The chaotic set and the cross section for chaotic scattering in three degrees of freedom

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\textit{New Journal of Physics} \textbf{12} (2010) 103021 (31pp)
Received 9 April 2010
Published 14 October 2010
Online at http://www.njp.org/
doi:10.1088/1367-2630/12/10/103021

Abstract. This article treats chaotic scattering with three degrees of freedom, where one of them is open and the other two are closed, as a first step towards a more general understanding of chaotic scattering in higher dimensions. Despite the strong restrictions, it breaks the essential simplicity implicit in any two-dimensional time-independent scattering problem. Introducing the third degree of freedom by breaking a continuous symmetry, we first explore the topological structure of the homoclinic/heteroclinic tangle and the structures in the scattering functions. Then we work out the implications of these structures for the doubly differential cross section. The most prominent structures in the cross section are rainbow singularities. They form a fractal pattern that reflects the fractal structure of the chaotic invariant set. This allows us to determine structures in the cross section from the invariant set and, conversely, to obtain information about the topology of the invariant set from the cross section. The latter is a contribution to the inverse scattering problem for chaotic systems.

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1. Introduction

Chaotic scattering with two degrees of freedom is fairly well understood [1]–[6], both for hard chaos (hyperbolicity) and for soft chaos in terms of Smale’s horseshoe construct [7, 8]. In a time-independent Hamiltonian system with two degrees of freedom, Smale’s horseshoe displays the invariant manifolds that qualitatively separate the dynamics. On an appropriate surface of section, these invariant sets become smooth curves. This has two advantages: (i) we can study objects easily if they can be drawn on paper and (ii) they separate the phase space dynamics if they close or go to infinity in both directions.

Scattering functions [8]–[10] and cross sections [11, 12] have been analysed both statistically and geometrically, and the inverse scattering problem has been tackled [9, 13] (for general background information, see the textbooks [14]–[16]).

Now the effort must be directed towards higher-dimensional systems, as they are relevant in astrophysics [17, 18] or chemistry [19]–[21]. How do we proceed to generalize this success in description of chaotic scattering to more than two degrees of freedom? There are some previous important steps, particularly by Wiggins and coworkers [22]–[24], but also by Ott and coworkers [25]. The former develops a formal theory that is difficult to apply but gives important foundations of the problem. The latter show that a straightforward generalization of the three-disc system in triangular configuration to a four-sphere problem in tetrahedral configuration is feasible, but the invariant manifolds are low dimensional and thus not relevant to some physical problems, as they are difficult to detect. We have suggested in an earlier paper that it can be useful to have a gradual approach to a change in dimension by breaking a continuous symmetry of the problem [26].

In this paper, we shall follow this last suggestion and apply it to the simplest possible three degrees of freedom configuration, with two bound and only one open degree of freedom. Despite this strong restriction, we are now definitely beyond the situation where Smale’s theory can be used, and systems of that kind are not without interest. We might consider guiding channels with one open degree of freedom, or we can consider equivalently three interacting particles in one dimension, under conditions where asymptotically one pair must always be bound.

We shall focus on the topological structure of the invariant set rather than on details of trajectories, because the former properties tend to be generic, i.e. robust and embody the most relevant information about the chaotic system [13]. We are thus looking for some generalization of the horseshoe to higher dimensions. A simple generalization does not exist, as can be
seen from the work of Wiggins [23]. The basic reason is that the dimension of the invariants manifolds of hyperbolic points is very low.

We proceed by analysing the transition from a system which has an $O(2)$ symmetry group in the three-dimensional (3D) position space, reducing the problem for a fixed value of the angular momentum to a system with two degrees of freedom. We shall then introduce in the reaction region (i.e. in the region where the asymptotic Hamiltonian is not valid) a symmetry breaking term. This will allow us to start our analysis with a continuous stack of horseshoes corresponding to different values of the angular momentum and observe how the structure evolves as the invariance breaks down. We then study the implications for scattering functions and for the doubly differential cross sections. The fractal structure of singularities in the latter, i.e. the rainbow structures, is directly related to the structure of the chaotic set, leading to an additional important contribution to the corresponding inverse scattering problem. Indeed we shall also see that the basic idea developed is not limited to three degrees of freedom, nor to one open degree of freedom, but only these aspects will be commented on.

We shall illustrate our procedures with three examples. The first is a channel with harmonic walls in two directions that deforms to some more complicated potential in some compact region of configuration space. This is equivalent to two pairs of particles bound by harmonic forces and interacting with each other weakly. The second example is a bottle-shaped billiard that either is connected to a channel billiard or has an opening that separates the interior from the exterior in some plane in configuration space. Finally, for numerical convenience, we shall use a $\delta$ kicked system of two degrees of freedom, which is topologically equivalent to the Poincaré maps of the first system.

As far as the physical implications are concerned, it does not seem easy to emulate systems with such restrictions and no significant friction, although it might become feasible with Bose–Einstein condensates at some point in the future. The alternatives in celestial mechanics imply higher dimensions and/or more complicated asymptotes, as is the case with the breaking of the Jacobi invariant in [26]. Yet the results are certainly useful for semi-classical considerations, such as e.g. the ones used in [27] to design and interpret a microwave experiment.

The paper is structured as follows. In section 2, we shall define the class of three degree of freedom systems, which we shall consider as well as the specific examples we shall use. Next we proceed to construct the invariant sets and study them as a function of the symmetry breaking. In section 4, we derive the scattering functions, that is, the behaviour of outgoing asymptotes as a function of the incoming ones. This will allow us to discuss the rainbow effects in the doubly differential cross sections in section 5. We finally proceed to comment on the scope of our results as well as implications for semi-classics.

2. The class of systems considered and the model systems

We consider a scattering system with three degrees of freedom where one of them is open and the other two are closed. We imagine that the first degree of freedom is a translational degree of freedom between the projectile and the target, the second degree of freedom is a vibrational degree of freedom and the third one is a rotational degree of freedom.

The first particular model system of this class that we use is a rotationally symmetric channel containing an additional short-range potential representing some obstacle (the target)
sitting in the otherwise empty channel. Accordingly the total Hamiltonian of the system splits, as always in scattering systems, into a free Hamiltonian $H_0$ describing the asymptotic free motion (in this particular case it is the motion in the empty channel) and an additional interaction $W$, which is the short-range scattering potential, i.e.

$$H = H_0 + W.$$  \hspace{1cm} (1)

We imagine that the channel runs straight in one direction and we use the coordinate $q$ along the channel, and $p$ is the momentum conjugate to $q$. In the transverse direction, the motion of the projectile is confined by the channel and we assume that the potential that represents the walls of the channel is quadratic in the transverse coordinates. Because of the rotational symmetry of the empty channel, one natural choice is to use cylindrical coordinates $\rho$ and $\theta$ and their conjugate momenta $p_\rho$ and $L$, and also to include in the free Hamiltonian the quadratic potential and the transverse kinetic energy in these coordinates. Since the radial motion is an oscillation, it is sometimes more convenient to use action and angle variables $I$ and $\phi$ for the radial degree of freedom. We will switch freely between these two possibilities according to which one is more convenient at the moment. The asymptotic Hamiltonian written in cylindrical position and momentum coordinates is

$$H_0 = p^2/2 + p_\rho^2/2 + L^2/(2\rho^2) + \rho^2/2.$$  \hspace{1cm} (2)

We choose units of time such that the transverse oscillation frequency in the empty channel is one. To describe the obstacle, we use later as a model of demonstration the potential

$$W = -\frac{\exp(-D)}{D},$$  \hspace{1cm} (3)

where

$$D^2 = q^2 + \rho^2(\sin^2 \theta + (1 + A)^2 \cos^2 \theta) + 1.$$  \hspace{1cm} (4)

The extra constant, taken as one, avoids singularities in the potential. Very important for the following is the parameter $A$ that measures the deviation of the interaction potential from rotational symmetry. For $A = 0$, we have perfect symmetry and, since the free Hamiltonian $H_0$ is also symmetric, the total system is symmetric, the angular momentum $L$ is conserved and the system can be reduced to two degrees of freedom. For the value $L = 0$, the symmetric system reduces to the one used in [11]. This reference also contains a physical interpretation of similar potential models.

