Atom scattering off a vibrating surface: An example of chaotic scattering with three degrees of freedom

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Abstract

In this article, we study the classical chaotic scattering of a He atom off a harmonically vibrating Cu surface. The three degrees of freedom (3-dof) model is studied by first considering the non-vibrating 2-dof model for different values of the energy. We calculate the set of singularities of the scattering functions and study its connection with the tangle between the stable and unstable manifolds of the fixed point at an infinite distance to the Cu surface in the Poincaré map for different values of the initial energy. With these manifolds, it is possible to construct the stable and unstable manifolds for the 3-dof coupled model considering the extra closed degree of freedom and the deformation of a stack of maps of the 2-dof system calculated at different values of the energy. Also, for the 3-dof system, the resulting invariant manifolds have the correct dimension to divide the constant total energy manifold. By this construction, it is possible to understand the chaotic scattering phenomena for the 3-dof system from a geometric point of view. We explain the connection between the set of singularities of the scattering function, the Jacobian determinant of the scattering function, the relevant invariant manifolds in the scattering problem, and the cross-section, as well as their behavior when the coupling due to the surface vibration is switched on. In particular, we present in detail the connection between the changes in the structure of the caustics in the cross-section and the changes in the zero level set of the Jacobian determinant of the scattering function.

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Introduction

The atom-surface scattering is a complex problem in nonlinear dynamics. The process of elastic chaotic scattering of an atom by surfaces has been studied in detail for Hamiltonian systems with 2-dof \[1–4\]. The chaotic scattering in 2-dof Hamiltonian systems is well understood because the corresponding Poincaré map acts on a domain of dimension 2. Moreover, the stable and unstable manifolds of the most relevant fixed points built up a homoclinic/heteroclinic tangle, which is the central element of the skeleton of the whole dynamics. These stable and unstable manifolds are of dimension 1 in the Poincaré map, i.e., they are also of codimension 1, and as such, they form division lines in the domain which direct the dynamics in the map. Analogous considerations also hold in the corresponding constant energy manifold for the flow since codimensions of their respective stable and unstable manifolds are equal in maps and flows. For a detailed discussion of the importance of homoclinic/heteroclinic trajectories, see chapter 3 in \[5\] and \[6\]. A pictorial illustration of the corresponding tangles can be seen in chapters 13 and 14 in \[7\].

Also, for some systems with more dof it is possible to apply the same geometric and topological ideas to construct dividing invariant manifolds with more dimensions but still codimension 1 and homoclinic/heteroclinic tangles, see the Ref. \[8, 9\]. There has been recent progress in chaotic scattering to study the 3-dof problem when it is close to a symmetric system, or equivalently close to a partially integrable system \[10\]-\[14\]. The main idea behind the analysis in those systems is that the principal phase space structures that direct the dynamics in the 3-dof system are quite robust under perturbations of the system. Then we expect these principal structures to survive qualitatively and change only slowly under small perturbations of the symmetry. Accordingly, we start with the symmetric 3-dof system, which can be considered a stack of 2-dof systems, and turn on smoothly the perturbations, thereby converting the stack of 2-dof systems into an irreducible 3-dof system.

The aim of this article is to extend the study of the atom scattering to the case when the surface oscillates, and the scattering is inelastic. In particular, we study the origin of the changes in the caustics in the double differential cross-section.

The studied model is an extension of a 2-dof model proposed in \[1, 2\], and it considers the vibration of the surface as an additional oscillatory degree of freedom. This consideration adds a new closed degree of freedom that exchanges energy, then the chaotic scattering becomes inelastic. In this work, we study the connections between the impenetrable stable and unstable manifolds of codimension 1 in the 3-dof system, the Jacobian determinant of the scattering function, and the rainbow singularities of the double differential cross-section from the geometrical and topological point of view.

The organization of the paper is as follows. Section 2 is a brief review of the basic results of the 2-dof model for the elastic collisions of He atoms off a static corrugated Cu-surface. The construction of the scattering functions of the system is presented. Also, the tangle between the stable and unstable manifolds of the fixed point at an infinite distance to the Cu surface in the Poincaré map is given for different values of the initial energy of the incident particle. In section 3 we turn on the vibrations of the surface and construct the stable and unstable manifolds of the most important invariant subset for the
3-dof system, which describes the inelastic He scattering by the vibrating Cu surface. These invariant manifolds still are impenetrable barriers in the phase space. We calculate the scattering function for the 3-dof system for different initial particle energies and study the corresponding set of singularities and its Jacobian determinant. Finally, we explain the changes in the structure of the caustics in the cross-section associated with the change of the initial energy of the particle, based on the changes in the regions of continuity of the scattering function and the level zero set of its Jacobian determinant. Section 4 contains the final remarks.

2 The 2-dof model: Elastic He-Cu surface scattering

First, we study the simplest version of the model, i.e. a Hamiltonian system with 2-dof, such as in the works previously considered in detail [1–3]. This study serves as preparation for the next section, where we built up the 3-dof system as a pile of 2-dof system.

