\pi}{2} - 2\tan^{-1}\left(\exp(c\,\tau)\right)\right).$$

Here the unstable manifold of a rest point $(\theta, \theta) \in \mathbb{S}^1 \times \mathbb{S}^1$ equals the stable manifold of $(\theta, \theta + \pi)$, see Figure 4.1, right. As (θ, θ) and $(\theta, \theta + \pi)$ are uniquely connected in the positive time direction, one can uniquely connect the incoming and outgoing solutions (brake orbits) for the original o.d.e. (4.7). (See also the end of Subsection 4.4 below.)

4.4 Blowing up the energy surface at Hill's boundary

The Hill boundary $\partial\widehat{M}_E \subseteq \widehat{M}$ is a submanifold of codimension one. (All values E of our potential are regular values.) So (like in Subsection 3.2) blowing up Hill's region $\widehat{M}_E$ at $\partial\widehat{M}_E$ just reproduces $\widehat{M}_E$. The restriction of the trivial sphere bundle (4.2) to $\partial\widehat{M}_E \subseteq \partial\widehat{M}_E$ has the form

$$\partial\widehat{M}_E \times \mathbb{S}^{(n-1)d-1} \to \partial\widehat{M}_E\,.$$

4.3 Lemma (Hill's boundary)
For all energy values $E < 0$ the flow on $\widehat{\Sigma}_E$ leaves the fibers

$$(\pi_E)^{-1}(q_0) \subseteq \widehat{\Sigma}_E \qquad \left(q_0 \in \partial\widehat{M}_E\right)$$

invariant. The limit point (q_0, w) of the incoming brake orbit is uniquely connected by its unstable manifold to the limit point $(q_0, -w)$ of the outgoing brake orbit.

Proof: The sphere $(\pi_E)^{-1}(q_0)$ is invariant under the flow generated by the differential equation (4.5), since $\widetilde{G}_E(q) = 0$ for $q_0 \in \partial\widehat{M}_E$, so that $q' = 0$. The vector field $-\nabla U(q) \neq 0$ is an outward pointing normal to $T_q\partial\widehat{M}_E$. As $w' = F(q) - \langle F(q), w\rangle\, w$, the only rest points (q_0, w) of the flow on the sphere are the ones with w parallel or antiparallel to the force $F(q_0) = \nabla U(q_0)$. But the brake orbits have these incoming and outgoing directions as is seen by a Taylor expansion of Newton's equations $\ddot{q} = \nabla U(q)$ with $\dot{q}(0) = 0, q(0) = q_0$. $\square$

4.4 Remark (significance of the flow on $\widehat{\Sigma}_E$)
We take the general philosophy that one can concatenate two solution curves to the reparameterized flow on $\widehat{\Sigma}_E$ if

1. the ω–limit set of first is the α–limit set of the second, with their common limit point $R \in \widehat{\Sigma}_E$ being a rest point of the extended flow. Note that all the rest points are in $\partial\widehat{\Sigma}_E$.

2. Additionally, we demand that R does not belong to the ω– respectively α–limit sets of other solution curves (disregarding the constant solution R).

In this way we regain the standard brake orbit solutions for Newton's equations as follows. Let $q_0 \in \partial\widehat{M}_E$ be a brake point and consider the energy E Newtonian solution $q(t)$ for which $q(0) = q_0$ and consequently $\dot{q}(0) = 0$. This solution satisfies $q(-t) = q(t)$. In the reparameterized time and with rescaled velocities w this single brake curve blows up into the concatenation $\gamma_- * \gamma_0 * \gamma_+$ of three curves. The π_E projections of the two curves $\gamma_\pm$ lie in the interior of the Hill region where they are reparameterizations of $q(t)$, parameterized so that they approach q_0 as $t \to \pm\infty$. The middle curve γ_0 travels along the invariant sphere $(\pi_E)^{-1}(q_0)$, connecting the incoming normalized velocity $w = -\nabla U(q_0)/\|\nabla U(q_0)\|$ (the outward pointing normal to the Hill boundary) to the outgoing normalized velocity $w = +\nabla U(q_0)/\|\nabla U(q_0)\|$, taking infinite τ-time to do so. $\Diamond$

4.5 Blowing up the energy surface at collisions

We next consider the boundary component of $\widehat{\Sigma}_E$ defined in (4.2) projecting to Δ and thus set

$$\widehat{\Sigma}_{E,\Delta} := \left\{ x \in \widehat{\Sigma}_E \mid \pi_E(x) \in M \right\}.$$

That is, we defer the analysis of the boundary component at spatial infinity.
The blown up energy surface $\widehat{\Sigma}_{E,\Delta}$ has two types of boundary components, the one projecting to the collision set Δ and, for $E < 0$, the ones projecting to the boundary of Hill's region. Unlike in the last subsection, over Δ the vector field experiences a loss of smoothness:

4.5 Lemma
The smooth vector field $\widehat{X}_E : \widehat{\Sigma}_E \to T\widehat{\Sigma}_E$ defined by the right hand sides of (4.5) *continuously extends to a locally $C^{(1+\alpha)}$ Hölder continuous vector field*

$$\widehat{X}_{E,\Delta} : \widehat{\Sigma}_{E,\Delta} \to T\,\widehat{\Sigma}_{E,\Delta}\,.$$

Its flow leaves the boundary component of $\widehat{\Sigma}_{E,\Delta}$ over Δ invariant.

Proof: The factor $\frac{E+U}{1+U}$ of $\widetilde{G}_E$ has the constant limit 1 over Δ. The factor $U^{-\frac{1}{\alpha}}$ of $\widetilde{G}_E$ has been shown in Lemma 3.4 to extend to a $C^{(1+\alpha)}$ Hölder continuous function on the blow-up $\widehat{M_\Delta}$. Since it goes to zero at Δ, $\widetilde{G}_E$ extends to a $C^{(1+\alpha)}$ function on the blown up configuration space $\widehat{M_\Delta}$ (see (3.6)), vanishing over Δ. So by the first differential equation in (4.5) the flow leaves the boundary component of $\widehat{\Sigma}_{E,\Delta}$ over Δ invariant.

The argument for the force terms F is similar, using that the radial blow-up of (4.6) is smooth. $\square$

4.6 Corollary (smoothness of the flow)
The initial value problem $x' = \widehat{X}(x)$, $x(0) = x_0 \in \widehat{\Sigma}_{E,\Delta}$, derived from (4.5) *has unique local solutions in $C^1(D, \widehat{\Sigma}_{E,\Delta})$, with open domain $D \subseteq \mathbb{R}_\tau \times \widehat{\Sigma}_{E,\Delta}$ containing $\{0\} \times \widehat{\Sigma}_{E,\Delta}$.*

Proof:
The vector field $\widehat{X}_{E,\Delta}$ is in the Hölder space $C^{(1+\alpha)}\big(\widehat{\Sigma}_{E,\Delta}, T\,\widehat{\Sigma}_{E,\Delta}\big)$ with $\alpha > 0$ and thus fulfills the criterion of the theorem of Picard and Lindelöf. $\square$

4.7 Remark (smoothness of the flow)
We believe that the flow is $C^{(1+\alpha)}$ Hölder continuous, since the vector field is $C^{(1+\alpha)}$ Hölder continuous. However, we couldn't find such a result in the literature, and we didn't try to prove it. $\Diamond$

We now consider the flow at collisions more precisely. Every $\mathcal{C} \in \mathcal{P}_\Delta(N)$ defines a different type of how the particles meet, as the $\Xi_\mathcal{C}$ defined in (2.30) lead to the stratification

$$\Delta = \bigsqcup_{\mathcal{C} \in \mathcal{P}_\Delta(N)} \Xi_\mathcal{C} \tag{4.10}$$

of the thick diagonal Δ. For $q_0 \in \Xi_\mathcal{C} \subseteq \Delta^E_\mathcal{C}$, we use the $\mathcal{M}$–orthogonal decomposition $M = \Delta^E_\mathcal{C} \oplus \Delta^I_\mathcal{C}$ of configuration space, with dimensions given in (2.17). As $\Xi_\mathcal{C} \subseteq \Delta^E_\mathcal{C}$ is relatively open, we can use the local Cartesian coordinates $(q^E_\mathcal{C}, q^I_\mathcal{C})$ from (2.18) in a neighborhood $U_\mathcal{C} := U^E_\mathcal{C} \times U^I_\mathcal{C} \subseteq \Xi_\mathcal{C} \times \Delta^I_\mathcal{C}$ of q_0. Depending on the choice of $U^E_\mathcal{C}$, we can choose $U^I_\mathcal{C}$ so that

$$U_\mathcal{C} \cap \Delta = U^E_\mathcal{C} \quad \text{and} \quad U_\mathcal{C} \setminus U^E_\mathcal{C} \subseteq \widehat{M}^{\mathrm{int}}_E\,.$$