Next we need labels for the asymptotes of the system, i.e. the trajectories of the free motion described by $H_0$. The optimal possibility is to use five independent quantities that are all constant along the asymptotic trajectories. Since in any Hamiltonian system the energy $E$ is conserved, both under the free asymptotic dynamics and under the full dynamics, we use $E$ as one of these labels. Asymptotically the translational degree of freedom decouples from the other ones and the momentum $p$ becomes constant. We use $p$ as the second asymptotic variable. The sign of $p$ indicates in which direction the asymptotic motion runs, and therefore a comparison between the signs of initial and final $p$ distinguishes transmission and reflection. In addition, since $H_0$ is independent of $\theta$, the conjugate variable $L$ is conserved under the asymptotic dynamics and it is convenient to use it as the third label for asymptotic trajectories. To distinguish the various asymptotic trajectories with the same values of $E$, $p$ and $L$, we need two additional labels giving the relative phase shifts between the translational motion along the channel and the other two
motions. The systematic choice for these relative angles is the reduced phases constructed along the following idea. In action variables, we find for our particular system,

\[ H_0(p, I, L) = \frac{p^2}{2} + 2I + |L|. \]  

(5)

Then the asymptotic equations of motion for \( \phi \) and \( \theta \) are

\[ \frac{d\phi}{dt} = \frac{\partial H_0}{\partial I} = \omega_\phi(I, L) = 2, \]  

(6)

\[ \frac{d\theta}{dt} = \frac{\partial H_0}{\partial L} = \omega_\theta(I, L) = \pm 1. \]  

(7)

The sign appearing in equation (7) is the sign of the angular momentum. We define the reduced angles \( \psi \) and \( \chi \) belonging to \( \theta \) and \( \phi \), respectively, as

\[ \psi = \theta - \omega_\theta(I, L)q/p = \theta \mp q/p, \]  

(8)

\[ \chi = \phi - \omega_\phi(I, L)q/p = \phi - 2q/p. \]  

(9)

The sign in equation (8) is minus the sign of the angular momentum. A short calculation shows that these two reduced angles are constant under the asymptotic dynamics.

An equivalent possibility is the following. We use the values of the two coordinates \( \phi \) and \( \theta \) at the moment when the absolute value of \( q \) reaches some very large value (in the numerical examples, we use \( \|q\| = 8 \)). We call these two particular values, which serve as asymptotic labels, \( \chi \) and \( \psi \) again. We use the index ‘in’ for initial asymptotic conditions and the index ‘out’ for the labels of outgoing asymptotes.

Because it is simpler to handle iterated maps instead of flows, we will use Poincaré maps to represent the dynamics of the system and to explain many ideas (an elementary explanation of the concept of Poincaré maps is found in section 2.5 of [28]). For the channel problem, an appropriate intersection condition for the Poincaré map is to take the maximum of the cylindrical radial coordinate \( \rho \). This choice has the advantage of coinciding with the choice made for a billiard model, which we also use later. Almost all trajectories intersect this surface transversely an infinite number of times and asymptotically the return time to this surface becomes constant; note the constant value of \( \omega_\phi(I, L) = 2 \) in equation (6). The only exceptions are trajectories with action \( I = 0 \), which run along spirals of constant value of \( \rho \) without any radial oscillations.

In the domain of the map, we use the canonical coordinates \( q, p, \theta \) and \( L \).

An alternative version of the reduced angles \( \psi \) and \( \chi \) for the map is obtained as follows. For trajectories with the value \( p \) of the asymptotic longitudinal momentum select an interval of large absolute values of \( |q| \), say the interval \([Q, Q + |p|]\) where \( Q \) is sufficiently large to guarantee that the trajectory is already in the asymptotic region. Observe the trajectory of the map until it steps into this interval. For this point, define \( \chi = 2\pi(|q| - Q)/|p| \), and for \( \psi \), take the actual value of \( \theta \) in this point. Note that the initial point and the final point of the selected \( q \) interval can be identified for the purpose of asymptotic labelling since they describe the same trajectory (one is the image of the other point under the action of the map) and lead to the same value of the angle \( \chi \), since multiples of \( 2\pi \) are irrelevant. Therefore, this line of initial conditions has the topology of a circle. An analogous construction also works well for the Poincaré maps of other model systems.

The second model of demonstration used is a billiard model, which describes the scattering in a bottle. The boundary of the bottle will be defined with the aid of the following
functions,
\[
f(q) = \begin{cases} 
1.4\sqrt{1-q^2} & \text{for } q \leq 0, \\
 a_0q^{2.5} + a_1q^2 + 1.4 & \text{otherwise},
\end{cases}
\] (10)

\[
r(q, \theta) = 1 + A \cos(\theta) \cos\left(\frac{q\pi}{2q_0}\right)^2.
\] (11)

The boundary itself is given by
\[
\rho(q, \theta) = r(q, \theta)f(q).
\] (12)

Two-dimensional billiards with the border described by function (10) have been studied in [29] and a similar model in [30].

The values of the constants \(a_i\) are chosen to give a smooth boundary and to lead to an unstable quasi-periodic orbit in the plane \(q = 0\) so that there is a complete binary horseshoe for the reduced rotationally symmetric case for \(L = 0\). Convenient values turn out to be
\[
a_0 = \frac{14}{25}(3.49)^{-1/4},
\] (13)
\[
a_1 = -0.7,
\] (14)
\[
q_0 = (3.49)^{1/2}.
\] (15)

Also, this model has a parameter \(A\), which gives the distance from rotational symmetry, and again for \(A = 0\) we have perfect symmetry and the system can be reduced to one with two degrees of freedom.

The billiard dynamics are the usual ones with elastic reflection on the wall and free motion on the inside. The energy is a constant and proportional to the square of the momentum. Therefore, we can set the velocity \(\|v\| = 1\) without loss of generality. The Poincaré map of the bottle model is the usual Birkhoff map on the wall of the billiard (these are explained in [31]). We only use weak deformations of the bottle such that this map coincides with the intersection condition of maximal cylinder radius \(\rho\). Accordingly, we use in the domain of the map the same coordinates \(q, \theta\) and \(L\) as in the channel model.

The Birkhoff–Poincaré map of this system has a binary horseshoe instead of the ternary one of the other two examples, and it has a surface of no return at a finite value of \(q\), which makes it qualitatively different. Nevertheless, we will see that it belongs to the same class of systems.

Since it is a lot more convenient and faster to investigate maps instead of flows, we construct as the third model a closed form example of a map acting on the 4D domain with coordinates \(q, p, \theta\) and \(L\). This model is constructed in a way that it can serve as a prototype Poincaré map for the whole class of systems considered in this article. It is based on the usual scheme of kick and free flight. The generating function for the kick is
\[
G(q, \theta, \tilde{p}, \tilde{L}) = q\tilde{p} + \theta\tilde{L} + (L_{\text{max}} - \tilde{L})(1 + A \cos \theta)V(q),
\] (16)

with potential function
\[
V(q) = -e^{-q^2}.
\] (17)

We define the force function on the \(q\) coordinate as
\[
F(q) = -\frac{dV}{dq} = -2qe^{-q^2}.
\] (18)
And the kick map is implicitly given by
\begin{align}
\tilde{q} &= \frac{\partial G}{\partial \tilde{p}} \quad p = \frac{\partial G}{\partial q}, \\
\tilde{\theta} &= \frac{\partial G}{\partial \tilde{L}} \quad L = \frac{\partial G}{\partial \theta}.
\end{align}

To construct a complete step of the map, the particles will perform the first half of the free flight,
\begin{align}
q' &= q_n + p_n / 2, \\
\theta' &= \theta_n + L_n / 2, \\
p' &= p_n, \\
L' &= L_n.
\end{align}

Afterwards, we give this auxiliary coordinates the kick, given explicitly by the next set of equations,
\begin{align}
q'' &= q', \\
\theta'' &= \theta' - (1 + A \cos \theta') V(q'), \\
p'' &= p' + (L_{\text{max}} - L') \frac{(1 + A \cos \theta') F(q')}{1 + A V(q') \sin \theta'}, \\
L'' &= \frac{L' + L_{\text{max}} A V(q') \sin \theta'}{A V(q) \sin \theta' + 1}.
\end{align}

And finally, half a free flight is applied again,
\begin{align}
q_{n+1} &= q'' + p'' / 2, \\
\theta_{n+1} &= \theta'' + L'' / 2, \\
p_{n+1} &= p'', \\
L_{n+1} &= L''.
\end{align}

This concludes the action of the map. Every step is symplectic, and the map behaves qualitatively as the Poincaré map of the first example.

We use mainly the map model for the presentation and explanation of our ideas. Below, we compare some results of this map with the results of the other two models in order to convince ourselves that the map results are representative.