Let us consider the motion of a He atom coming in from the asymptotic region, and moving towards the interaction region where there is a static Cu surface. Let $z$ and $x$ be the spatial coordinates of the atom perpendicular and parallel to the surface, respectively (we consider a single tangential coordinate to the surface, i.e. in-plane scattering). The corresponding 2-dof Hamiltonian is

$$H_0(x, z, p_x, p_z) = \frac{p_x^2}{2m} + \frac{p_z^2}{2m} + V(x, z),$$

(1)

where the function $V(x, z)$ is a corrugated Morse potential with the functional form

$$V(x, z) = D(e^{-\chi z}(e^{-\chi z} - 2)) + 2e^{-\chi z}V_f(x),$$

$$V_f(x) = \sum_{G=1}^{4} V_G \cos \frac{G \pi x}{A}.$$ (2)

The constants $D$, $A$, $V_G$ and $\chi$ are taken from the table of Ref. [1]. Note that the potential is periodic in $x$ direction with period $P = 2A/G$. Therefore it is possible to think that $x$ is a compact variable restricted to a circle, and in this sense this dof can be considered a closed one.

In a scattering experiment, the particle starts in the asymptotic region and moves towards the interaction region, where the particle remains close to the surface for an interval of time, and finally moves back to the asymptotic region. The irregular behavior of the particle for a finite time interval and the sensibility of its trajectory to initial conditions is a phenomenon called transient chaos; more examples of this kind of phenomena are described in [15][18].

2.1 The scattering functions and the tangle

The scattering functions of the system contain useful information to analyze and compare the behavior of different scattering trajectories of the particles. These functions map initial asymptotic quantities to final asymptotic quantities,
similar to the measurements in a standard scattering experiment. This natural.
approach to detect and analyze essential structures in the phase space is similar
to other approaches based on trajectories like Lagrangian Descriptors and Fast
Lyapunov Indicators, see [19–22].

The main idea behind this detection is associated with the different behavior
between the trajectories in the invariant manifolds and the trajectories outside
of them. The trajectories in the stable manifold converge to its limit set; meanwhile,
the other trajectories close to the stable manifold go to other regions of
the phase space. In a scattering system, the trajectories starting in the sta-
ble manifold of some localized invariant set remain bounded for all \( t > 0 \) in
contrast to the trajectories close but not exactly in the stable manifold which
escape to the asymptotic region after a finite time. This characteristic property
allows identifying intersections between these stable manifolds and the domain
of the scattering functions as the position of the singularities of the scattering
functions. Similar considerations apply for the unstable manifold changing the
direction of time in the equation of motion. At the singularities, the considered
scattering functions lose differentiability or go to infinity. Let us investigate
these considerations in more detail for the present scattering system.

First, we consider the appropriate asymptotic variables for the scattering sys-
tem. Initially, in the incoming asymptotic region, the relevant initial conditions
of a He atom for the scattering process can be taken as an impact parameter
\( b \) measured relative to the \( x \) axis, an initial momentum \( \vec{p}_i \) forming an angle \( \theta_i \n\)
with respect to the \( z \) axis, and the initial energy \( E_0 \), which is asymptotically
the kinetic energy and is fixed by the given initial momentum.

In this case, we consider a beam of non-interacting particles, all with the
same initial energy \( E_0 \) and the same initial angle \( \theta_i \). Equivalently the value of
the asymptotic vector momentum is constant over the beam, whereas the initial
impact parameter \( b \) has a uniform random distribution over the beam. Also,
the time of arrival at the surface is random. The most useful scattering function
in the present set up is the final scattering angle \( \theta_f \) as a function of the initial
impact parameter \( b \). The impact parameter can be defined in the following
way: Let us imagine the system without potential. Then the entire trajectory
with specific initial conditions would be a straight line. This trajectory would
intersect the \( x \)-axis in a value \( x_s \). Since the potential is periodic in \( x \), with
period \( P = 2A/G \), its only necessary to consider its value mod \( P \). In this
spirit, we define the impact parameter as \( b = x_s \mod P \).

The Fig. 1 shows the graph of the final scattering angle \( \theta_f \) as a function of
the impact parameter \( b \) in the upper panel. The initial energy is \( E_0 = 2 \)
and the initial angle is \( \theta_i = 80^\circ \). Along the \( b \) axis, there is a fractal of points where
the scattering function \( \theta_f \) is not defined. A point with this property is called a
singularity of the scattering function.

In a neighborhood of a singular point, the value of the scattering function
oscillates more and more rapidly, as the singularity is approached. Close to
a singularity of the scattering function, i.e. in regions where the value of \( \theta_f \n\)
changes quickly, trajectories starting in this neighborhood spend more time in
the interaction region than trajectories starting far from the singularities. For
a detailed investigation of the scaling behavior of the scattering and delay time
functions in the neighborhood of a singularity, see [23].