With the definition (2.20) of $J^I_\mathcal{C}$ and regarding it as a function on $\Delta^I_\mathcal{C}$, we write the coordinate $q^I_\mathcal{C}$ in the form

$$q^I_\mathcal{C} = r\, Q^I_\mathcal{C} \quad \text{with } J^I_\mathcal{C}(Q^I_\mathcal{C}) = 1 \text{ and } r := \big(J^I_\mathcal{C}(q^I_\mathcal{C})\big)^{1/2}. \tag{4.11}$$

Assuming that $q_{\mathcal{C}}^I \neq 0$, this polar decomposition is unique and

$$\Delta_{\mathcal{C}}^I \setminus \{0\} \cong (0,\infty) \times S_{\mathcal{C}}^I \quad \text{with the sphere } S_{\mathcal{C}}^I := \big(J_{\mathcal{C}}^I\big)^{-1}(1)\,.$$

For any $q_0 \in \Xi_{\mathcal{C}}$ and any direction $Q_{\mathcal{C}}^I \in S_{\mathcal{C}}^I$ for which $q_0 + rQ_{\mathcal{C}}^I \notin \Delta$ if $r > 0$ is small enough, we thus attach a point to blow up the boundary. The last condition is only violated for the subset $S_{\mathcal{C}}^I \cap \Delta$, which by (4.10) is a finite union of submanifolds of codimension at least d in $S_{\mathcal{C}}^I$.

Although the potential U is in general not $(-\alpha)$–homogeneous in r for $q = q_0 + rQ_{\mathcal{C}}^I$, it has this property asymptotically as $r \searrow 0$: For $Q_{\mathcal{C}}^I \in S_{\mathcal{C}}^I \backslash \Delta$

$$W_{\mathcal{C}}(Q_{\mathcal{C}}^I) := \lim_{r\searrow 0} r^\alpha\, U(q_0 + rQ_{\mathcal{C}}^I) = \tfrac{1}{2} \sum_{C\in\mathcal{C}} \sum_{i\neq j\in C} U_{i,j}\big((Q_{\mathcal{C}}^I)_i - (Q_{\mathcal{C}}^I)_j\big) = U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I)$$

has values in $(0,\infty)$, so $W_{\mathcal{C}} = U_{\mathcal{C}}^I\big|_{S_{\mathcal{C}}^I}$ and

$$\nabla W_{\mathcal{C}}(Q_{\mathcal{C}}^I) = \nabla U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I) - \langle U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I), Q_{\mathcal{C}}^I\rangle Q_{\mathcal{C}}^I\,. \tag{4.12}$$

This limit does not depend on $q_0 \in \Xi_{\mathcal{C}} \subseteq \Delta_{\mathcal{C}}^E$ and defines a smooth function

$$W_{\mathcal{C}} : S_{\mathcal{C}}^I \setminus \Delta \to (0,\infty)\,.$$

To construct our collision manifold, we attached to the point $(q_0, Q_{\mathcal{C}}^I)$ of the configuration space boundary an $(n-1)d-1$–dimensional unit sphere of velocities $w = w_{\mathcal{C}}^E + w_{\mathcal{C}}^I$. The internal part is split further into the component $\langle w_{\mathcal{C}}^I, Q_{\mathcal{C}}^I\rangle Q_{\mathcal{C}}^I$ parallel to $Q_{\mathcal{C}}^I$ and the one perpendicular to it. In order to obtain a somewhat simpler form of the differential equation, we rescale the parallel part, setting

$$v_{\mathcal{C}}^I := \big(W_{\mathcal{C}}(Q_{\mathcal{C}}^I)\big)^{1/2} \langle w_{\mathcal{C}}^I, Q_{\mathcal{C}}^I\rangle \quad\text{and}\quad X_{\mathcal{C}}^I := w_{\mathcal{C}}^I - \langle w_{\mathcal{C}}^I, Q_{\mathcal{C}}^I\rangle Q_{\mathcal{C}}^I\,. \tag{4.13}$$

4.8 Remark (gradient-like flow)
We defined $v_{\mathcal{C}}^I$ to be $\langle w_{\mathcal{C}}^I, Q_{\mathcal{C}}^I\rangle$ rescaled by $\sqrt{W_{\mathcal{C}}(Q_{\mathcal{C}}^I)}$ in order that $v_{\mathcal{C}}^I$ becomes a Lyapunov function on the collision manifold $\Xi_{\mathcal{C}}$ when $w_{\mathcal{C}}^E = 0$. In this way the flow on the invariant manifold $\Xi_{\mathcal{C}} \cap \{w_{\mathcal{C}}^E = 0\}$ is gradient-like[8]. Condition $w_{\mathcal{C}}^E = 0$ is important since orbits in $\widehat{\Sigma}_E$ colliding with $\Xi_{\mathcal{C}}$ must satisfy this condition in the limit:

$$\lim_{\tau\to\infty} w_{\mathcal{C}}^E(\tau) = 0\,. \tag{4.14}$$

[8]**Definition [McG1]:** Let ψ be a flow on a complete metric space X. Suppose there is a continuous function $g : X \to \mathbb{R}$ such that $g(\psi(x,t)) < g(x)$ if $t > 0$ unless x is a rest point. Suppose further that the rest points of ψ are isolated. Then g is called **gradient-like**.
We use this definition, although in our case the rest points are not isolated.

In order to derive equation (4.14) we use that the limiting internal cluster energies [9] $\lim_{\tau\to\infty} H^I_C(\tau)$ (see (2.27)) exist and are finite for all $C \in \mathcal{C}$. (Their existence has been proven for a more general class of potentials in [FK, Corollary 5.7].) The existence of $\lim_{\tau\to\infty} U^E_C(\tau) \in \mathbb{R}$ for the external cluster energy is obvious. $\lim_{\tau\to\infty} U^I_C(\tau) = +\infty$ so the finiteness of the limit of $H^I_C(\tau)$ implies that $\lim_{\tau\to\infty} K^I_C(\tau) = +\infty$. On the other hand $\lim_{\tau\to\infty} K^E_C(\tau) \in \mathbb{R}$, since the cluster-external forces are bounded along the orbit. Consequently, viewed projectively, the ratio of internal and external speeds (*i.e.* of $\left[\sqrt{2K^I_C}, \sqrt{2K^E_C}\right]$) tends to $[1, 0]$. Now (4.14) follows from this fact, (2.29) and the definition (4.1) of $w = w^E_{\mathcal{C}} + w^I_{\mathcal{C}}$. $\diamondsuit$

4.9 Lemma (Dynamics at collisions)
For the time variable τ, see (4.3)*, and the coordinates* (4.11) *and* (4.13) *the restriction of the o.d.e.* (4.5) *to the $\mathcal{C}$ component of the boundary is of the form*

$$(r^I_{\mathcal{C}})' = 0 \quad , \quad (Q^I_{\mathcal{C}})' = \big(W_{\mathcal{C}}(Q^I_{\mathcal{C}})\big)^{-1/\alpha} X^I_{\mathcal{C}} \,, \tag{4.15}$$

$$(v^I_{\mathcal{C}})' = \big(W_{\mathcal{C}}(Q^I_{\mathcal{C}})\big)^{1/2-1/\alpha} \left[(1-\tfrac{\alpha}{2})\left(\|w^I_{\mathcal{C}}\|^2 - \langle w^I_{\mathcal{C}}, Q^I_{\mathcal{C}}\rangle^2\right) - \tfrac{\alpha}{2}\|w^E_{\mathcal{C}}\|^2\right], \tag{4.16}$$

$$\begin{aligned}(X^I_{\mathcal{C}})' = {} & F^I_{\mathcal{C}}(Q^I_{\mathcal{C}}) - \langle F^I_{\mathcal{C}}(Q^I_{\mathcal{C}}), Q^I_{\mathcal{C}}\rangle Q^I_{\mathcal{C}} - \langle F^I_{\mathcal{C}}(Q^I_{\mathcal{C}}) + W_{\mathcal{C}}(Q^I_{\mathcal{C}})^{-1/\alpha} Q^I_{\mathcal{C}}, w^I_{\mathcal{C}}\rangle X^I_{\mathcal{C}} \\ & - W_{\mathcal{C}}(Q^I_{\mathcal{C}})^{-1/\alpha}\langle X^I_{\mathcal{C}}, w^I_{\mathcal{C}}\rangle Q^I_{\mathcal{C}} \,,\end{aligned} \tag{4.17}$$

$$(q^E_{\mathcal{C}})' = 0 \quad \textit{and} \quad (w^E_{\mathcal{C}})' = -\langle F^I_{\mathcal{C}}(Q^I_{\mathcal{C}}), w^I_{\mathcal{C}}\rangle\, w^E_{\mathcal{C}} \,. \tag{4.18}$$

In particular, the boundary component $r = 0$, is flow-invariant and so is its submanifold $r = 0 = w^E_{\mathcal{C}}$. Finally $v^I_{\mathcal{C}}$ is strictly increasing on this submanifold at points at which $w^I_{\mathcal{C}}$ and $Q^I_{\mathcal{C}}$ are linear independent.