3. The topological structure of the chaotic invariant set

Since the interaction potential of equation (3) or of equation (17) is negative, there are trajectories with negative energy yet arbitrarily close to zero, going out extremely far and returning. Therefore our first example system has no points without return. Its outermost
periodic orbits lie at $q = \pm \infty$. They are trajectories oscillating transverse to the channel and rotating at constant value of $q$, where $q$ is arbitrarily far away. Because any displacement of $q$ leads to an equivalent transverse oscillation, these transverse trajectories come in a whole continuum of copies. In the Poincaré map, they lead to fixed points at $q = \pm \infty$, $p = 0$ and these points are parabolic, i.e. neutrally stable in linear approximation. However, the nonlinearities of the map at finite values of $q$ make these points nonlinearly unstable, and they have stable and unstable invariant manifolds. The stable manifolds consist of trajectories that go out to infinity monotonically, i.e. the absolute value of $q$ increases monotonically while at the same time the value of the momentum $p$ converges to zero. Asymptotically, all energy of the motion goes to the transverse motion. The unstable manifolds consist of trajectories doing the same under the time reversed motion. In this sense, the trajectories belonging to the invariant manifolds of the points at infinity converge to the periodic trajectories described above. In the domain of the map, these manifolds are the separatrix lines between motion going monotonically away and motion that returns.

The map model described as the third example of demonstration in the previous section is in this respect similar to the channel. It also does not have values of $q$ of no return.

In contrast, the bottle model has a surface of no return, the surface of the bottle neck. The trajectories lying on this surface forever serve as the outermost fixed points in the Poincaré map. The set of trajectories staying in the plane of the bottle neck, and also the trajectories with $p = 0$ in the asymptotic region of the channel, form an example of what Wiggins [23] calls a normally hyperbolic invariant manifold, abbreviated NHIM. Let us explain this set first for the case of the bottle, since in this case we have an NHIM in its original form.

For fixed energy, all the orbits that stay forever in the plane of the bottle neck form a 2D continuum. Firstly, there are such orbits for all possible values of the angular momentum and, secondly, for each such orbit there also exist corresponding orbits rotated by an arbitrary angle. These trajectories are neutrally stable under perturbations of initial conditions that keep them in the bottle neck plane. In the domain of the Poincaré map, all of these trajectories form a 2D surface, which is the NHIM in the domain of the map. In the direction perpendicular to the bottle neck, all of these trajectories are unstable and they have stable and unstable manifolds. The union of these invariant manifolds taken over the whole 2D continuum of bottle neck trajectories form the stable and unstable manifolds of the NHIM that we will call $W^s$ and $W^u$. They are 3D surfaces in the 4D domain of the map. Therefore these surfaces are dividing surfaces; they divide trajectories that pass the bottle neck from trajectories that return. For more details and consequences for scattering see [22], or for applications see [24].

In the example of the channel, we have a slightly modified version of an NHIM. Trajectories in the empty channel or in the asymptotic region of the channel having $p = 0$ stay forever in the plane of a fixed value of $q$; they are trajectories in the 2D oscillator potential forming the empty channel. In a harmonic oscillator, all trajectories are periodic; they are ellipses. The ones for a fixed value of the total energy are a 2D continuum where each individual trajectory can be distinguished by its value of the angular momentum and by the orientation of the ellipse. Again, such trajectories are neutrally stable under perturbations that keep the value $p = 0$. The difference between the channel and the bottle example is that in the channel case the trajectories that form the NHIM are also neutrally stable in the $q$ direction, at least in linear approximation. If we include the nonlinearities caused by the asymptotic tail of the attractive scattering potential, they become unstable and have stable and unstable manifolds. The union of these invariant manifolds forms again the invariant manifolds of the whole NHIM. They are
dividing surfaces that separate trajectories going out monotonically from returning trajectories. In this respect, the map model behaves like the Poincaré map of the channel model.

To investigate the chaotic set of the models, we start with the case of $A = 0$ and later on break the symmetry. For $A = 0$ the $\theta$ dependence of the dynamics decouples from the rest of the dynamics, $L$ becomes a conserved quantity and the map reduces to a 2D map in the coordinates $q$ and $p$, where $L$ serves as a parameter. Because of its importance in what follows, we show this reduced map in explicit form for the map model with the potential function from equation (17),

$$q_{n+1} = q_n + p_n - (q_n + p_n/2) \exp(-(q_n + p_n/2)^2)(L_{\text{max}} - L),$$  

(33)

$$p_{n+1} = p_n - 2(q_n + p_n/2) \exp(-(q_n + p_n/2)^2)(L_{\text{max}} - L).$$  

(34)

The $L$ value determines the strength of the force of the kick, becoming negligible for $L \approx L_{\text{max}}$. This corresponds to all energy spent on rotational motion, and almost no development for the horseshoe, as can be seen on the sequence of plots of the homoclinic tangle for this reduced map in figure 1.

To construct the horseshoe, we plot the stable manifold and the unstable manifold of both the fixed point at $+\infty$ and of the one at $-\infty$. To plot the whole interval $q \in [-\infty, +\infty]$ on a finite range, we use the horizontal coordinate $z = \tanh(q)$, which is convenient to get informative plots (figure 2). The intersection points between a stable and an unstable manifold are trajectories that converge forward in time and also backward in time to a fixed point of the map. An intersection between the manifolds of the same fixed point is called the homoclinic point, and an intersection between the manifolds of different fixed points is called the heteroclinic point. The whole structure of the manifolds is called homoclinic/heteroclinic tangle; many times only the expression ‘homoclinic tangle’ or simply ‘tangle’ is used for short, even when it also contains heteroclinic points. The existence of a homoclinic tangle is the topological criterion for chaos in the system. It implies the existence of an uncountable set of unstable trajectories. For more details of the role of homoclinic tangles and the importance for scattering and transport problems, see the book by Wiggins [23].

Because of symmetry in our example, the manifolds of point $-\infty$ are obtained from the ones of the point at $+\infty$ by inversion about the origin. The time-reversal symmetry in the maps also permits one to obtain the stable manifolds from the unstable ones by the reflection $p \rightarrow -p$. From these symmetry properties also follows the existence of a trajectory oscillating transverse to the channel at $q = 0$. It leads to a fixed point of the map at $q = 0$ and $p = 0$. We call this fixed point the inner fixed point. In total, the map has three fixed points where the outer two are symmetry related and therefore we call the resulting homoclinic structure a ternary symmetric horseshoe.

When changing $L$, we have the usual development scenario starting from a complete horseshoe for $L = 0$ up to a parabolic line when $L$ reaches its maximal limiting value $L_{\text{max}}$ allowed by total energy. In our particular example, we have

$$L_{\text{max}} = 6.23.$$  

(35)

Next we define the fundamental area $R$ for the horseshoe. Let us start with the local branches of the manifolds of the two outer fixed points and let them grow longer continuously in a completely symmetric pattern. Then at some length we obtain the first intersection points; for
Figure 1. The Poincaré maps for the discrete dynamical system in the axial symmetric case ($A = 0$). The $L$ parameter regulates the degree of development of the horseshoe. Note also the reduction of the phase space occupied by the horseshoe as $L$ increases. The line $C$ on (a) is chosen so that its preimage is an adequate domain for scattering functions.
Figure 2. The same as figure 1, but after compactifying the \( q \)-axis using the function \( \text{arctan}(q) \).
symmetry reasons they are located at $q = 0$. At this moment, let us stop the process of growth. The result is a curvilinear quadrilateral, which we call the fundamental rectangle $R$.

The intersection pattern between some local segment of an unstable manifold (e.g. the piece between an outer fixed point and the next corner of $R$) and the whole fractal bundle of stable manifolds already contains complete information of the whole tangle formed by the manifolds of the outer fixed points, and the knowledge of such local intersection patterns is sufficient. We will make use of this idea for the reconstruction of important properties of the tangle from scattering data. The use of these for determining the development of the horseshoe is thoroughly explained in [13].

In figure 1(a), we included an additional thick line labelled C that runs parallel to one of the local segments of unstable manifolds but just outside $R$. Note that the intersection pattern between C and the bundle of segments of the stable manifolds coincides exactly with the intersection pattern between the local segment of the unstable manifold and the bundle of segments of stable manifolds. Accordingly, also the intersection pattern along the line C contains all the important information about the whole tangle. The iterated preimages of line C play an important role in the following as asymptotic initial conditions for scattering trajectories.