For this kind of systems, the set of singularities of the scattering functions is a
fractal Cantor set, and it is generated by a chaotic invariant set of the dynamics
Figure 1: The scattering functions $\theta_f(b)$ and $\theta_f(\phi_i, b)$ on colour scale for initial energy $E_0 = 2$ and the initial angle $\theta_i = 80^\circ$. The value of the angle $\theta_f$ oscillates as a function of the impact parameter $b$, and it is constant as a function of the phase $\phi_i$ associated with the vibration of the surface, which is taken here as static. The initial phase $\phi_i$ represents the phase shift between the particle motion and the oscillator representing the vibrations, see the section 3. At present, the angle $\phi$ does not change in the scattering process in this section; the surface is static, and the scattering is elastic. The graph of the scattering function $\theta_f(\phi_i, b)$ will be useful in the next section to compare the results of the elastic and the inelastic system.
Figure 2: Fractal set of singularities of the scattering function in the $b - E_0$ plane, i.e. in the domain of this function for the 2-dof system. We can see the regions of continuity, which are the gaps of the fractal. For every value of the initial energy $E_0$, the singularities reflect the stable manifolds $W_{sE_0}$ of the chaotic invariant set. The horizontal line at $E_0 = 2$ intersects the same set of singularities as the scattering functions in Fig. 1. The region of continuity marked yellow will serve in the subsections 3.1 and 3.3 as example region.

In the phase space $[23]$. The trajectories corresponding to the singularities end with a final momentum in the $z$-direction of value zero because these trajectories are the intersections between the stable manifolds $W_{sE_0}$ of a chaotic invariant set with the set of asymptotic initial conditions for a fixed value of $E_0$, see the Figs. 2 and 3.

In Fig. 2 a plot of the position of the fractal set of singularities of $\theta_f$ in the $b - E_0$ plane is presented, again the initial angle is $\theta_i = 80^\circ$. To each point of the set of singularities, there belongs a trajectory that gets trapped forever in the interaction region, and those trajectories lie on the stable manifold of some invariant subset, a “periodic orbit” at infinity in this case. Note that first, there is a large region of continuity, reaching up to infinite values of the energy. In addition, there is an infinite number of regions of continuity for small values of the particle energy $E_0$. In the figure, the largest inner region of continuity is marked by a yellow color, this region serves in subsections 3.1 and 3.3 as an example region of continuity for the case when the perturbation is switched on. The yellow region in Fig.2 corresponds to the two vertical regions of continuity in Fig.1, which are located around the $b$ values 0.6 and 0.72, respectively. In the following, we will call the yellow region and the corresponding regions of continuity in the scattering functions the region $R$.

In the general case, there is a small number of fundamental periodic orbits, such that the tangle built up by these orbits is dense in the whole chaotic
Figure 3: The tangle between the stable and unstable manifolds of the point at infinity for different values of the initial energy \( E_0 \) of the 2-dof model describing the elastic scattering of He from a static Cu surface. The blue line is a segment of the stable manifold \( W^{s}_{E_0} \), and the red line is a segment of the unstable manifold \( W^{u}_{E_0} \). The tangle between \( W^{s}_{E_0} \) and \( W^{u}_{E_0} \) changes as \( E_0 \) increases.

invariant set. Then it is sufficient to study the tangle formed by the fundamental orbits only. In most cases, these orbits are the periodic orbits oscillating over the outermost saddles of the potential. However, in the present case, where the potential is of the form given in Eq. (2) there is a small extra problem that it has an attractive asymptotic tail, and then the outermost localized orbit of the flow or the outermost fixed point of the corresponding Poincaré map sits at infinity.

Formally this fixed point at infinity has neutral linear stability, i.e. it is parabolic. However, it is nonlinearly unstable and forms stable and unstable manifolds and tangles (chaotic saddles) of the usual topological structure \([11,12]\).

In an appropriate Poincaré section, the unstable manifold is obtained as the reflection of the stable manifold in the line \( p_z = 0 \); this is a consequence of the time-reversal symmetry of the Hamiltonian dynamics. To visualize the tangle, we construct the Poincaré map with the intersection condition \( x \mod P = 0 \). By \( W^{s}_{E_0} \) and \( W^{u}_{E_0} \) we denote the stable and unstable manifolds of the point at infinity on the Poincaré map, i.e the point with \( p_z = 0 \) and \( z \to \infty \). The Fig. 3 displays the tangle for various values of initial energy \( E_0 \), and thereby shows the development scenario of this tangle, as a function of \( E_0 \). The sequence of plots shows the typical scenario of development for a binary Smale horseshoe.

Let us consider now the dimension of the relevant geometrical phase space
objects that play an essential role in the scattering process. The structure of the tangle between the stable and unstable manifolds determines the chaotic scattering of the system. The Poincaré map has dimension 2, the dimension of the stable and unstable manifolds $W^s_{E_0}$ and $W^u_{E_0}$ in the map is 1. Moreover, these manifolds are natural barriers that direct the dynamics on the map, since they are lines of codimension 1. The dynamics of points on a lobule defined by segments of stable and unstable manifolds are determined by the structure of the tangle between stable and unstable manifolds. The image of a lobule visible in the plots under the Poincaré map is the next lobule [24]. Moreover, the iterations of the lobules rotate around an inner fixed point in the Poincaré map. This fixed point corresponds to a periodic orbit trapped in the periodic potential of the surface [3].