Proof: We derive these identities from the differential equation (4.5), beginning with (4.15). For $q = q_0 + rQ^I_{\mathcal{C}} \in \widehat{M}$

$$r' = \frac{\langle q^I_{\mathcal{C}}, (q^I_{\mathcal{C}})'\rangle}{r} \overset{(4.5)}{=} \widetilde{G}_E(q)\,\langle Q^I_{\mathcal{C}}, w^I_{\mathcal{C}}\rangle \,. \tag{4.19}$$

As $r \searrow 0$, $\widetilde{G}_E(q_0 + rQ^I_{\mathcal{C}}) \searrow 0$ (asymptotically linearly), whereas $\|Q^I_{\mathcal{C}}\|_{\mathcal{M}} = 1$ and $\|w^I_{\mathcal{C}}\|_{\mathcal{M}} \le 1$, proving $r' = 0$ on the boundary. Similarly,

$$(Q^I_{\mathcal{C}})' = \left(\frac{q^I_{\mathcal{C}}}{r}\right)' \overset{(4.19)}{=} \frac{\widetilde{G}_E(q)}{r}\left(w^I_{\mathcal{C}} - \langle Q^I_{\mathcal{C}}, w^I_{\mathcal{C}}\rangle Q^I_{\mathcal{C}}\right) \xrightarrow{r\searrow 0} \frac{w^I_{\mathcal{C}} - \langle Q^I_{\mathcal{C}}, w^I_{\mathcal{C}}\rangle Q^I_{\mathcal{C}}}{\big(W_{\mathcal{C}}(Q^I_{\mathcal{C}})\big)^{\frac{1}{\alpha}}} \,.$$

To derive (4.16), based on Definition (4.13) we write the derivative of $v^I_{\mathcal{C}}$ as the sum $(v^I_{\mathcal{C}})' = I + II + III$ with

$$I := \left(\big(W_{\mathcal{C}}(Q^I_{\mathcal{C}})\big)^{1/2}\right)' \langle w^I_{\mathcal{C}}, Q^I_{\mathcal{C}}\rangle \quad \text{and} \quad II := \big(W_{\mathcal{C}}(Q^I_{\mathcal{C}})\big)^{1/2}\,\langle (w^I_{\mathcal{C}})', Q^I_{\mathcal{C}}\rangle \,.$$

[9] Here we use a simplified notation for the values of observables along orbits.

Using (4.12) and (4.15),

$$I = \tfrac{1}{2}\big(W_{\mathcal{C}}(Q_{\mathcal{C}}^I)\big)^{-1/2-1/\alpha}\Big\langle \nabla U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I) - \langle \nabla U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I), Q_{\mathcal{C}}^I\rangle\, Q_{\mathcal{C}}^I\,,\, w_{\mathcal{C}}^I\Big\rangle\, \langle w_{\mathcal{C}}^I, Q_{\mathcal{C}}^I\rangle\,,$$

whereas by (4.5) and the definition (4.4) of F

$$II = \tfrac{1}{2}\big(W_{\mathcal{C}}(Q_{\mathcal{C}}^I)\big)^{-1/2-1/\alpha}\Big\langle \nabla U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I) - \langle \nabla U_{\mathcal{C}}^I(Q_{\mathcal{C}}^I), w_{\mathcal{C}}^I\rangle w_{\mathcal{C}}^I\,,\, Q_{\mathcal{C}}^I\Big\rangle\,.$$

So by $(-\alpha)$–homogeneity of $U_{\mathcal{C}}^I$

$$I + II = -\tfrac{\alpha}{2}\,\big(W_{\mathcal{C}}(Q_{\mathcal{C}}^I)\big)^{+1/2-1/\alpha}\big(1 - \langle w_{\mathcal{C}}^I\,,\, Q_{\mathcal{C}}^I\rangle^2\big)\,.$$

In this expression we substitute $1 = \|w\|^2 = \|w_{\mathcal{C}}^I\|^2 + \|w_{\mathcal{C}}^E\|^2$. Finally, by (4.15)

$$III = \big(W_{\mathcal{C}}(Q_{\mathcal{C}}^I)\big)^{1/2}\,\langle w_{\mathcal{C}}^I, (Q_{\mathcal{C}}^I)'\rangle = \big(W_{\mathcal{C}}(Q_{\mathcal{C}}^I)\big)^{+1/2-1/\alpha}\big(\|w_{\mathcal{C}}^I\|^2 - \langle w_{\mathcal{C}}^I\,,\, Q_{\mathcal{C}}^I\rangle^2\big)\,,$$

proving (4.16).

The proof of (4.17) uses (4.15) and $(w_{\mathcal{C}}^I)' = F_{\mathcal{C}}^I(Q_{\mathcal{C}}^I) - \langle F_{\mathcal{C}}^I(Q_{\mathcal{C}}^I), w_{\mathcal{C}}^I\rangle w_{\mathcal{C}}^I$.

In (4.18) the equation $(q_{\mathcal{C}}^E)' = 0$ follows, since $(q_{\mathcal{C}}^E)' = \widetilde{G}_E(q) w_{\mathcal{C}}^E$, with the scaling factor $\widetilde{G}_E(q)$ being zero at the boundary.
The equation for $(w_{\mathcal{C}}^E)'$ is a consequence of $(w_{\mathcal{C}}^E)' = \Pi_{\mathcal{C}}^E F(q) - \langle F(q), w\rangle\, w_{\mathcal{C}}^E$, where the velocity w has norm one and the force term $F(q)$ goes to $F(Q_{\mathcal{C}}^I)$ for $q = q_0 + rQ_{\mathcal{C}}^I$ in the limit $r \searrow 0$, whereas $\Pi_{\mathcal{C}}^E F(q) \to 0$ for the external force. $\Box$

4.6 Blowing up the energy surface at infinity

The configuration sphere $\mathbb{S}$ at spatial infinity is the disjoint union of $\widehat{\mathbb{S}} = \mathbb{S}\backslash\Delta$ and $\mathbb{S} \cap \Delta$, where the last set corresponds to non-trivial clusters whose barycenters tend to infinity. We treat $\widehat{\mathbb{S}}$ first.

4.6.1 The case of single particles

We first consider the motion of n single particles approaching $\widehat{\mathbb{S}}$, which in our center of mass configuration space can happen for energies $E \geq 0$ if $n \geq 2$. For $n = 2$ we have $\widehat{\mathbb{S}} = \mathbb{S}$. In the Figure 3.3 for three particles on the line, $\widehat{\mathbb{S}}$ corresponds to the six segments of the outer circle.
Instead of $q = r\,Q \in \widehat{M}$ we use the polar coordinates (z, Q) near infinity, with

$$z := r^{-\alpha} \quad \text{and} \quad \overline{q} := z\,Q = r^{-\alpha}\,Q = r^{-\alpha-1}q\,. \tag{4.20}$$

The configuration space is mirror-symmetric: $\widehat{M} = \{(z, Q) \mid q \in \widehat{M}\}$.