Now we will discuss the chaotic structure of the three degrees of freedom system. We begin with $A = 0$. Then the surfaces of the various values of $L$ are dynamically independent and we obtain a fractal structure in the full dimensional domain of the map with its coordinates $q$, $p$, $L$ and $\theta$ in a two-step process. Firstly, we pile up the tangles for the various values of $L$, obtaining a fractal tangle in a 3D embedding space and, secondly, we form the Cartesian product of this object with a circle representing the fourth coordinate $\theta$. Accordingly, also the value of $L$ orders the pile of 2D horseshoes naturally from the complete case, with $L$ near zero, to the integrable system, with $L$ near $L_{\text{max}}$. When we view this family of systems as just one geometrical object, the family of invariant manifolds form smooth 2D surfaces in the 3D embedding space with the coordinates $q$, $p$ and $L$. For brevity, we call this structure the 3D tangle. Now let us restrict our attention to intersections between the unstable and stable manifolds. The basic pattern is a transverse intersection between 2 2D surfaces in a 3D embedding space, as shown schematically in figure 3. A point of interest is that the tangential intersections of the lower-dimensional horseshoe become extremal points in the $L$ direction of the intersection curve shown in figure 3. The whole curve belongs to the ‘hyperbolic component’ of the invariant set.

So far we have ignored the $\theta$ coordinate. To include it for the symmetric case of $A = 0$, we simply form the Cartesian product of the structures described above with a circle representing this cyclic coordinate. Thereby the manifolds become 3D surfaces in the 4D embedding space. The elementary transverse intersection structures between the surfaces $W^u$ and $W^s$ are smooth 2D surfaces. Each one of their points has 1D unstable and stable directions and two neutral directions. Because the manifolds themselves are folded to fractal structures, we obtain a fractal
Figure 3. A plot of the intersection of stable and unstable manifolds in the \((p, q, L)\) space when \(A = 0\). The \(L\) value gives the degree of development of the horseshoe for every \((q, p)\) plane. After stacking these in order, we obtain two intersecting two-dimensional manifolds. In the end, we consider a direct product with a circle for the \(\theta\) coordinate.

repetition of the elementary intersection structures, which we call the tangle in the 4D domain of the Poincaré map. The dimension of this tangle can be anything between two and four, depending on how exactly the manifolds turn and fold. For an argument we present later, remember that this dimension is larger than two.

Finally, we consider the changes implied by a moderate breaking of the rotational symmetry. To understand this, let us return to figure 3 and imagine its product with a circle. Then we see the transverse intersection of 2 3D surfaces in a 4D embedding space. Because the intersection is transverse, it is structurally stable. This means that, under small deformation, the intersection pattern remains qualitatively the same. This argument applies to all the transverse homoclinic intersections appearing in the development scenario of the horseshoe. However, it does not apply to the non-hyperbolic structures near the surface of KAM islands.

Hence, when the parameter \(A\) is slightly different from zero, we can understand that relevant qualitative properties of this structure remain unchanged. The structure of the whole 4D tangle is therefore robust. This stability, together with the transversality of the intersection, is inherited from the leaves of the symmetric system in a way that is only possible for systems that can be connected continuously to the symmetric systems and that are not far from the symmetric case. This may appear restrictive at first, but even so we can cover a broad range of physically relevant problems.

4. Scattering functions

Scattering functions are interesting objects in their own right and we need them as auxiliary concepts to explain and motivate the ideas on the singularities in the cross sections, which are more accessible to experiments.

A scattering function gives one of the outgoing asymptotic labels, or several of them, as a function of initial asymptotic conditions. It is advantageous to study outgoing actions like variables as a function of initial angular variables; this is exactly the version of the scattering functions we need to understand the properties of the cross sections. As explained before, every asymptotic trajectory in the Poincaré map can be labelled as \(p, L, \psi\) and \(\chi\). It is always understood that the total energy \(E\) is kept fixed at one particular value.
The scattering function that we will now describe in detail gives the outgoing momentum $p_{\text{out}}$ and the angular momentum transfer $\Delta L = L_{\text{out}} - L_{\text{in}}$ as a function of $\chi_{\text{in}}$ and $\psi_{\text{in}}$ for fixed values of $p_{\text{in}}$, $L_{\text{in}}$ and $E$. The domain of this function is the 2D torus with the coordinates $\chi_{\text{in}}$ and $\psi_{\text{in}}$. The periodicity of the function follows thereby.

First let us study the symmetric case $A = 0$ and show some numerical examples for the model map. In this case, the angle $\psi$ is irrelevant and, because of angular momentum conservation, the function $\Delta L$ is identically zero. Then the domain of the scattering function is an interval of length $2\pi$ in the angle $\chi_{\text{in}}$, and this interval is represented by the line $C$ in figure 1(a). Remember that $C$ is the iterated image of an asymptotic line of fixed $p$ where $q$ changes over an interval of length $p$, which corresponds to an interval of $\chi_{\text{in}}$ of length $2\pi$.

As a consequence, the scattering function has singularities on a fractal set and intervals of continuity in between. The singularities correspond to the intersection of the line of initial conditions with stable manifolds. Since preimages of intersections with invariant manifolds are again intersections with the same manifolds, the intersection pattern of this line of initial conditions coincides with the fractal pattern of intersections of the line $C$ with the stable manifolds of the horseshoe. If the asymptotic part of the trajectory starts on a stable manifold of the horseshoe, and the actual scattering trajectory converges to a periodic orbit and does not come out of the interaction region with a longitudinal kinetic energy larger than zero, then the outgoing asymptotic conditions are ill-defined, and therefore the scattering function has a singularity. The pattern of singularities is the pattern of intersections of the line $C$ with stable manifolds and is a smooth image of the fractal pattern in the tangle. In this way, asymptotically obtained scattering functions carry information on the topological structure of the tangle sitting in the interaction region [13].

We have to ensure that the line of initial conditions maps to a line equivalent to the line $C$ in the horseshoe plots and not to a line intersecting the outer tendril further out, where it does not scan the whole structure. As the line $C$ moves further away from $R$, we lose more and more intersection points in the line, until it is so far out that it no longer intersects the bundle of stable manifolds. Here it is essential to use a value of $p_{\text{in}}$ sufficiently small. The actual line used for the numerical examples of the scattering functions and cross section data will be the 312th preimage of the line $C$ shown in the figure, which is sufficiently far out to be considered asymptotic. This line is given by

$$T^{-312}C = \{(q, p) \mid q \in [-6.962, -6.912], p_{\text{in}} = 0.05\},$$

where $T$ is the Poincaré map. If the line of initial conditions intersects the fractal structure only partially, then it still would contain the complete information because of the self-similarity of the fractal structure. However, then the reconstruction would pose some additional technical problems, which we want to avoid. Typical structures for the scattering functions on a 1D domain are presented in figures 4 and 5.

In a given plot of a scattering function, we recognize intersections with the stable manifolds as initial conditions that lead to $p_{\text{out}} = 0$. They represent boundaries between transmission ($p_{\text{out}} > 0$) and reflection ($p_{\text{out}} < 0$).

In preparation for the asymmetric case, we have to include the role of the coordinate $\psi$. For $A = 0$, the fractal of singularities in the 2D domain of the scattering function is the Cartesian product of a 1D fractal along the $\chi$ direction described above with a circle in the $\psi$ direction. The intervals of continuity have the structure of strips that run in the $\psi$ direction around the domain. The natural domain of the higher-dimensional scattering functions is the product of the
Figure 4. The $p_{\text{out}}$ scattering function for $A = 0$ (axial symmetric case). The independent variable is $q_{\text{in}}$, the entrance phase.
Figure 5. An illustration of the self-similarity of the scattering function $p_{\text{out}}$ with parameter $L_{\text{in}} = 0.00$. This case has a complete horseshoe, so the function reveals the structure of a Cantor set in the singular values.
preimage of the line \( C \) described above with the circle of \( \psi \) values. It is a 2D torus if we recall that the initial and final points of the line \( C \) should be identified.

Let us break the rotational symmetry and recall the robustness mentioned at the end of the previous section. For \( A \), small the important intervals of continuity still have the same qualitative structure, they are only deformed continuously. Only the non-hyperbolic dust around KAM islands is changed immediately for \( A \neq 0 \). In this sense, the qualitative structure of the fractal of singularities is still close to a product of a 1D fractal with a circle.

With increasing value of \( A \), intervals of increasing size and lower level in the fractal hierarchy are changed qualitatively insofar as they are disrupted into fragments that no longer have the structure of stripes winding around the domain in the \( \psi \) direction. Only for \( A \approx 0.5 \) are the last large intervals of continuity destroyed. Thereby the last remnants of the product structure of the fractal are lost and the fractal is transformed into a truly higher dimensional fractal. In this paper, we shall not investigate this new structure but restrict our consideration to smaller values of \( A \).

So far we have seen that all topological information on the chaotic tangle is contained in asymptotic scattering data and that a measurement of scattering functions and their analysis is one way for the asymptotic observer to obtain this information. The scattering functions present a kind of shadow image of the chaotic invariant set cast into the outgoing asymptotic region. However, the measurement of scattering functions is difficult or impossible in many real scattering experiments and therefore we now have to go one step further to cross sections that are the quantity measured in most of the traditional scattering experiments.