The situation in the constant energy manifold is equivalent. Here all relevant dimensions are higher by 1, but the codimensions remain the same. The constant energy manifold has dimension 3, the stable and unstable manifolds have dimension 2, and they form a partition of the constant energy manifold. The considered model keeps the value of the codimensions of the important objects that direct the dynamics when the vibration of the surface is included, and the system is 3-dof.

3 The 3-dof model: the inelastic scattering case

To construct the 3-dof Hamiltonian associated with the vibrating copper surface, we include an oscillatory term with a single frequency $\omega$. Then, to convert the system into a time-independent one, we replace $\omega t$ by the phase variable $\psi$ of an oscillator and include its conjugate action variable $I$ into the Hamiltonian. Once we have the time-independent three degrees of freedom version of the system, it is possible to apply the ideas developed in Refs. [11,12] to study the scattering process.

The construction of the 3-dof model starts from the time-independent 2-dof one. We include a surface oscillation in the direction $z$ of the form $B_z \cos \omega t$, replace $\omega t$ by the new coordinate $\psi$ and approximate

$$V(x, z + B_z \cos \psi) \approx V(x, z) + B_z \cos \psi \frac{\partial V(x, z)}{\partial z}.$$ 

The Hamiltonian model of the complete system is the sum of three terms: the Hamiltonian of the 2-dof model (see Eqs. (1) and (2)), a term for the free surface oscillator, and a term for the interaction between the oscillating surface and the incident particle.

$$H(x, z, \psi, p_x, p_z, I) = \frac{1}{2m} \left( p_x^2 + p_z^2 \right) + V(x, z) + I \omega + B_z \cos \psi \frac{\partial V(x, z)}{\partial z}. \quad (3)$$

The dof associated with the vibration of the surface is a closed one by construction, while the potential $V(x, z)$ is periodic in $x$, and accordingly, the associated $x$-dof can also be considered to be a closed one. In this sense, the 3-dof system has 1 open and 2 closed dofs. The main effect of the interaction
term is a possible energy transfer between the surface oscillator and the incident particle. Whether the particle gains or loses energy depends on whether the $z$ components of the surface velocity and the particle velocity have the opposite or same sign in the moment of approach. Therefore, the final particle energy is, in general, no longer equal to the initial particle energy. For a simple model to explain this energy transfer between a vibrating target and a scattered particle, see Refs. [25][26].

An essential question in all scattering problems is to make an appropriate choice of the asymptotic labels. For an $n$-dof Hamiltonian system, the asymptotes should be labeled by $2n - 1$ independent quantities, which are conserved by the asymptotic dynamics. For a detailed explanation of this issue and general information on the appropriate choice of asymptotic labels, we refer the interested reader to section 2.1 of Ref. [27].

In the present case, a right choice of the 5 asymptotic labels is as follows: the first 2 labels are either the particle momenta $p_x$ and $p_z$, or equivalently the initial kinetic energy $E_0$ and the incident angle $\theta_i$ between the $z$ axis and the initial momentum $p_0$. A third label consists of the impact parameter $b$, the fourth label is a relative phase shift $\phi$ between the particle motion and the oscillator representing the vibrations, that can be defined, formally, as $\phi = \dot{\psi} - \omega z/p_z$ (note that this quantity is constant under the asymptotic motion), and as the last asymptotic label one can use either the initial oscillator action $I$, or the total system energy, i.e., including that of the oscillator. However, this last quantity is irrelevant since the action $I$ never enters any significant quantity; therefore, we will ignore the value of $I$.

In the following, $E_0$ will denote the value of $H_0$, i.e., the particle energy. Its value in the asymptotic region will be the kinetic energy of the particle, its value along an incoming asymptote will be $E_0$, and its value along an outgoing asymptote will be $E_f$.

### 3.1 The scattering function and its Jacobian determinant

The scattering function in the 3-dof case is again a map from the set of all possible initial asymptotes to some magnitudes characterizing the final asymptotes. In the present case, the domain of this map is a 5-dimensional set. However, we have already indicated that the initial action $I$ is irrelevant, and then it will not be considered. Moreover, also in the 3-dof case, we think of an incoming beam where the initial vector momentum, or equivalently $E_0$ and $\theta_i$, is well defined, and where the quantities $b$ and $\phi_i$ have a random distribution with constant density. The most interesting quantities to measure along the outgoing asymptotes are the final energy $E_f$ of the particle and the trajectory inclination $\theta_f$ (equivalently, we could use the final vector momentum).