In these coordinates the sphere at infinity corresponds to $z = 0$. We set

$$\overline{G}_E(\overline{q}) := z^{1+1/\alpha}\, \widetilde{G}_E(q) = z^{1+1/\alpha}\, \widetilde{G}_E(z^{-1/\alpha}Q) = z\, \tfrac{E+zU(Q)}{1+zU(Q)} U^{-1/\alpha}(Q) \quad (4.21)$$

(compare with (4.3)) and rewrite the force term (4.4):

$$\overline{F}(\overline{q}) := F(q) = z \tfrac{\mathcal{M}^{-1}\nabla U(Q)}{2(1+zU(Q))\, U(Q)^{\frac{1}{\alpha}}}\,.$$

The differential equation (4.5) then takes the form

$$\overline{q}' = \overline{G}_E(\overline{q})\,\big(w - (1+\alpha)\langle w, Q\rangle\, Q\big) \quad , \quad w' = \overline{F}(\overline{q}) - \langle \overline{F}(\overline{q}), w\rangle\, w \qquad (4.22)$$

and in polar coordinates (z, Q) one gets

$$z' = -\overline{G}_E(\overline{q})\,\langle Q, w\rangle \quad , \quad Q' = \tfrac{\overline{G}_E(\overline{q})}{z}\,(w - \langle Q, w\rangle\, Q)\,.$$

By looking at $\overline{G}_E$ in (4.21), we conclude that the right hand sides of these differential equations are real-analytic for $Q \in \widehat{\mathbb{S}}$ and $z \in [0, \infty)$. At spatial infinity, that is, at $z = 0$, they reduce to

$$z' = 0 \quad , \quad Q' = E\, U^{-1/\alpha}(Q)\,(w - \langle Q, w\rangle\, Q) \quad , \quad w' = 0\,.$$

In particular the boundary component of $\widehat{\Sigma}_E$ over $\widehat{\mathbb{S}}$ is invariant under the flow. Whereas $Q' = 0$ for $E = 0$, for $E > 0$ this is the case if and only if $w \in \{-Q, Q\}$. These velocities w then correspond to the negative/positive time asymptotics of non-clustering particles.
Similar to the case of two bodies treated in Subsection 4.3, the unparametrized motion takes place on the invariant great circle $\mathbb{S} \cap \mathrm{span}(Q, w)$ in configuration space. The reparameterization is given by integrating the factor $E\, U^{-1/\alpha}(Q)$.

- If these do not meet Δ, then the span is a half-circle. As in Subsection 4.3, we cannot connect asymptotically free solutions of the original Hamiltonian differential equation (2.6) via the flow at infinity. The reason is that (unlike the collision orbits and the brake orbits) they converge to the *stable* manifold. That is nice, because this would not have a sensible physical interpretation (observe that then the original time variable t diverges as τ does).

- Otherwise the trajectory can be asymptotic to points $Q \in \Delta \cap \mathbb{S}$, where $U^{-1/\alpha}(Q)$ vanishes. This leads us to the next point, the blow-up for non-trivial clusters at spatial infinity.

4.6.2 The case of non-trivial clusters

We now consider trajectories in M that approach a point $q_0 \in \Delta \cap \mathbb{S}$. In the Figure 3.3 for three particles on the line, this part of the boundary of blown up configuaration space $\widehat{M}$ corresponds to the twelve small quarter circle segments near the the outer circle.
By the stratification (4.10) of Δ, $q_0 \in \Xi_{\mathcal{C}} \cap \mathbb{S}$ for a unique $\mathcal{C} \in \mathcal{P}_\Delta(N)$, with $\mathcal{C} \neq \mathcal{C}_{\max}$, since total collision occurs at $0 \in M$. $\Xi_{\mathcal{C}}$, defined in (2.30), is a relatively open (and dense) subset of the linear subspace $\Delta^E_{\mathcal{C}}$. So by (2.17) it is a manifold of dimension $d(|\mathcal{C}|-1)$, with a number $2 \le |\mathcal{C}| \le n-1$ of clusters. It follows that $\Xi_{\mathcal{C}} \cap \mathbb{S}$ is open in a $\big(d(|\mathcal{C}|-1)-1\big)$–dimensional sub-sphere of $\mathbb{S}$. Its blow-up is a fiber bundle

$$B_{\mathcal{C}} \;\longrightarrow\; \Xi_{\mathcal{C}} \cap \mathbb{S} \;\text{ , with typical fiber } S_+^{d(n-|\mathcal{C}|)}\,, \tag{4.23}$$

the plus sign meaning the half-sphere of incoming directions.[10] So it is a manifold whose dimension coincides with the one of $\mathbb{S}$, as it should, being part of $\partial\widehat{M}$.

Next we construct coordinates on the half-sphere $S_+^{d(n-|\mathcal{C}|)}$at q_0. The important result will be that, with the Cartesian coordinates $(q^E_{\mathcal{C}}, q^I_{\mathcal{C}})$ near $\Xi_{\mathcal{C}}$, $q^I_{\mathcal{C}}$ can be used.

We use the polar coordinates (z,Q) of $\overline{M} = M \sqcup \mathbb{S}$ near $\mathbb{S}$ with $z := 1/r > 0$ for $q = r\,Q \in M\backslash\{0\}$), and $z=0$ on $\mathbb{S}$. The metric used is

$$\big\|(z_1,Q_1)-(z_2,Q_2)\big\| := \sqrt{|z_1-z_2|^2 + \|Q_1-Q_2\|^2} \qquad \big((z_j,Q_j) \in [0,\infty)\times\mathbb{S}\big).$$

For a unit vector $Q^I_{\mathcal{C}} \in S^I_{\mathcal{C}}$ we set $(q^E_{\mathcal{C}}, q^I_{\mathcal{C}}) := (c\,q_0,\, d\,Q^I_{\mathcal{C}})$ and consider the distance of

$$(z_1,Q_1) := \Big(\|q^E_{\mathcal{C}} + q^I_{\mathcal{C}}\|^{-1}\,,\; \tfrac{q^E_{\mathcal{C}}+q^I_{\mathcal{C}}}{\|q^E_{\mathcal{C}}+q^I_{\mathcal{C}}\|}\Big) \quad \text{and} \quad (z_2,Q_2) := (0,q_0)\,.$$

In the limit $c \nearrow \infty$, with $d \ge 0$ fixed their difference is asymptotic to

$$(z_1,Q_1)-(z_2,Q_2) = \big(c^2+d^2\big)^{-1/2}, \tfrac{cq_0+dQ^I_{\mathcal{C}}}{\sqrt{c^2+d^2}} - q_0\big) \;\sim \big(\tfrac{1}{c}, \tfrac{d}{c}\,Q^I_{\mathcal{C}}\big)\,,$$

which we write as $(\frac{1}{c}, \frac{d}{c}\,Q^I_{\mathcal{C}}) = R\,\big(\cos(\varphi), \sin(\varphi)\,Q^I_{\mathcal{C}}\big)$ (so that $\|(\frac{1}{c}, \frac{d}{c}\,Q^I_{\mathcal{C}})\| = R$ with $R = \sqrt{1+d^2}/c \searrow 0$). As

$$q^I_{\mathcal{C}} = d\,Q^I_{\mathcal{C}} = \tan(\varphi) Q^I_{\mathcal{C}}\,,$$

in the limit $d \nearrow \infty$ the $\mathcal{C}$–internal cluster coordinates $q^I_{\mathcal{C}}$ parameterize the half-sphere at q_0 of the bundle (4.23). In that limit the distance between the positions

[10] In general, (4.23) is a non-trivial bundle. However, here we argue only semi-locally so that this does not play a role in our analysis.

of any pair of particles in different clusters of $\mathcal{C}$ goes to infinity, whereas the difference of particle positions in the same cluster is constant.
From (4.5) we get in this limit and for the cluster-internal potential $U_\mathcal{C}^I$ (see (2.26)), the differential equation

$$(q_\mathcal{C}^I)' = \widetilde{G}_{E,\mathcal{C}}(q_\mathcal{C}^I)\, w_\mathcal{C}^I \quad , \quad (w_\mathcal{C}^I)' = F_\mathcal{C}(q_\mathcal{C}^I) - \langle F_\mathcal{C}(q_\mathcal{C}^I), w_\mathcal{C}^I\rangle\, w_\mathcal{C}^I, \tag{4.24}$$

with

$$\widetilde{G}_{E,\mathcal{C}}(q_\mathcal{C}^I) := \tfrac{E+U_\mathcal{C}^I(q_\mathcal{C}^I)}{(1+U_\mathcal{C}^I(q_\mathcal{C}^I))\,(U_\mathcal{C}^I(q_\mathcal{C}^I))^{\frac{1}{\alpha}}} \quad \text{and} \quad F_\mathcal{C}(q_\mathcal{C}^I) := \tfrac{\mathcal{M}^{-1}\nabla U_\mathcal{C}^I(q_\mathcal{C}^I)}{2(1+U_\mathcal{C}^I(q_\mathcal{C}^I))\,(U_\mathcal{C}^I(q_\mathcal{C}^I))^{\frac{1}{\alpha}}}\,.$$

So up to a common time reparameterization by $1/\big((1+U_\mathcal{C}^I)((U_\mathcal{C}^I)^{\frac{1}{\alpha}}\big)$, the clusters in $\mathcal{C}$ only interact internally. To see this, note that, up to that factor, $\widetilde{G}_{E,\mathcal{C}}$ and $F_\mathcal{C}$ depend affinely on $U_\mathcal{C}^I$.

The motion of the cluster centers occurs with a velocity vector $w_\mathcal{C}^E$ that is a constant of the motion.