5. The cross section

The measurement of scattering functions needs control over the canonically conjugate variables \( p, L \) and \( \chi, \psi \). In classical mechanics, this could be done in principle. However, it is not done in the usual scattering experiment. More important, in quantum mechanics this preparation is forbidden even in principle, and if we want to develop concepts and ideas that have some chance to be transferred to quantum dynamics, we cannot use quantities needing the simultaneous preparation of canonically conjugate variables. What is done in most scattering experiment is the following: one half of the phase space variables (normally the actions) is prepared as sharp as possible and the other conjugate half (the conjugate angles) is completely unspecified. In our case this means that for fixed total energy \( E \) we prepare \( p_\text{in} \) and \( L_\text{in} \) to specific values and do not have any control over the reduced angles \( \chi_\text{in} \) and \( \psi_\text{in} \). Their values have a distribution with constant density over the whole domain, \( \mathbb{T}^2 \). The detector measures the final values \( p_\text{out} \) and \( L_\text{out} \) for each outgoing particle and we monitor the relative probability \( \sigma(p_\text{out}, \Delta L) \) to find a given combination of values of \( p_\text{out} \) and \( \Delta L \), normalized by the incoming flux. This relative probability is called the doubly differential cross section. For more general information on cross sections, see some textbooks on scattering theory such as [32] or [33]; for an application, consult [12].

In the previous section, we have seen that the scattering function with values \( p_\text{out}(\chi_\text{in}, \psi_\text{in}), \Delta L(\chi_\text{in}, \psi_\text{in}) \) contains the fractal structure of the horseshoe. If we can measure this function directly, then we have the necessary data to reconstruct the pattern of the horseshoe and our version of the inverse problem is solved [13]. If we can only measure cross sections, we must find out how the fractal pattern of the scattering function is transferred to some recognizable pattern in the cross section.
In the beam of incoming projectiles, the weight on the $\chi_{\text{in}}, \psi_{\text{in}}$ torus is constant and the scattering function maps this initial weight on some interval in the range of this function having the coordinates $p_{\text{out}}$ and $\Delta L$, and the image weight is exactly the cross section $\sigma(p_{\text{out}}, \Delta L)$. Therefore, to obtain the value of $\sigma$ for a particular combination of the values of $p_{\text{out}}$ and $\Delta L$, we first search for all preimages $\chi_k, \psi_k$ of the image point. Each preimage gives the contribution

$$g_k(p_{\text{out}}, \Delta L) = \frac{1}{|\text{Det } \partial (p, \Delta L)/\partial (\chi, \psi)|}.$$  \hfill (37)

Then the value of the cross section is just the sum of these weights over all the contributing preimage points, i.e.

$$\sigma(p_{\text{out}}, \Delta L) = \sum_k g_k(p_{\text{out}}, \Delta L).$$  \hfill (38)

From equation (37), we see that the cross section has singularities at image points where the Jacobian of this map is zero, i.e. points that are locally not invertible. They are caustics of the projection of the graph of the function into the image space. The corresponding singularities in the cross section are called rainbow singularities, for their effect on the light scattering off water drops. Now we shall focus on these singularities. Each interval of continuity of the scattering functions leads to one copy of a typical rainbow singularity in the cross section. This allows us to see the fractal structure of the chaotic invariant set in the cross section. For systems with two degrees of freedom, this idea has been worked out in detail in \cite{11, 12} and in this section we explain the higher-dimensional generalization.

The determinant of the derivatives of the scattering function is zero exactly for such values of $p_{\text{out}}$ and $\Delta L$ for which two trajectories fall together and disappear. Accordingly, these singularities are the lines across which the number of contributing trajectories, i.e. the number of preimages, changes by 2. Now we will construct a simple analytical normal form for these singularity lines and compare it with the numerical results for the three model systems presented in section 2.

First we need an analytical model for the scattering function in one interval of continuity, which is as simple as possible but still produces the generic form of singularity in the cross section. As explained in section 4, the domain of the scattering function is the 2D torus with the coordinates $\chi_{\text{in}}$ and $\psi_{\text{in}}$. For a small deviation from symmetry, a typical interval of continuity is a strip running around the torus in the $\psi$ direction. In the $\chi$ direction, the strips run in the symmetric case over a limited range only, let us say from $\chi_0 - \delta$ up to $\chi_0 + \delta$, where $\chi_0$ is the position of the middle of the strip. The value of $p_{\text{out}}$ is maximal in the middle of the interval, let us say it has the value $p_0$ in the middle, and it goes to zero on the boundaries of the interval of continuity. Accordingly, the simplest model function for $p_{\text{out}}$ in the symmetric case is

$$p_{\text{out}} = p_0 - (\chi_0 - \chi_{\text{in}})^2,$$  \hfill (39)

where the variables are scaled such that $\delta^2 = p_0$. For the asymmetric case we add a $\psi$-dependent term. This term must be $2\pi$ periodic and for simplicity we take the lowest Fourier contribution only, resulting in

$$p_{\text{out}} = p_0 - (\chi_0 - \chi_{\text{in}})^2 + b \cos(\psi_{\text{in}})$$  \hfill (40)
for the general case with broken symmetry. Here, for each given value of $\psi$, the variable $\chi$ is restricted to such values that result in a positive value for $p_{\text{out}}$. This restriction defines the deformed interval of continuity for the case of broken symmetry.

The function $\Delta L$ is identically zero in the symmetric case. For the case of broken symmetry, we will consider first the very simple model function

$$\Delta L = a \sin(\psi_{\text{in}})$$

without $\chi$ dependence and the version with $\chi$ dependence,

$$\Delta L = a \sin(\psi_{\text{in}})/(1 - c(\chi_{\text{in}} - \chi_{0})).$$

The small perturbative parameters $b$ and $c$ will be considered to be of the same order.

Now we consider the preimages of these scattering model functions. First, as the simplest possibility, combine equations (39) and (41). In equation (39), we find two possible real preimage values of $\chi$ as long as $p_{\text{out}} < p_{0}$ and zero real preimage values if $p_{\text{out}} > p_{0}$. Exactly at $p_{\text{out}} = p_{0}$, two preimages collide and turn from real to imaginary: as physical solutions they disappear. Accordingly, the line $p_{\text{out}} = p_{0}$ is a caustic line in this case. In equation (41), we find two real values of $\psi$ for $|\Delta L| < a$ and zero preimages for $|\Delta L| > a$. Along the lines $\Delta L = a$ and $-a$, the two solutions collide and turn from real to imaginary. Therefore, these two lines are also caustic lines for this simple case. In total, we find four preimages inside the rectangle delimited by the lines $p_{\text{out}} = 0$ and $p_{0}$ and $\Delta L = a$, and $-a$ and zero preimages outside this rectangle (see figure 6). Of course, the caustic structure of this very simple case is not structurally stable; it changes qualitatively under small deformations of the scattering functions. Along generic caustic lines, the number of solutions changes by 2 and not by 4. Therefore, we need to add the appropriate perturbations to the scattering functions to turn the caustic structure into a structurally stable one. We have to see next that the transitions from equation (39) to

Figure 6. The diagrams of the regions divided by a rainbow singularity. The numbers indicate the quantity of preimages of the region for each point.

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equation (40) and from equation (41) to equation (42) are the appropriate perturbations to turn the caustic lines into generic and structurally stable ones.

Next, let us combine equations (40) and (41). In this case, the function for \( \Delta L \) still produces the degenerate caustic lines \( \Delta L = a \) and \(-a\). If we invert equation (40) and we eliminate the \( \psi \) dependence by inserting from equation (41), then we obtain for \( \chi \) the equation
\[
\chi_{\text{in}} = \chi_0 \pm \sqrt{p_0 - p_{\text{out}} \pm b \sqrt{1 - \Delta L^2/a^2}}.
\]  
(43)

First we see the caustic lines \( \Delta L = a \) and \(-a\), which are already known from the inversion of equation (41). In addition, we also see that solutions collide and turn from real to complex along the ellipse given by the equation
\[
a^2(p_0 - p_{\text{out}})^2 + b^2 \Delta L^2 = a^2 b^2.
\]  
(44)

In total, for the combination of equations (40) and (41), the behaviour of the preimages is as follows. Outside the strip delimited by the lines \( \Delta L = a \) and \(-a\), the number of real preimages is zero. Let us now look at the interior of this strip. For values of \( p_{\text{out}} \) outside the ellipse and at the side of larger values, we find zero real preimages in \( \chi \); inside the ellipse, we find two preimages; and for values of \( p_{\text{out}} \) between zero and the ellipse, we find four preimages. The result is that the perturbation introduced in equation (40) is able to modify the degenerate caustic line \( p_{\text{out}} = p_0 \) into a structurally stable curve. However, the two caustic curves \( \Delta L = a \) and \(-a\) stay in their structurally unstable form.