For the numerical calculations, we consider a fixed value of the surface oscillation frequency $\omega = 0.05$ and proceed similarly to the 2-dof system. As long as the oscillation amplitude $B_z = 0$, the initial energy of the particle $E_0$ is equal to its final value $E_f$. However, as soon as $B_z \neq 0$ (for the following numerical examples, the value of the oscillation amplitude is fixed, $B_z = 0.001$), the energy $E_f$ can be different from $E_0$, and the scattering process becomes inelastic. A convenient quantity to characterize final asymptotes is the energy transfer $\Delta E = E_f - E_0$. For the present system, a meaningful set of 2 scattering functions are: $\Delta E(b, \phi_i)$ and $\theta_f(b, \phi_i)$, both depending on $b$ and $\phi_i$ while keeping...
Figure 4: Scattering function $\theta_f(b,\phi_i)$ for $\theta_i = 80^\circ$ and the 6 values of the incident energy, $E_0 = 1.9, 2.0125, 2.1, 2.16, 2.175, 2.45$ in the parts (a), (b), (c), (d), (e) and (f) respectively. The structure of the fractal set of singularities changes when the value of $E_0$ is increased. In comparison with the unperturbed case of Fig.1, where the scattering functions are independent of $\phi_i$, here, this symmetry is broken by the perturbation, and new structures with different topology appear, namely annular regions of continuity.
Figure 5: Scattering function $\Delta E(b, \phi_i)$ for $\theta_i = 80^\circ$ and the 6 values of the incident energy, $E_0 = 1.9, 2.0125, 2.1, 2.16, 2.175, 2.45$ in the parts (a), (b), (c), (d), (e) and (f) respectively.
and $\theta_i$ fixed, like the beam already described above.

Some numerical examples, corresponding to the cases $E_0 = 1.9, 2.0125, 2.1, 2.16, 2.175$ and $2.45$ are shown in Figs. 4 and 5, where Fig. 4 shows $\theta_f$ and Fig. 5 shows $\Delta E$. The incoming angle is always kept fixed at $\theta_i = 80^\circ$. As can be seen, the structure of the set of singularities of the scattering functions changes as the value of the initial energy $E_0$ is increased, and the sequence of $E_0$ values used in the figures demonstrates well the fundamental pattern of these changes. For $E_0 = 1.9$, two basic structures are seen: First, vertical strips along the $\phi$ direction, which are qualitatively similar to the strips that are observed in the uncoupled 2-dof case, i.e., $B_z = 0$. And second, disks are around a central point.

The complement of the set of singularities is the set of regions of continuity of the scattering functions. If the value of $E_0$ is increased, the structure of strips and circles changes. This change reflects the changes in the structure of the associated tangle between the stable and unstable manifolds of the 3-dof system.

As we will see in subsection 3.3 in the domain of the scattering functions, i.e., in the $b-\phi_i$ plane an important subset related with the caustics in the cross-section is the level zero set of the determinant of the Jacobian matrix of the scattering function, see Ref. [28]. This determinant of the Jacobian is defined as

$$\det J = \left| \frac{\partial(\theta_f, \Delta E)}{\partial(b, \phi_i)} \right| = \frac{\partial \theta_f}{\partial b} \frac{\partial \Delta E}{\partial \phi_i} - \frac{\partial \theta_f}{\partial \phi_i} \frac{\partial \Delta E}{\partial b}$$

(4)

The level zero set of the determinant of the Jacobian is form by curves in the domain of the scattering function. In each region of continuity, there must be at least one curve fulfilling this condition because in Fig. 1, each region of continuity has one vertical $\det J = 0$ line in its interior. Next, imagine that we include the perturbation with an extremely small value of $B_z$. Then in Eq. 4, only the first product on the righthand side matters, since the second product is of second order in $B_z$. That is, we have $\det J = 0$ lines when $\frac{\partial \theta_f}{\partial \phi_i} = 0$. This means the above mentioned vertical $\det J = 0$ lines are not affected and remain the same in the limit of very small values of $B_z$. However, the $\phi$ dependent perturbation also introduces small changes of $\Delta E$, and the functional form of the perturbation as given in Eq. 3 makes it understandable that these small dependencies go like $\sin \phi_i$. Then we have relative extrema of $\Delta E$ at $\phi_i = \pi/2$ and $\phi_i = 3\pi/2$. This introduces a new type of $\det J = 0$ lines, which we call the horizontal lines. It depends strongly on the size of the stripes of continuity at which value of $B_z$ these horizontal lines suffer qualitative changes in their structure. In addition, the perturbation mainly affects the dependence of $\Delta E$ on $\phi_i$, and therefore we expect that with increasing values of $B_z$ first, the horizontal $\det J = 0$ lines are strongly affected whereas the vertical $\det J = 0$ lines are more robust.