Like in Subsections 4.5 and the present one, with the half-sphere bundle $B_\mathcal{C}$ from (4.23), the boundary component $B_\mathcal{C} \times S^{(n-1)d-1}$ of the blown-up energy surface $\widehat{\Sigma}_E$ is invariant under the flow, which by the same arguments is continuously differentiable.
$\mathcal{C}$-internal collisions that would lead to components with a $\mathcal{D} \in \mathcal{P}(N)$ with $\mathcal{D}$ strictly coarser than $\mathcal{C}$ only can occur in the temporal limits $\tau \to \pm\infty$.
The same statement holds for $\|q_\mathcal{C}^I(\tau)\| \to \infty$, that is escape to spatial infinity.[11]

5 Topology of the blown up configuration space

Here we are going to determine the homeomorphism type of the total boundary blow up $\partial\widehat{M}_\Delta$, with $\widehat{M}_\Delta$ defined in Lemma 3.2. For the proof we use a variant of the Graf partition of configuration space M devised by Gian Michele Graf in [Gr], see also [DG, Sect. 5.2].

5.1 Definition ([Kn, Sect. 12.6]) *For $\delta \in (0,1)$, let*

$$J^{(\delta)} : M \to \mathbb{R} \quad , \quad J^{(\delta)}(q) := \max\big\{ J_\mathcal{C}^E(q) + \delta^{|\mathcal{C}|} \;\big|\; \mathcal{C} \in \mathcal{P}(N) \big\}\,.$$

The **Graf partition** *of the configuration space M is the family of subsets*

$$\Xi_\mathcal{C}^{(\delta)} := \Big\{ q \in M \;\Big|\; J_\mathcal{C}^E(q) + \delta^{|\mathcal{C}|} = J^{(\delta)}(q) \Big\} \qquad \big(\mathcal{C} \in \mathcal{P}(N)\big). \tag{5.1}$$

[11] In Figure 3.3 for collisions these correspond to the twelve dark green points near the outer circle. For escape to spatial infinity, they are represented by the twelve points on that circle.

5.2 Remark (Graf partition)

1. These atoms are closed, and we obtain a measure theoretic partition of M: $\bigcup_{\mathcal{C}\in\mathcal{P}(N)} \Xi_{\mathcal{C}}^{(\delta)} = M$, For $\mathcal{C} \neq \mathcal{D}$ the Lebesgue measure of $\Xi_{\mathcal{C}}^{(\delta)} \cap \Xi_{\mathcal{D}}^{(\delta)}$ is zero, since the values of $J_{\mathcal{C}}^E + \delta^{|\mathcal{C}|}$ and $J_{\mathcal{D}}^E + \delta^{|\mathcal{D}|}$ coincide only on quadrics in M.

2. Moreover, there is a $\delta_0 \in (0,1)$ so that for all $\delta \in (0, \delta_0]$, the Graf partition (5.1) has the property that for $\Xi_{\mathcal{C}}^{(\delta)} \cap \Xi_{\mathcal{D}}^{(\delta)} \neq \emptyset$, the cluster decompositions $\mathcal{C}$ and $\mathcal{D}$ are **comparable**, *i.e.*, $\mathcal{C} \preccurlyeq \mathcal{D}$ or $\mathcal{C} \succcurlyeq \mathcal{D}$ (see [Kn, Lemma 12.52]). $\diamondsuit$

5.3 Theorem *For $n \geq 2$ particles,*

1) $S^{(n-1)d-1} \setminus \Delta$ *is homeomorphic to* $\partial\, \Xi_{\mathcal{C}_{\min}}^{(\delta)}$*,*

2) *whereas* $\partial\, \Xi_{\mathcal{C}_{\min}}^{(\delta)}$ *is homeomorphic to* $\partial \widehat{M}_\Delta$*.*

Proof:
1) We first construct homeomorphisms

$$H^{(\delta)} : S^{(n-1)d-1} \setminus \Delta \;\to\; \partial\, \Xi_{\mathcal{C}_{\min}}^{(\delta)} \qquad \big(\delta \in (0, \delta_0)\big)$$

to the boundary of the free atom $\Xi_{\mathcal{C}_{\min}}^{(\delta)}$. With the rays

$$R_s := \{\lambda s \mid \lambda > 0\} \;\subseteq\; M \qquad (s \in S^{nd-1} \setminus \Delta)$$

$H^{(\delta)}(s)$ is defined as the unique intersection point in $R_s \cap \partial\, \Xi_{\mathcal{C}_{\min}}^{(\delta)}$. In fact,

1. $R_s \cap \partial\, \Xi_{\mathcal{C}_{\min}}^{(\delta)}$ is non-empty:
   (a) As $n \geq 2$, there exists a set partition $\mathcal{D} \in \mathcal{P}_\Delta(N)$, and the difference
   $$\left[J_{\mathcal{C}_{\min}}^E + \delta^n\right] - \left[J_{\mathcal{D}}^E + \delta^{|\mathcal{D}|}\right] = J_{\mathcal{D}}^I + \delta^n - \delta^{|\mathcal{D}|} \tag{5.2}$$
   is strictly increasing along the ray R_s and goes to $+\infty$, since the continuous map $\lambda \mapsto J_{\mathcal{D}}^I(\lambda s)$ equals $j\lambda^2$, with $j = J_{\mathcal{D}}^I(s) > 0$ if $s \in S^{(n-1)d-1} \setminus \Delta$ (and $j = 0$ in the excluded case $s \in S^{(n-1)d-1} \cap \Delta_{\mathcal{D}}^E \subseteq S^{(n-1)d-1} \cap \Delta$).
   (b) Conversely, $\lim_{\lambda \searrow 0} J_{\mathcal{D}}^I(\lambda s) + \delta^n - \delta^{|\mathcal{D}|} = \delta^n - \delta^{|\mathcal{D}|} < 0$ in (5.2), since $|\mathcal{D}| < n$ and $\delta \in (0,1)$.

2. $R_s \cap \partial\, \Xi_{\mathcal{C}_{\min}}^{(\delta)}$ consists of one point only, and the intersection is transverse. This follows since for $\lambda_0 s \in \Xi_{\mathcal{C}_{\min}}^{(\delta)} \cap \Xi_{\mathcal{D}}^{(\delta)}$, (5.2) is strictly increasing at $\lambda_0 s$, so that $\lambda s \in \Xi_{\mathcal{C}_{\min}}^{(\delta)}$ for $\lambda > \lambda_0$. Of course, $\lambda_0 s$ can belong to more than two atoms in the partition, see Figure 5.1. Then that boundary point lies in the intersection of more than one quadric, but R_s is transversality to all of them.

3. By that transversality property, $H^{(\delta)}$ is continuous. $H^{(\delta)}$ is injective, since the rays R_s and $R_{s'}$ are mutually disjoint for $s \neq s' \in S^{(n-1)d-1}$.
   As the atom $\Xi^{(\delta)}_{\mathcal{C}_{\min}}$ is closed and disjoint from Δ, the same is true for its boundary $\partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}}$. Since $\bigcup_{s\in S^{(n-1)d-1}\setminus\Delta} R_s = \widehat{M} = \mathbb{R}^{(n-1)d}\setminus\Delta$, $H^{(\delta)}$ is surjective.
   The inverse of $H^{(\delta)}$ is continuous, too, since the intersection of the rays R_s with the sphere is transverse, too.

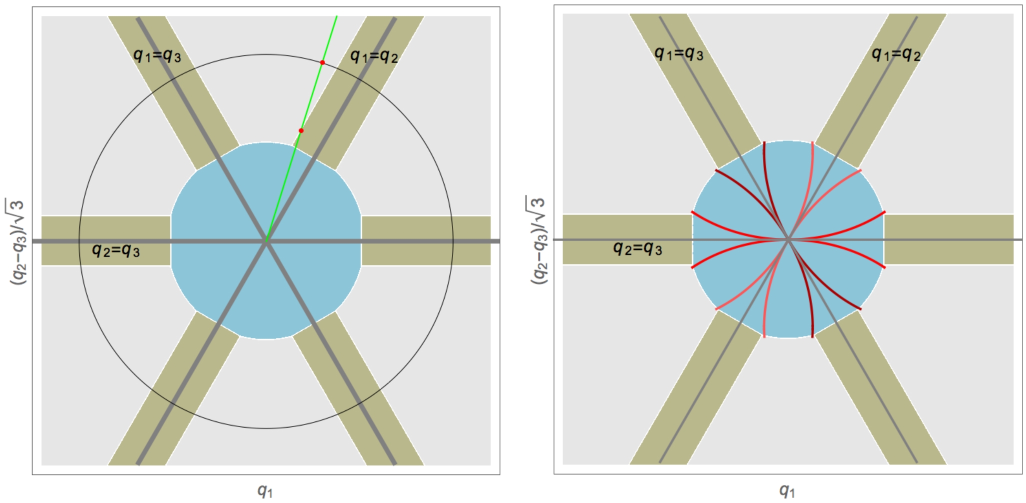

Figure 5.1: A Graf partition of the configuration space of $n = 3$ particles in $d = 1$ dimension, in center of mass system. Left: the homeomorphism between $S^1\setminus\Delta$ and $\partial\Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$, induced by the rays R_c (green), with $\Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$ in gray. Right: curves S_{ch}, parametrised by $\delta < \delta_0$, corresponding to intersections of three atoms (red)

Incidentally, we proved that $H^{(\delta)}$ is even locally bi-Lipschitz.