Next, let us combine equations (39) and (42). Equation (39) has the caustic line \( p_{\text{out}} = p_0 \), as before. Inserting equation (39) into equation (42) leads to the following equation for \( \psi \),
\[
\sin(\psi_{\text{in}}) = \Delta L (1 \pm c \sqrt{p_0 - p_{\text{out}}})/a,
\]  
(45)

which in turn leads to the caustic curves
\[
\Delta L = \pm a (1 \pm c \sqrt{p_0 - p_{\text{out}}})^{-1}.
\]  
(46)

In the relevant region of \( p \) values, the curves given by this equation come close to parabolas centred at \( \pm a \). Now the preimage structure is as follows. We find zero real preimages for \( p_{\text{out}} > p_0 \). Therefore, let us concentrate on the strip of \( p_{\text{out}} \) values between zero and the line \( p_{\text{out}} = p_0 \). In the region of small values of \( \Delta L \) between the two approximate parabolas, we find four real preimages; inside the two approximate parabolas we find two real preimages; and in the rest of the strip, we find zero real preimages. The perturbation introduced in equation (42) is able to turn the degenerate caustic lines \( \Delta L = a \) and \(-a\) into structurally stable curves.

Last, let us check that the combination of equations (40) and (42) produces structurally stable caustic curves only. Eliminating the variable \( \psi_{\text{in}} \) and making the substitution \( x = \chi_0 - \chi_{\text{in}} \), we obtain the following polynomial in \( x \),
\[
P(x) = x^4 + A x^2 + B x + C,
\]  
(47)

where
\[
A = 2(p_{\text{out}} - p_0) + b^2 \Delta L^2 c^2/a^2,
\]  
(48)
\[
B = -2b^2 \Delta L^2 c/a^2,
\]  
(49)
\[
C = (p_{\text{out}} - p_0)^2 + b^2 (\Delta L^2/a^2 - 1).
\]  
(50)
Figure 7. In (a), we represent an annular region that spans a quadratic maximum. In (b), we emphasize the singular set of the projection into a two-dimensional manifold. The domain of the scattering function is labelled D. The numbers represent the number of inverse preimages for the projection. Compare with figures 6 and 8(d).

In the following, we use the abbreviation \( D = \Delta L^2 / a^2 - 1 \). A polynomial has colliding solutions whenever its discriminant is zero, see e.g. section II.4 and in particular Lemma 4.7 in [34]. In the case of the polynomial of (47), the discriminant is given by

\[
\text{Dis} = -27 B^4 - 4 A^3 B^2 + 16 A^4 C + 144 A B^2 C - 128 A^2 C^2 + 256 C^3.
\]  

(51)

We will evaluate the resulting complicated expression in \( p \) and \( x \) perturbatively in the small quantities \( b \) and \( c \). The lowest-order contributions come in order 4 and are

\[
\text{Dis}_4 = 256 b^4 (p_{\text{out}} - p_0)^2 D^2.
\]  

(52)

This discriminant is zero along the lines \( p_{\text{out}} = p_0, \Delta L = a \) and \( \Delta L = -a \). All these three lines come with multiplicity 2. It is the same caustic structure as we obtained with the combination of equations (39) and (41).

Next we keep all contributions up to order 6 combined in \( b \) and \( c \) and leave out the irrelevant constant factor 256\( b^4 \). The result is

\[
\text{Dis}_6 = b^2 D^2 + (p_{\text{out}} - p_0)^2 D^2 + 2(p_{\text{out}} - p_0)^3 (\Delta L^2 / a^2 + 1) \Delta L^2 c^2 / a^2.
\]  

(53)

The real zeros of these last expressions in the \( (p_{\text{out}}, \Delta L) \) plane are sketched in figure 6. We have also produced a theoretical plot for the curve of the zeros of expression (53) with parameter \( a \) set on the value 1, whereas the small parameters \( b \) and \( c \) take the value 0.1 (see figure 8(d)). In these plots, the various regions of the plane are marked by the number of real preimages of the original equations (40) and (42). Here, all structural instabilities of the caustic curves are removed. Note that this figure coincides with the projection singularities of the ring-shaped mountain shown in figure 7. The projection is highlighted on the left side. Figures 8(a), (b) and (c) show for comparison the rainbow structure in the cross section coming from a single interval of continuity of the scattering function for the three examples introduced in section 2. Panel (a) belongs to the channel with obstacle, panel (b) to the map model and panel (c) to the bottle billiard.

We see that for all the three examples the rainbow singularity in the cross section has the same qualitative structure as the curves described by (53). This motivates us to propose (53) as
Figure 8. Different isolated rainbow singularities corresponding in each case to a single domain of continuity of the scattering functions, for the different systems presented and the solution for the zeros of the $D_{i6}$ polynomial.

(a) Rainbow singularity for the channel system.  

(b) Rainbow singularity for the map.  

(c) Rainbow singularity for the billiard.  

(d) As a comparison, the zeros of the polynomial $D_{i6}$, equation 54. The parameters are $a = 1, b = c = 0.1$.

the normal form of the rainbow singularity in the double differential cross section for the class of scattering systems considered in this paper.

The shape of the normal form induces a ring-shaped mountain. Since a ring-shaped mountain can be considered half a torus, our projection is half the well-known projection singularity pattern of the torus (see figure 6.13 of [35]).

For moderate breaking of the symmetry, each interval of continuity, which is still some strip running around the torus in the $\psi$ direction, produces in the cross section one copy of the typical rainbow singularity. Of course, for each individual interval it takes different values of the parameters. The total set of singularities seen in the cross section coming from all intervals is expected to consist of a superposition of a fractal of shifted and continuously deformed copies of the normal form. In principle, there should be an infinite number of them. Practically, we can resolve a finite number up to some finite level of hierarchy of the underlying fractal. Let us turn next to some numerical examples for the cross section.

To obtain figures 8–10, we have done a coarse graining of the domain of the cross section, which is similar to what any real detector in an experiment does. The domain is divided into many small rectangles and the counts in any one of these rectangles are registered. Each rectangle can be considered as one detector channel. High count rates are indicated in the figure by a darker colour. Note that there are high count rates also in some detector channels, which do not contain contributions from the true singularity itself. In particular the detector channels near the cusp of the inner singularity line show this behaviour. They are the ones roughly connecting
Figure 9. The rainbow singularities for the map system generated by equation (16). The parameters are \( A = 0.010 \) and \( L_{in} = 1.0383 \). We show the structure of the projection of the half-torus repeated as far as resolution goes.

Figure 10. The rainbow singularities for the system generated by the function \( G(q, \theta, \tilde{p}, \tilde{L}) \) (equation (16)). The parameters are \( A = 0.015 \) and \( L_{in} = 1.5575 \).

After studying the projections of these points, we recognize the shape of the half-toroidal mountains (see figures 9 and 10). These figures have been obtained by simulating a great quantity of trajectories with initial conditions uniformly distributed on the torus. Then we have selected points on the histogram of final conditions which show a much higher count than their neighbours, as seen in figures 9 and 10. If we compare them with the black outline in figure 7, we can see the projection of the same basic pattern repeated an infinite number of times. For a symmetric case, we can see the domains of continuity in smoothly changing
Figure 11. The scattering function for the map generated by the function in expression (16) with $A = 0.000$ and $l_{in} = 1.0383$ on the torus of initial conditions. As $L$ is conserved, we only show the $p_{out}$ component.

colours in figure 11, which partitions the torus into a fractal family of stripes. Each typically has an extremal set of measure zero and shows up as a rainbow singularity in the cross section. As the symmetry gets broken, the embedding remains stable, although the discontinuities bend and may form rings (see figures 12 and 13), or even multiply punctured domains. Then we observe distinct shapes besides the circular rings, which should also represent a complete partition of the domain. It should be noted that the smoother parts of the function still have a ring-shaped domain of continuity and that they are the main contributors to the cross section. Therefore, the experimentally detectable signature of the partitions of the domain is still a family of ring-shaped sets.

6. Final remarks

By asymptotic measurements, we observe which rainbow contributions are present or absent and conclude which corresponding intervals of continuity in the scattering function contribute, and finally we draw conclusions about the structure of the chaotic invariant set in the Poincaré map of the system. In particular, we can change a parameter of the system, for example the symmetry breaking parameter $A$, and follow important changes of the chaotic set, at least in the lower levels of the hierarchy of the fractal structure. For further analysis of the resulting data, two promising possibilities exist.