The Fig. 6 shows a numerical example for the dependence of the $\det J = 0$ curves on $E_0$ for a fixed value of $B_z$ where we use again our previous value $B_z = 0.001$. The 6 parts (a), (b), (c), (d), (e), (f) of the figure correspond to the energy values also used in Figs. 4 and 5. Regions with $\det J > 0$ are coloured black while regions with $\det J < 0$ are shown white. The curves $\det J = 0$ are the boundary curves between white and black regions. Remember that $b$ and $\phi_i$ are periodic variables and that, therefore, opposite boundaries of the figure should be identified to turn the domain into a torus. We are mainly interested in the
Figure 6: Signature of det $J$ for the scattering functions. The black regions have det $J > 0$, the white regions have det $J < 0$. The green lines correspond to vertical det $J = 0$ lines in the region of continuity $R$. The orange lines are the deformation of the horizontal lines det $J = 0$ in the region $R$. The blue lines are the boundaries of the region $R$. 
region \( R \) and therefore curves in \( R \) are marked by color. The \( \det J = 0 \) curves coming from the curves \( \partial \theta / \partial b = 0 \) of the unperturbed case (i.e., the case \( B_z = 0 \)) are marked green. Such curves will also be called vertical \( \det J = 0 \) curves in the following. The \( \det J = 0 \) curves coming from the curves \( \partial \Delta E / \partial \phi = 0 \) in the limit \( B_z \to 0 \) are marked orange. Such \( \det J = 0 \) curves will also be called deformations of the horizontal \( \det J = 0 \) curves in the following. In addition, the boundaries of the region \( R \) are marked blue. First, observe the robustness of the vertical \( \det J = 0 \) line but also the robustness of the two horizontal \( \det J = 0 \) lines in the largest region of continuity. In this largest region of continuity, we never observe any interesting changes in the topology of the region itself or the \( \det J = 0 \) lines for moderate values of \( B_z \).

In order to show the typical scenario for a change of the topology of regions of continuity and related changes of the \( \det J = 0 \) lines, we focus our attention on one region of continuity, namely the one which is coloured yellow in Fig.2 and which has been already called the region \( R \). In Fig.2 it is the largest region of continuity besides the infinite outer region of continuity. At the lowest energy \( E_0 = 1.9 \), the region \( R \) consists of two components. Compare them with an intersection between a horizontal line at \( E_0 = 1.9 \) in Fig.2 and the yellow region in this figure. Of course, because of the nonzero perturbation, the two components wiggle a little as a function of \( \phi \), but they still have the same topology as in the unperturbed case, compare part (b) of Fig.1. Each one of the 2 components still has its vertical \( \det J = 0 \) curve (colored green), which also still has the same topology as in the unperturbed case.

We also observe the relatively large sensitivity of the horizontal \( \det J = 0 \) curves against perturbations. Only in the largest outer region of continuity, the horizontal curves are almost the same as in the uncoupled case of perturbation zero. They are two almost horizontal lines near \( \phi = \pm \pi/2 \). In contrast, in all the smaller regions of continuity, the horizontal lines are deformed strongly and have changed their topology such that they can no longer be recognized easily as curves having developed from horizontal lines. This behavior illustrates how the onset of strong deformations of the horizontal \( \det J = 0 \) lines depends on the size of the region of continuity; smaller regions are more sensitive to perturbations. We also see that the value \( B_z = 0.001 \) is the appropriate one to see the essential behavior of the \( \det J = 0 \) lines in the region \( R \).

Now let us observe in more detail the transformation of the \( \det J = 0 \) curves within \( R \) under a variation of the energy \( E_0 \). When we increase \( E_0 \) then the gap separating the two components of \( R \) becomes smaller, and at a critical value of \( E_0 \) the gap breaks near \( \phi_i = 3\pi/2 \). At this moment, the gap changes its topology from a stripe running around \( \phi_i \) direction to a disc contractible to a point. Accordingly, also \( R \) changes its topology from two disconnected stripes running around in \( \phi_i \) direction to a connected set. At the same time, a new vertical \( \det J = 0 \) curve is created running between the two extremal points in \( \phi_i \) of the disc-shaped gap. See part (b) of the figure. With \( E_0 \) increasing further, the gap shrinks, and the right vertical \( \det J = 0 \) curve and the new middle \( \det J = 0 \) curve come closer see part (c) of the figure. At another critical value of \( E_0 \), these two vertical \( \det J = 0 \) curves touch at \( \phi_i = 3\pi/2 \), and change their topology as shown in part (d) of the figure. They change from two curves running around in \( \phi_i \) direction to a single contractible loop. Next, the gap disappears completely, as can be seen in part (e) of the figure, while also with increasing \( E_0 \), the contractible green \( \det J = 0 \) curve shrinks and finally
disappears. Simultaneously the right orange curve shrinks and disappears. The result is shown in part (f) of the figure. In the end, we have a single region of continuity running around in $\phi_i$ direction and containing a single vertical $\det J = 0$ curve also running around in $\phi_i$ direction. Thereby the scenario of the fusion of two typical regions of continuity into a single one is finished. This scenario is the direct generalization of the 2-dof scenario of the fusion of intervals of continuity, as described in Ref. [29]. For other regions of continuity similar transformations and fusions happen under a change of the energy.