So for $\delta_1 < \delta_2 \in (0, \delta_0)$ the boundaries $\partial\,\Xi^{(\delta_1)}_{\mathcal{C}_{\min}}$ and $\partial\,\Xi^{(\delta_2)}_{\mathcal{C}_{\min}}$ are homeomorphic. Furthermore, $\mathrm{int}\big(\Xi^{(\delta_1)}_{\mathcal{C}_{\min}}\big) \supseteq \Xi^{(\delta_2)}_{\mathcal{C}_{\min}}$ if $\delta_0 \leq 1/2$, and $\lim_{\delta\searrow 0}\Xi^{(\delta)}_{\mathcal{C}_{\min}} = \widehat{M}$ in the sense of Hausdorff distance, since $0 < |\mathcal{D}| < n$ for $\mathcal{D} \in \mathcal{P}_\Delta(N)$ so that in (5.2)

$$0 < \delta_1^{|\mathcal{D}|} - \delta_1^n < \delta_2^{|\mathcal{D}|} - \delta_2^n \quad \text{and} \quad \lim_{\delta\searrow 0}\left(\delta^{|\mathcal{D}|} - \delta^n\right) = 0. \tag{5.3}$$

2) To relate the boundaries $\partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}}$ and $\partial\widehat{M}_\Delta$, we use homeomorphisms different from $H^{(\delta_1)}\circ(H^{(\delta_2)})^{-1} : \partial\,\Xi^{(\delta_2)}_{\mathcal{C}_{\min}} \to \partial\,\Xi^{(\delta_1)}_{\mathcal{C}_{\min}}$, since the limit of the latter for $\delta_1 \searrow 0$ is not well-behaved. Instead we show existence of a smooth vector field

$$v : \widehat{M}\setminus\Xi^{(\delta_0)}_{\mathcal{C}_{\min}} \to \mathbb{R}^{d(n-1)}, \tag{5.4}$$

whose time t flow restricts to locally Lipschitz homeomorphisms

$$\partial\,\Xi^{(\delta_2)}_{\mathcal{C}_{\min}} \to \partial\,\Xi^{(\delta_1)}_{\mathcal{C}_{\min}} \qquad \big(\delta_1 \in (0,\delta_2] \text{ with } \delta_2-\delta_1=t\big). \tag{5.5}$$

Every point $q \in \widehat{M} \setminus \Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$ belongs to $q \in \partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}}$, for some $\delta \in (0,\delta_0)$.

Furthermore q (exactly) belongs to $\bigcap_{\ell=0}^k \partial\,\Xi^{(\delta)}_{\mathcal{D}_\ell}$ with $\mathcal{D}_0 := \mathcal{C}_{\min}$ and $k \in \mathbb{N}$. According to Remark 5.2.2 these set partitions are mutually comparable. So by reordering we can assume that the chain

$$\mathrm{ch} := \{\mathcal{D}_0,\ldots,\mathcal{D}_k\} \text{ is ordered: } \mathcal{D}_0 \preccurlyeq \mathcal{D}_1 \preccurlyeq \ldots \preccurlyeq \mathcal{D}_k, \quad (1 \le k \le n-1). \tag{5.6}$$

Conversely, every such chain (5.6) defines a semialgebraic set $S_{\mathrm{ch}} \subseteq \widehat{M} \setminus \Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$, consisting of the q that for some $\delta \in (0,\delta_0)$ simultaneously belong to all $\partial\,\Xi^{(\delta)}_{\mathcal{D}_\ell}$, see Figure 5.1, right. Finally, the set of all chains (5.6) gives rise to a set partition of $\widehat{M} \setminus \Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$ by the S_{ch}. In fact, these semialgebraic sets are submanifolds, of codimension $k-1$.

For a chain (5.6) the corresponding projections (2.16) are pairwise commuting. So the level sets $(J^I_{\mathcal{D}_\ell} - J^I_{\mathcal{D}_{\ell-1}})^{-1}(\delta^{|\mathcal{D}_\ell|} - \delta^{|\mathcal{D}_{\ell-1}|})$ are pairwise $\mathcal{M}$-orthogonal and define smooth functions

$$\tilde f_\ell : U_{\mathrm{ch}} \longrightarrow \mathbb{R}^+ \;\;,\;\; \big(J^I_{\mathcal{D}_\ell} - J^I_{\mathcal{D}_{\ell-1}}\big)^{-1}\big(\delta^{|\mathcal{D}_\ell|} - \delta^{|\mathcal{D}_{\ell-1}|}\big) \ni q \longmapsto \delta \qquad (\ell = 1,\ldots,k)$$

on a suitable neighborhood $U_{\mathrm{ch}} \subseteq \widehat{M} \setminus \Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$ of S_{ch} that have non-vanishing gradients. Formulated differently, the vector fields

$$\tilde v_\ell : U_{\mathrm{ch}} \to \mathbb{R}^{(n-1)d} \quad,\quad \tilde v_\ell := \tfrac{-\nabla \tilde f_\ell}{\|\nabla \tilde f_\ell\|^2_{\mathcal{M}}} \qquad (\ell = 1,\ldots,k)$$

are pairwise $\mathcal{M}$-orthogonal, with Lie derivatives $L_{\tilde v_i} \tilde f_\ell = -\delta_{i,\ell}$. Therefore there exists a unique linear combination

$$v_{\mathrm{ch}} := \sum_{\ell=1}^k c_\ell\, \tilde v_\ell : U_{\mathrm{ch}} \to \mathbb{R}^{(n-1)d}$$

of the vector fields so that $L_{v_{\mathrm{ch}}} f_\ell = -\delta_{i,\ell}$ for the functions

$$f_\ell : U_{\mathrm{ch}} \longrightarrow \mathbb{R}^+ \quad,\quad \big(J^I_{\mathcal{D}_\ell}\big)^{-1}\big(\delta^{|\mathcal{D}_\ell|} - \delta^n\big) \ni q \longmapsto \delta \qquad (\ell = 1,\ldots,k) \tag{5.7}$$

that satisfy

$$f_\ell\big(\partial\,\Xi^{(\delta)}_{\mathcal{D}_\ell} \cap U_{\mathrm{ch}}\big) = \delta$$

(note that $J^I_{\mathcal{D}_0} = J^I_{\mathcal{C}_{\min}} = 0$, so that $J^I_{\mathcal{D}_\ell} = \sum_{m=1}^{\ell}(J^I_{\mathcal{D}_m} - J^I_{\mathcal{D}_{m-1}})$). In particular, v_{ch} is tangential to S_{ch}. Actually we define the neighborhood U_{ch} by the condition that for some constant $c > 1$

$$\tfrac{f_i(q)}{f_j(q)} \in (1/c, c) \qquad (i,j = 1,\ldots,k). \tag{5.8}$$

Note this still guarantees that $S_{\rm ch} \subseteq U_{\rm ch}$. Of course for $k = 1$, the restriction (5.8) is vacuous.

$c > 1$ is chosen small enough so that $U_{\rm ch} \cap U_{\rm ch'} = \emptyset$ if the chains ch and ch$'$ contain incompatible atoms.

Combining the vector fields $v_{\rm ch}$ by a partition of unity subordinate to the $U_{\rm ch}$, we get a vector field (5.4) on $\widehat{M} \setminus \Xi^{(\delta_0)}_{\mathcal{C}_{\min}}$. It induces a local flow Φ, mapping level surfaces to level surfaces.

Restricting the local flow to initial conditions in $\partial\,\Xi^{(\delta_2)}_{\mathcal{C}_{\min}}$, we obtain the family of homeomorphisms (5.5). Their limit for $\delta_1 \searrow 0$ exists (see below) and leads to a homeomorphism with the boundary blow up $\partial\widehat{M_\Delta}$.

Existence of the limit is seen as follows:

(a) Along a Φ trajectory at time $t \geq 0$, (5.8) transforms into $\frac{f_i(q)-t}{f_j(q)-t}$. So if $q \in U_{\rm ch} \setminus S_{\rm ch}$, then its trajectory will ultimately leave $U_{\rm ch}$. This implies that near the escape time limit we can assume that $\Phi_t(q) \in S_{\rm ch'}$ for some subchain ch$'$.