Firstly, we can try to construct a symbolic dynamics for the system. For systems with two degrees of freedom, a description of the development scenario of the chaotic set in terms of a development parameter related to an approximate symbolic dynamics has been presented for binary and for ternary symmetric horseshoes in [13] and [36], respectively. This description was based on a rather simple approximation for the symbolic dynamics. In the meantime, for chaotic sets of 2D maps, more sophisticated approximations for the symbolic dynamics have been developed [37, 38]. It is worth generalizing all these developments for the 4D maps encountered in the present paper.

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Secondly, we can measure the weight of the contributions to the structures in cross sections and scattering functions coming from the various levels of hierarchy of the underlying fractal. Thereby we extract scaling factors of this fractal. The distribution of these scaling factors can be analysed by thermodynamical methods to extract the statistical measures of the chaos of the systems. For the thermodynamical methods, see [39, 40]. For the application of these methods to chaotic scattering with two degrees of freedom and its cross section, see [41].

By knowing which rainbow singularities are present and which ones are missing compared to the complete case, and by knowing the scaling factors between contributions from the various levels of the hierarchy, we have knowledge about the topology of the horseshoe and about the measures of chaos in 2D cases.

All our considerations have been restricted so far to the case where only one degree of freedom is open and all other degrees of freedom are closed. This situation implies the following property of the system: for any value of the total energy, the closed degrees of freedom can swallow all energy such that for the open degree of freedom only energy zero remains.

**Figure 12.** The scattering function for the map generated by the function in expression (16) with $A = 0.010$ and $L_{\text{in}} = 1.0383$ on the torus of initial conditions. This gives the rainbow singularities depicted in figure 9.
Therefore, for any positive value of the total energy the motion of the open degree of freedom can come to a stop at infinity (when the potential is attractive without outer barrier) or at the outermost potential barrier (in cases where it exists, where the potential is repulsive for large distances). In this sense, the existence of at least one closed degree of freedom implies that for any positive value of the total energy the system sits exactly on a channel threshold. As a consequence, we have the dividing surfaces of dimension 3 (in the domain of the Poincaré map) formed by such trajectories and the intersection of the stable and unstable dividing surfaces forms the chaotic set described before. The elementary intersection set between two hypersurfaces of codimension 1 is a set of codimension 2. If the dividing surfaces form fractal folds, then we have a fractal collection of elementary intersection patterns and the complete intersection set has a codimension less than 2. In our particular case, this property guarantees that the chaotic invariant set in the Poincaré map has a dimension larger than 2.

The situation is different if no closed degree of freedom exists. Imagine a system with only open degrees of freedom and an attractive potential. Then, for positive values of the total energy,
it is impossible to have trajectories that go out arbitrarily far and where at the same time the velocity goes to zero. However, such trajectories are exactly the ones that form the homoclinic tangle in the case investigated in this paper and cause the fractal structure in the scattering functions and in the cross section. This consideration shows that the structures described in this paper will not necessarily exist in systems without closed degrees of freedom.

Of course, topological chaos can exist in systems with only open degrees of freedom. One system of this type with three degrees of freedom, investigated in the past [25, 42], is scattering of a point particle off four hard spheres situated at the four corners of a tetrahedron. When the radius of the spheres is small compared to their distance, all periodic orbits are completely unstable and we have hyperbolicity. In the 4D Poincaré map, this implies the existence of hyperbolic periodic points, but excludes the existence of NHIMs. The invariant manifolds of the hyperbolic points are 2D; their elementary intersection structures are points. Even when the manifolds are folded to form some fractal structure, the complete intersection structure between stable and unstable manifolds is a fractal built up of points. Then, in general, the dimension of this intersection structure is small and does not cause much observable structure in scattering functions. According to [25], the intersection structure in the 4D domain of the Poincaré map should have at least dimension 2 in order to cause easily observable effects in generic scattering functions.

The choice of our class of systems has also favourable consequences for the cross sections. Naturally, we look at the doubly differential inelastic cross section as a function of two action-type variables. In section 5, we studied the cross section as a function of angular momentum transfer and of the outgoing momentum of the open degree of freedom. Because of the conservation of total energy and because of the monotonous dependence of the energy of the oscillating degree of freedom on its action, we could equally well express the same cross section as a function of angular momentum transfer and the final action of the oscillating degree of freedom. The use of the outgoing momentum has the advantage that its sign indicates immediately whether a particular trajectory describes transmission or reflection. Therefore, we stay with the variable $p_{\text{out}}$ in the cross section. However, because of the above-mentioned considerations, we treat $p_{\text{out}}$ as if it would be an action variable. Because of energy conservation, these two action-like variables of the cross section are restricted to a finite interval of possible values. On the boundaries of intervals of continuity of the scattering function, $p_{\text{out}}$ goes to zero. In the interior of intervals of continuity, the scattering function is smooth. Then this function necessarily has generic extrema in the interior and has lines along which the determinant of derivatives is zero. This guarantees the existence of the rainbow structures described above.

Again the situation can be different for scattering systems with open degrees of freedom only. For simplicity, think of the scattering of a points particle off a localized potential in a 3D position space. For the moment, consider the rotationally symmetric case where the azimuth angle is irrelevant. Then the possibility exists that in each interval of continuity of the scattering function, the deflection angle goes monotonically from minus infinity to plus infinity without any generic extremal points. As has been pointed out in [43], this situation can also happen in cases of chaotic systems. Then the fractal chaotic set in the phase space does not leave fractal traces in the cross section.

What happens for even more degrees of freedom, let us say $N$? We can make some comments for the class of systems where we have one open degree of freedom coupled strongly to one closed degree of freedom and any number of further degrees of freedom.
that are only coupled weakly to the first two degrees of freedom. Let us assume again that there is a parameter $A$ that gives the strength of this coupling and that we have again a limiting case $A = 0$ where these additional degrees of freedom are decoupled from the first two, and for simplicity also decoupled among themselves and where accordingly the system can be reduced to one with two degrees of freedom. In this case, we find a $(2N - 4)$-dimensional NHIM in the $(2N - 2)$-dimensional domain of the Poincaré map. It is stable in one direction, unstable in one direction and neutrally stable in the remaining $(2N - 4)$ directions. The development degree of the horseshoe of the reduced system depends on the amount of energy in the reduced system. Because it depends on the value of the conserved actions of the remaining degrees of freedom, we can use one of the remaining neutral directions as the development parameter of the horseshoe and in total again obtain a pile of 2D horseshoes similar to the 3D tangle described before for the three degrees of freedom case. In particular, we can apply the same arguments of robustness as before. The difference is that now we have to form the Cartesian product of this 3D structure with $(2N - 5)$ neutral directions, which are partially action directions and partially angle directions. The domain of the scattering function is now an $(N - 1)$-dimensional torus of initial relative phase shifts between the $N$ degrees of freedom and its range is an $(N - 1)$-dimensional interval of final actions. Take our previous quantities $L$, $\theta$, $\chi$ and $\Delta L$ to be $(N - 2)$ component quantities.

Under small breaking of the symmetric case $A = 0$, the robustness argument indicates again that the coarse structure of the scattering function should be stable; the lower the level of hierarchy in the fractal structure, the more stable the situation should be. The $(N - 1)$-fold differential cross section is the relative probability to obtain some combination of final actions for a constant density of the initial phase shifts. The rainbow singularities are again the projection singularities of the graph of the scattering function under projection on the range. The elementary rainbow structure coming from a single interval of continuity of the scattering function is now an $(N - 2)$-dimensional surface in the $(N - 1)$-dimensional domain of the cross section. We plan a more detailed discussion of the general case in a future publication.

So far, everything has been explained for classical dynamics. Therefore, the question remains about how our results are reflected in quantum systems, like the ones presented in [44]. We have analysed the cross section as a function of the outgoing action for fixed total energy. This was appropriate, since classically the actions of the closed degrees of freedom are continuous variables. In this point, quantum mechanics is essentially different. In our models, asymptotically the open degree of freedom is decoupled from the two closed degrees of freedom (see, for example, equation (2)). Accordingly, in the asymptotic region, the transverse motion, i.e. the state of the two closed degrees of freedom, must be in one of the discrete quantum states of this bound subsystem. For example, in equation (2), the transverse motion is a 2D harmonic oscillator with its usual quantization of the action according to $I = (n + 1/2)\hbar\omega$. For other particular models of the closed transverse degrees of freedom, similar restrictions apply. On the other hand, this discreteness of the asymptotic transverse states provides a natural channel decomposition of the $S$-matrix and the scattering amplitude, where we start from a particular asymptotic initial transverse state and study the transitions to various other energetically allowed final asymptotic transverse states. The open longitudinal degree of freedom does not have similar restrictions; its asymptotic energy can be any positive value. Thus, scanning the action of the closed degrees of freedom is impossible in quantum dynamics. The appropriate procedure is to select particular initial and final states of the closed degrees of freedom and to vary the total
energy continuously, i.e. study the cross sections for the various channel-to-channel transitions as a function of the total energy. In these quantities, we expect to see structures, in particular sequences of scattering resonances, related to the classical chaotic set. So far, we have not studied such implications and they are not the subject of this paper.