In connection with Figs. 1, 4, 5, let us consider the fractal dimension $D$ of the set of singularities of the scattering functions and its dependence on parameters like $B_z$ or $E_0$. First, in Fig. 1, the fractal has a simple product structure; it consists of a collection of lines running in $\phi$ direction. Each line has dimension 1. In $b$ direction, we have a Cantor set with a fractal dimension $D_b$ which lies between 0 and 1. Therefore we find in total a dimension $D = D_b + 1$. When we compare Figs. 1 and 4, then we see that locally, the structure of the singularity set remains the same, and this suggests that also the dimension remains the same. In Ref. [30] a 4-dimensional model map for a 3-dof scattering system, has been investigated. When in this model map, a perturbation parameter $\epsilon$ is changed from 0 to 1, then the system changes from partially integrable to uniformly hyperbolic. In this system, the fractal dimension as a function of $\epsilon$ has been calculated and plotted in Fig. 5 of Ref. [30]. This dimension stays approximately constant in the interval $\epsilon \in [0, 0.1]$, which is the regime of small perturbation where the product structure essentially survives and starts to drop for higher perturbation. The dimension drops lower than the value 1 as soon as the system becomes hyperbolic. The model map from Ref. [30] is typical for the whole class of systems perturbed away from partial integrability. Therefore the present system should have similar behavior also. In contrast to this discreet map model system, the present system is always far away from complete hyperbolicity. Therefore in the present system, we can never see any interesting changes in the fractal dimension of the singularity set.

### 3.2 Stable and unstable manifolds in the 3-dof problem

Let us discuss the construction of the tangle between the stable and unstable manifolds in the 4-D Poincaré map for the 3-dof case following the ideas developed in Refs. [11, 12] for systems with one open and 2 dof. To explain the construction, we start with the case of zero oscillation amplitude, i.e., $B_z = 0$. In this case, the particle energy $E_0$ is conserved, and each slice, $E_0 = \text{constant}$, in the 4-D Poincaré map is invariant. The tangle in each one of such slices was already discussed in section 2 (see Fig. 3). Now, the higher dimensional tangle can be obtained in a two-step process. First, we form a stack with all curves taken from the whole continuum of 2-dof tangles, where the value of $E_0$ is the stack parameter. This union creates a 3-D object.

Second, we add to this object the phase variable of the oscillator by forming a Cartesian product of the 3-D stack with a circle representing the still missing variable $\psi$. In this way, we end up with a tangled structure in the 4-D domain of the Poincaré map for the 3-dof system; see Fig. 7. Notice, that this is still only for zero oscillator amplitude, $B_z = 0$.

In the 2-dof case of section 3 the tangle was created, starting from the fixed point at infinity ($z = \infty, p_z = 0$), by plotting the associated stable and unstable
Figure 7: The Cartesian product of the pile of 2-D tangles with the energy $E_0$ as stack parameter and a circle representing the angle $\psi$ form the tangle between the stable and unstable manifolds for the 3-dof system in the Poincaré map.

manifolds. The stack of these fixed points on the Poincaré maps corresponds to a vertical line on the plot, and the Cartesian product of this line with the circle corresponding to the oscillator phase generates an invariant cylinder at infinity.

In the 3-dof case, the analog of the central fixed point of the 2-dof tangle is a 2-D invariant surface. If the fixed point at infinity were hyperbolic, the resulting 2-D surface in the 4-D stack and the Cartesian product construction would be a normally hyperbolic invariant manifold (NHIM). In our case, this object is formally not a NHIM, but it plays an analogous role. For general information on NHIMs and their role in dynamical systems, see for example [9,31].

The stable and unstable manifolds $W^s/u$ of the invariant surface at infinity are also obtained by the same stack-and-product process as

$$W^{s/u} = \bigcup_{E_0} W^{s/u}_{E_0} \times S^1.$$  

(5)

Let us now consider the dimension of these manifolds. The dimension of the stable and unstable manifolds in the 2-dof case is 2 in the flow or 1 in the map. The pile of the stable and unstable manifolds, parametrized by the initial particle energy $E_0$, is a surface with dimension 3 in the flow or dimension 2 in the map. Then forming the product with a 1-D circle results in a 4-D surface in the flow of the 3-dof system or a 3-D surface in the domain of the map. Most important: The codimension of the stable and unstable manifolds is 1 in any case, and then the stable and unstable manifolds create a partition in the constant total energy manifold of the 3-dof system, and also in the domain of the Poincaré map. The invariant manifolds $W^{s/u}$ are impenetrable hypersurfaces that direct the flow similar to what happens in the 2-dof systems. Moreover, the stable/unstable manifold is the union of the trajectories with zero momentum in the $z$-dof in the incoming/outgoing asymptotic region.