(b) For $q \in S_{\rm ch}$ with $f_\ell(q) = \delta$ by definition $\lim_{t\nearrow\delta} f_\ell \circ \Phi_t(q) = 0$ ($\ell = 1, \ldots, k$). This implies that $\lim_{t\nearrow\delta} \Phi_t(q) \in \Delta$ exists:

   - The external coordinates $\big(\Phi_t(q)\big)^E_{\mathcal{D}_k}$ are independent of t, since (5.7) depends only on internal $\mathcal{D}_k$ coordinates, and by $\mathcal{M}$-orthogonality of the projections (2.16).
   - The internal coordinates $\big(\Phi_t(q)\big)^I_{\mathcal{D}_k}$ go to zero as $t \nearrow \delta$.

(c) For the same reason, the map

$$\Phi^{(\delta)} : \partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}} \to \Delta \quad , \quad q \mapsto \lim_{t\nearrow\delta} \Phi_t(q) \tag{5.9}$$

is continuous. It is surjective, since the Hausdorff distance of these two subsets of M goes to zero as $\delta \searrow 0$. It is not injective (not even in the case $n = 2$, since then $\Delta = \Delta^E_{\mathcal{C}_{\max}} = \{0\}$, whereas $\partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}} \cong S^{n-1}$).

(d) We recall the definition $S^I_{\mathcal{C}} = \big(J^I_{\mathcal{C}}\big)^{-1}(1)$ of the internal unit sphere for $\mathcal{C} \in \mathcal{P}(N)$ (which is of dimension $d(n - |\mathcal{C}|) - 1$).
For $q \in \partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}} \cap \overline{S}_{\rm ch}$ and $\ell = 1, \ldots, k$, the unit vectors $N^{(\delta)}_{\mathcal{D}_\ell}(q)$ given by

$$N^{(\delta)}_{\mathcal{D}_\ell} : \partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}} \cap \overline{S}_{\rm ch} \to S^I_{\mathcal{D}_\ell} \quad , \quad N^{(\delta)}_{\mathcal{D}_\ell}(q) = \lim_{t\nearrow\delta} \frac{(\Phi_t(q) - \Phi^{(\delta)}(q))^I_{\mathcal{D}_\ell}}{\|(\Phi_t(q) - \Phi^{(\delta)}(q))^I_{\mathcal{D}_\ell}\|} \tag{5.10}$$

exist, and obviously depend only on $\mathcal{D}_\ell \in \mathcal{P}_\Delta(N)$, not on the chain ch to which $\mathcal{D}_\ell$ belongs. This is important since the closure $\overline{S}_{\mathrm{ch}}$ of S_{ch} used in the definition of the domain can intersect other $S_{\mathrm{ch}'}$. Moreover, the maps $N^{(\delta)}_{\mathcal{D}_\ell}$ are continuous, and $N^{(\delta)}_{\mathcal{D}_\ell}(q)$ is perpendicular to $\Delta^E_{\mathcal{C}_\ell}$.

By the above arguments, on the subsets $\partial\, \Xi^{(\delta)}_{\mathcal{C}_{\min}} \cap S_{\mathrm{ch}}$, indexed by the ch,

(e) Together, $\Phi^{(\delta)}(q)$ and the $N^{(\delta)}_{\mathcal{D}_\ell}(q)$ $(\ell = 1, \ldots, k)$ define a point in $\partial \widehat{M}_\Delta$. So (5.9) and (5.10) define a continuous map

$$\Psi^{(\delta)} : \partial\, \Xi^{(\delta)}_{\mathcal{C}_{\min}} \to \partial \widehat{M}_\Delta$$

The (continuous and surjective) blow-down $\beta : \widehat{M}_\Delta \to M$ maps $\widehat{M}_\Delta$ onto Δ, whereas it is the identity on $\widehat{M} = M \setminus \Delta$. It has the property

$$\beta \circ \Psi^{(\delta)} = \Phi^{(\delta)} . \tag{5.11}$$

(f) We finally prove that $\Psi^{(\delta)}$ is a homeomorphism.

- To show that it is a surjection, we use that the right hand side of (5.11) is a surjection. For the chains $\mathrm{ch} = \{\mathcal{D}_0, \mathcal{D}_1\}$ of length $k = 1$ the restriction of $\Psi^{(\delta)}$ to $\partial\, \Xi^{(\delta)}_{\mathcal{C}_{\min}} \cap S_{\mathrm{ch}}$ maps onto $\mathrm{int}(\beta^{-1}(\Xi_{\mathcal{D}_1})) \subseteq \partial \widehat{M}_\Delta$, since then the vector field on U_{ch} is ultimately radial, so that the t-dependent unit vector in (5.10) becomes constant. But the union of these interiors is dense in $\widehat{M}_\Delta$, which, together with the continuity of $\Psi^{(\delta)}$, shows that this map is onto.
- To prove injectivity of $\Psi^{(\delta)}$, by the Φ-invariance of the sets S_{ch} it suffices to consider points $q_1, q_2 \in \Psi^{(\delta)} \cap S_{\mathrm{ch}}$ and conclude that they coincide if their images coincide. Using (a) above, we can further assume that $v(q_i) = v_{\mathrm{ch}}(q_i)$. This property is then preserved by the forward flow. By the first bullet point in (b), we can also assume (by diminishing $\delta > 0$, if necessary) that their external $\mathcal{D}_k$ coordinates coincide. Now if $q_1 \neq q_2$, there is a largest $\ell \in \{1, \ldots, k\}$ such that $(q_1)^I_{\mathcal{D}_\ell} \neq (q_2)^I_{\mathcal{D}_\ell}$. The nontrivial rotation of the plane spanned by $(q_1)^I_{\mathcal{D}_\ell}$ and $(q_2)^I_{\mathcal{D}_\ell} \in \Delta^I_{\mathcal{D}_\ell}$ mapping the first to the second point maps the vector field v along the forward orbit $t \mapsto \Phi_t(q_1)$ onto the one of the forward orbit of q_2. Thus

$$N^{(\delta)}_{\mathcal{D}_\ell}(q_1) \neq N^{(\delta)}_{\mathcal{D}_\ell}(q_2),$$

since (by diminishing $\delta > 0$ again, if necessary), we can assume that $N^{(\delta)}_{\mathcal{D}_\ell}(q_i)$ is not perpendicular to $q^{(\delta)}_{\mathcal{D}_\ell}$.

- Although the continuous bijection $\Psi^{(\delta)}$ does not have a compact domain, its inverse is continuous, too. Namely the intersections of $\partial\,\Xi^{(\delta)}_{\mathcal{C}_{\min}}$ with closed balls in M of radius $r > 0$ are compact, and exhaust the domain as $r \to \infty$ As the restrictions of $\Psi^{(\delta)}$ are homeomorphisms onto their images (since $\widehat{M}_\Delta$ is Hausdorff), this shows that $\Psi^{(\delta)}$ itself is a homeomorphism. $\square$

5.4 Corollary
For $d = 1$ dimensions, $\partial\widehat{M}_\Delta$ is homeomorphic to $n!$ disjoint copies of $\mathbb{R}^{n-2}$.

Proof: This follows from Theorem 5.3, since for $d = 1$ the set Δ is a union of $\binom{n}{2}$ hyperplanes $\{q \in \mathbb{R}^{n-1} \mid q_i = q_j\}$ $(1 \le i < j \le n)$, so that $S^{n-2} \setminus \Delta$ is the disjoint union of $n!$ relatively open spherical simplices, given by the ordering of the coordinates $(q_1, \ldots, q_n)$. These are in turn homeomorphic to $\mathbb{R}^{n-2}$. $\square$

A Appendix: Manifolds with corners

We follow [AMN] and [Me] in our presentation. Manifolds with corners are modeled on the m–dimensional cylinders

$$\mathbb{R}^m_k := [0,\infty)^k \times \mathbb{R}^{m-k} \subseteq \mathbb{R}^m \qquad (k \le m \in \mathbb{N}_0).$$

Their subsets

$$L_I := \{x = (x_1, \ldots, x_m) \in \mathbb{R}^m_k \mid x_i = 0 \text{ if } i \in I\} \qquad (I \subseteq \{1, \ldots, m\}) \quad \text{(A.1)}$$

will be used to define submanifolds.