The essential point for the analysis of the quantum mechanical cross section is the wave dynamical analogue to classical rainbows. One essential difference between classical dynamics and quantum dynamics is how the contributions from the various initial conditions are summed. In classical dynamics, the cross section of equation (38) itself is a sum over the contributing initial conditions. In a semi-classical approximation to quantum dynamics or when using Feynman’s path integral version of the quantum propagator, we first form a scattering amplitude as a sum over contributing trajectories and then form the cross section or scattering probability as the absolute square of the amplitude. Therefore, the resulting cross section is a double sum over the trajectories and contains first a sum over diagonal terms that has the structure of the classical cross section plus the non-diagonal terms that are interferences between the various contributing trajectories. If in a rainbow two trajectories fall together, then in a semi-classical treatment of the scattering amplitude we have to apply some uniformization that replaces the contribution of the two trajectories by an Airy function. This gives the wave dynamical analogue of the classical square root singularity.

Accordingly, two things might be done in a wave dynamical treatment. Firstly, the interference pattern in the wave cross section can be analysed. For some attempts in this direction, see [41, 45], where the semi-classical scattering from three soft potential mountains has been used as an example for demonstration. Secondly, a decomposition of the scattering amplitude into Airy-type contributions might be tried, in order to recover at least the first few hierarchical levels of the fractal pattern of rainbows. To our knowledge, this has not been done so far, but might be worth trying.

Acknowledgments

This work has been supported by CONACyT under Grant number 79988 and DGAPA under Grant number PAPIIT-DGAPA 110110 and by a doctoral scholarship grant also from CONACyT to K Zapfe. We thank Kevin Mitchell for useful comments on the manuscript.

References

[1] Tel T and Ott E (eds) 1993 Chaos 3(4) (whole issue)
[2] Jung C and Pott S 1989 Classical cross section for chaotic potential scattering J. Phys. A: Math. Gen. 22 2925
[3] Jung C and Scholz H J 1988 Chaotic scattering off the magnetic dipole J. Phys. A: Math. Gen. 21 2301
[4] Eckhardt B 1987 Fractal propierties of scattering singularities J. Phys. A: Math. Gen. 20 5971
[5] Rapoport A and Rom-Kedar V 2008 Chaotic scattering by steep repelling potentials Phys. Rev. E 77 029901
[6] Mitchell K A and Delos J B 2007 The structure of ionizing electron trajectories for hydrogen in parallel fields Physica D 229 9
[7] Smale S 1967 Differentiable dynamical systems Bull. Am. Math. Soc. 73 747
[8] Büttikofer T, Jung C and Seligman T H 2000 Extraction of information about periodic orbits from scattering functions Phys. Lett. A 76 265
[9] Tapia H and Jung C 2003 Inelastic inverse scattering problem Phys. Lett. A 313(3) 198–210
[10] Jung C, Merlo O and Seligman T H 2004 Symmetry properties of periodic orbits extracted from scattering data Chaos 14 969
[11] Jung C, Orellana-Rivadeneyra G and Luna-Acosta G A 2004 Reconstruction of the chaotic set from classical cross section data J. Phys. A: Math. Gen. 38 567
[12] Schelin A B, de Moura A P S and Grebogi C 2008 Transition to chaotic scattering: Signatures in the differential cross section Phys. Rev. E 78 046204
[13] Jung C, Lipp C and Seligman T H 1999 The inverse scattering problem for chaotic hamiltonian systems Ann. Phys. 275 151
[14] Ramm A G 1992 Multidimensional Inverse Scattering Problems (Harlow: Longman Scientific/Wiley)
[15] Gladwell G M L 1993 Inverse Problem in Scattering. An Introduction (Dordrecht: Kluwer)
[16] Akhariev B N and Sucko A A 1990 Potential and Quantum Scattering. Direct and Inverse Problems (Berlin: Springer)
[17] Contopoulos G and Efstathiou K 2004 Escapes and recurrence in a simple Hamiltonian system Celest. Mech. Dyn. Astron. 88 163
[18] Waalkens H, Burbanks A and Wiggins S 2005 Escape from planetary neighbourhoods Mon. Not. R. Astron. Soc. 361 763
[19] Waalkens H and Wiggins S 2010 Geometrical models of the phase space structures governing reaction dynamics Reg. Chaos. Dyn. 15 1
[20] Ezra G S and Wiggins S 2009 Phase-space geometry and reaction dynamics near index 2 saddles J. Phys. A: Math. Gen. 42 205101
[21] Waalkens H, Schubert R and Wiggins S 2008 Wigner’s dynamical transition state theory in phase space: classical and quantum Nonlinearity 21 R1
[22] Uzer T, Jaffe C, Palacian J, Yanguas P and Wiggins S 2002 The geometry of reactions dynamics Nonlinearity 15 957
[23] Wiggins S 1994 Normally Hyperbolic Invariant Manifolds in Dynamical Systems (Berlin: Springer Verlag)
[24] Waalkens H, Burbanks A and Wiggins S 2004 A computational procedure to detect a new type of high-dimensional chaotic saddle and its application to the 3D Hill’s problem J. Phys. A: Math. Gen. 37 257
[25] Chen Q, Ding M and Ott E 1990 Chaotic scattering on several dimensions Phys. Lett. A 115 93
[26] Benet L, Broch J, Merlo O and Seligman T H 2005 Symmetry breaking: a heuristic approach to chaotic scattering in many dimensions Phys. Rev. E 71 036225
[27] Dietz B, Papenbrock T, Mößner B, Reif U and Richter A 2008 Bouncing ball orbits and symmetry breaking effects in a three-dimensional chaotic billiard Phys. Rev. E 77 046221
[28] Jackson E A 1989 Perspectives of Nonlinear Dynamics (Cambridge: Cambridge University Press)
[29] Jung C, Mejia-Monasterio C, Merlo O and Seligman T H 2004 Self pulsing effect in chaotic scattering New J. Phys. 6 48
[30] Hansen P, Mitchell K A and Delos J B 2006 Escape of trajectories from a vase-shaped cavity Phys. Rev. E 73 066226
[31] Chernov N and Markarian R 2006 Chaotic Billiards vol 127 (Mathematical Surveys and Monographs) (Rhode Island: American Mathematical Society)
[32] Taylor J R 1972 Scattering Theory (New York: Wiley)
[33] Newton R G 1982 Scattering Theory of Waves and Particles (Berlin: Springer)
[34] Kendig K 1977 Elementary Algebraic Geometry (Berlin: Springer)
[35] Ozorio de Almeida A M 1988 Hamiltonian Systems: Chaos und Quantization (Cambridge: Cambridge University Press)
[36] Rückerl B and Jung C 1994 Scaling properties of a scattering system with an incomplete horseshoe J. Phys. A: Math. Gen. 27 55
[37] Mitchell K A and Delos J B 2006 A new topological technique for characterizing homoclinic tangles Physica D 221 170
[38] Mitchell K A 2009 The topology of nested homoclinic and heteroclinic tangles Physica D 238 737
[39] Tel T 1990 *Directions in Chaos* (Singapore: World Scientific) chapter 3
[40] Beck C and Schlögel F 1993 *Thermodynamics of Chaotic Systems* (Cambridge: Cambridge University Press)
[41] Jung C and Tel T 1991 Dimension and escape rate of chaotic scattering from classical and semiclassical cross section data *J. Phys. A: Math. Gen.* 24 2793
[42] Korsch H J and Wagner A 1991 Fractal mirror images and chaotic scattering *Comp. Phys.* 5 497
[43] de Moura A P and Grebogi C 2002 Rainbow transition in chaotic scattering *Phys. Rev. E* 65 035206
[44] Mitchell K A and Ilan B 2009 Nonlinear enhancement of the fractal structure in the escape dynamics of Bose-Einstein condensates *Phys. Rev. A* 80 043406
[45] Jung C 1990 Fractal properties in the semiclassical scattering cross section of a classically chaotic system *J. Phys. A: Math. Gen.* 23 1217