A.1 Definition *Let $U \subseteq \mathbb{R}^m_k$ and $V \subseteq \mathbb{R}^{m'}_{k'}$ be open, and $f : U \to V$.*

- *f is called* **smooth** *if for some open neighbourhood $\tilde{U} \subseteq \mathbb{R}^m$ of U there exists $\tilde{f} \in C^\infty(\tilde{U}, \mathbb{R}^{m'})$ with $\tilde{f}|_U = f$.*
- *f is called a* **diffeomorphism***, if it is a smooth bijection with f^{-1} smooth.*

A.2 Definition (manifolds with corners) *Let X be a Hausdorff space.*

- *An* **(m–dimensional) corner chart** *(U, ϕ) on X is a homeomorphism $\phi : U \to V$, with V open in $\mathbb{R}^m_k$.*
- *Corner charts (U_1, ϕ_1) and (U_2, ϕ_2) on X are* **compatible** *if for $U := U_1 \cap U_2$*

$$\phi_2 \circ \phi_1^{-1} : \phi_1(U) \to \phi_2(U)$$

is a diffeomorphism.

- *A* **(corner) atlas** $\{(U_i, \phi_i) \mid i \in I\}$ *on* X *is a family of pairwise compatible charts* (U_i, ϕ_i) *on* X *of equal dimension with* $\bigcup_{i \in I} U_i = X$.

- *Corner atlases on* X *are* **equivalent** *if their union is a corner atlas on* X. *A* **corner structure** *on* X *is an equivalence class of corner atlases of* X.

- *A paracompact Hausdorff space* X *with a corner structure consisting of* m*–dimensional corner charts is an* **(m–dimensional) manifold with corners**.

- *For* $\partial_\ell \mathbb{R}^m_k := \{x \in \mathbb{R}^m_k \mid$ *of* $x_1, \ldots, x_k,$ *exactly* ℓ *vanish*$\}$,

  $$\partial_\ell X := \{p \in X \mid \text{coordinates at } p \text{ map to } \partial_\ell \mathbb{R}^m_k\}$$

  and the **boundary** $\partial X := \partial^1 X$ **of** X *for* $\partial^\ell X := \overline{\partial_\ell X}$.

Unlike for manifolds with boundary, the Cartesian product of two manifolds with corners is naturally a manifold with corners.

A.3 Definition (submanifolds of manifolds with corners)

- *A subset* $S \subseteq X$ *of an* m*-dimensional manifold with corners is a* **weak submanifold** *if for every* $x \in S$ *there exist* $k \in \{1, \ldots, m\}$ *and a corner chart* $\phi : U \to \Omega \subseteq \mathbb{R}^m_k$ *with* $x \in U$ *such that* $\phi(S \cap U)$ *is a submanifold of* $\mathbb{R}^m$. *Then the* **dimension of** S **at** x *is* $\dim(\phi(S \cap U))$ *at* $\phi(x)$.

- *A weak submanifold* $S \subseteq X$ *is a* **submanifold** *(in the sense of manifolds with corners) if, additionally there are integers* $m' \leq m$ *and* $k' \leq m'$, *and a matrix* $G \in \mathrm{GL}(m, \mathbb{R})$ *such that*

  (a) $G \cdot \left(\mathbb{R}^{m'}_{k'} \times \{0\}\right) \subseteq \mathbb{R}^m_k$

  (b) The chart ϕ *maps* $S \cap U$ *bijectively to the intersection of this linear submanifold with* Ω, *in other words* $\phi(S \cap U) = G \cdot \left(\mathbb{R}^{m'}_{k'} \times \{0\}\right) \cap \Omega$.

- *A submanifold* $S \subseteq X$ *is a* p**–submanifold** *if for* $x \in X$ *there exists a corner chart* (U, ϕ) *at* x *and* $I \subseteq \{1, \ldots, m\}$ *with, see Definition* (A.1)

  $$\phi(S \cap U) = L_I \cap \phi(U).$$

  Then $|I|$ *is the* **codimension of** S **at** x *and* $|I \cap \{1, \ldots, k\}|$ *is the* **boundary depths of** S **at** x.

So a p-submanifold S of X is a closed submanifold that has a tubular neighborhood: $S \subseteq U \subseteq X$ that is locally of product form.

References

[Ai] Martin Aigner: Combinatorial Theory. Classics in Mathematics, Springer 1997

[AMN] Bernd Ammann, Jérémy Mougel, Victor Nistor: A comparison of the Georgescu and Vasy spaces associated to the n-body problems. Annales Henri Poincaré **23**, 1141–1203 (2022)

[De] Robert L. Devaney: Singularities in classical mechanical systems. In: Ergodic theory and dynamical systems I. Birkhäuser, Boston, MA, 1981

[DG] Jan Dereziński, Christian Gérard: Scattering Theory of Classical and Quantum N-Particle Systems. Texts and Monographs in Physics. Berlin: Springer 1997

[DMMY] Nathan Duignan, Richard Moeckel, Richard Montgomery, Guowei Yu: Chazy-type asymptotics and hyperbolic scattering for the n-body problem. Archive for Rational Mechanics and Analysis **238**, 255–297 (2020)

[ElB] Mohamed Sami ElBialy: Collision singularities in celestial mechanics. SIAM journal on mathematical analysis **21**, 1563–1593 (1990)

[FK] Stefan Fleischer, Andreas Knauf: Improbability of Collisions in n-Body Systems. Archive for Rational Mechanics and Analysis **234**, 1007-1039, (2019)

[FKM] Jacques Féjoz, Andreas Knauf, Richard Montgomery: Lagrangian Relations and Linear Point Billiards, Nonlinearity **30**, 1326–1355 (2017)

[Gr] Gian Michele Graf: Asymptotic completeness for N-body short range quantum systems: A new proof. Commun. Math. Phys. **132**, 73–101 (1990)

[He] Douglas Heggie: A global regularisation of the gravitational N-body problem. Celestial mechanics **10**, 217–241 (1974)

[Hi] Morris W. Hirsch: Differential Topology. Graduate Texts in Mathematics, Vol. 33. Berlin, Heidelberg, New York: Springer 1988

[KK] Andreas Knauf, Markus Krapf: The non-trapping degree of scattering. Nonlinearity **21**, 2023–2041 (2008)

[KM] Andreas Knauf, Richard Montgomery: Compactifying the three-body problem. [In preparation]

[Kn] Andreas Knauf: Mathematical Physics: Classical Mechanics. Springer, New York, 2018.

[LI] Ernesto A. Lacomba, Luis A. Ibort: Origin and infinity manifolds for mechanical systems with homogeneous potentials. Acta Applicandae Mathematica **11**, 259–284 (1988)

[LS] Ernesto A. Lacomba, Carles Simó: Boundary manifolds for energy surfaces in celestial mechanics. Celestial Mechanics **28**, 37–48 (1982)

[Le] Georges Lemaître: Regularization of the Three Body Problem. Vistas in Astronomy **1**, 207–215 (1955)

[LC] Tullio Levi-Civita: Sur la résolution qualitative du problème restreint. Acta Mathematica **30**, 305–327 (1906)

[MM] John N. Mather, Richard McGehee: Solutions of the collinear four body problem which become unbounded in finite time. Dyn. Syst., Theor. Appl., Battelle Seattle 1974 Renc., Lect. Notes Phys. **38**, 573–597 (1975)

[McG1] Richard McGehee: Triple collision in the collinear three-body problem. Invent. Math. **27**, 191–227 (1974)

[McG2] Richard McGehee: Double collisions for a classical particle system with nongravitational interactions. Commentarii Mathematici Helvetici **56**, 524–557 (1981)

[McG3] Richard McGehee: A stable manifold theorem for degenerate fixed points with applications to celestial mechanics. J. Differential Equations **14**, 70–88 (1973)

[Me] Richard Melrose: Differential analysis on manifolds with corners. Book in preparation (1996)

[MM] Richard Moeckel, Richard Montgomery: Symmetric Regularization, Reduction, and Blow-Up of the Planar Three-Body Problem. Pac. J. Math. **262**, 129–189 (2013)

[Mo] Jürgen Moser: Regularization of Kepler's problem and the averaging method on a manifold. CPAM **23**, 609–636 (1970)

[Ro] Clark Robinson: Homoclinic Orbits and Oscillations for the Planar Three-body Problem. J. Differential Equations **52**, 356–377 (1984)

[Va] András Vasy: Propagation of singularities in three-body scattering. Astérisque **262**, 157 p. (2000)

[Wald] Jörg Waldvogel: A new regularization of the problem of three bodies. Celestial Mechanics **6**, 221–231 (1972)

[Wa] Qiu-Dong Wang: The global solution of the n–body problem. Celestial Mechanics and Dynamical Astronomy **50**, 73–88 (1991)

[Wall] C.T.C. Wall: Differential Topology, Cambridge studies in advanced mathematics, Cambridge University Press, 2016