So far, we have described the construction of the tangle for the 3-dof problem in the case of zero coupling, i.e., for $B_z = 0$. What happens when the coupling is switched on? If we would have a usual NHIM, then we could quote the theorem of Fenichel on the persistence of NHIMs and their stable and unstable manifolds, see, for example, Refs. [31,33]. However, in the present case, the invariant surface is stacked up by linearly parabolic points, which are only nonlinearly unstable. On the other hand, in this case, the interaction (see Eq. (2)) goes to

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zero exponentially for large values of $z$. Therefore, the invariant surface itself at infinity is not affected by the interaction. The tangle of the stable and unstable manifolds coming from the points at infinity contains hyperbolic components and in general, also nonhyperbolic components, as it is generally found in usual incomplete horseshoe constructions. The general experience indicates that for scattering processes, the hyperbolic part of the chaotic saddle dominates. In addition, the nonhyperbolic parts are less important and are influencing only very high levels of hierarchical in the resulting fractal structure. However, the hyperbolic parts are robust under small perturbations of the system, while the nonhyperbolic parts may change already under the smallest perturbations.

In total, we can expect that the stack of tangles maintains its large-scale structure also under moderate perturbations of the system, and therefore also under moderate coupling strengths between the particle dofs and the oscillator dof. As a result, the intersection of the perturbed stack with a plane surface should be similar to the intersection of the unperturbed stack with a curved surface. In this sense, the stack construction method provides us with a valid idea of the higher dimensional tangle and is also able to explain the dynamics of the system with coupling.

Now, we can understand from another point of view the changes in the structure of the set of singularities in the scattering functions for the coupled 3-dof system in Figs. 4, 5, 6. When the 3-dof system contains a perturbation, then the symmetry in the angle $\phi$ is broken, and the manifold $W^s$ is deformed and loses its symmetry with respect to $\phi$. And its intersection with the set of initial conditions change. If we change the set of initial conditions in the phase space, then the pattern of intersections is different. The plots of the various parts in Figs. 4, 5, 6 are scattering functions for different sets of initial conditions (different $E_0$), and their singularities show the pattern of the intersection of the stable manifold.

With the help of Fig. 2 and our new understanding, we can give still another interpretation of the change of the regions of continuity of the scattering functions under perturbations. Depending on the value of $\phi_i$, the value of the particle energy $E_0$ changes. Thereby the particle can change in Fig. 2 from the initial value of $E_0$ to a modified value of $E_0$, and this modification depends on $\phi_i$. Imagine that the initial value lies around 2, e.g., at the value 2.0125 used in parts (b) of the Figs. 4, 5, 6. Here the region $R$ is very close to the value where it switches in Fig. 2 from having 2 components to having 1 component. For $\phi_i$ values around $-\pi/2$ the particle energy is increased (see Fig. 4(b)) and correspondingly the system runs into the situation where along the $b$ direction $R$ has 1 component and for $\phi_i$ values around $\pi/2$ the particle energy is decreased (see again Fig. 4(b)) and the system runs into the situation where along the $b$ direction $R$ has 2 components. This is exactly what we observe in the parts (b) of the Figs. 4, 5, 6. Considerations of this type only hold for weak perturbations where the homoclinic/heteroclinic tangle still has the stack structure.

### 3.3 The cross-section and its connection with the scattering functions

We assume an incoming beam, as explained before. The detector should measure the distribution of the values of the outgoing particle energy $E_f$, or equivalently and even better, the energy transfer $\Delta E$ and the outgoing angle of inclination...
θ_f. This detector registers neither the outgoing phase shift φ_f nor the value of the outgoing impact parameter b_f. The result in this type of measurement is the doubly differential cross-section \( \frac{d\sigma}{d\theta d\Delta E} (\theta_f, \Delta E) \) for fixed values of the initial energy \( E_0 \) and fixed initial angle of incidence \( \theta_i \).

Now, let us discuss the geometrical connection between the scattering function and the cross-section. Remember that the relevant scattering function for the construction of the cross-section is the function whose domain and range are the \( b - \phi_i \) and \( \Delta E - \theta_f \) planes, respectively. This function can be viewed as a graph in the Cartesian product of the 2-D domain with the 2-D range, i.e., in the 4-D \( (b, \phi_i, \Delta E, \theta_f) \) space. The incoming beam represents a constant density on the domain, and the function maps this density into the range. The differential cross-section defined above is the resulting density in the range. This connection is expressed as follows

\[
\frac{d\sigma}{d\theta d\Delta E} (\theta_f, \Delta E) = \sum_i \left| \frac{\det \left( \frac{\partial (\theta_f, \Delta E)}{\partial (b, \phi_i)} \right)}{\det \left( \frac{\partial (\theta_f, \Delta E)}{\partial (b, \phi_i)} \right)} \right|^{-1},
\]  

where the sum runs over all preimage points in the domain, i.e., in the \( b - \phi_i \) plane, leading to the values \( \theta_f, \Delta E \) in the range of the scattering function. It is clear that the cross-section has singularities where the projection of the graph into the range is singular, i.e., where the determinant of the Jacobian matrix of the scattering function appearing in the previous equation is zero, i.e., they are the lines already studied in subsection 3.1 and Fig.6. The resulting singularities in the cross-section are the well-known rainbow singularities of the differential cross-section, and they are the lines over which the number of preimages changes (in general by 2). In a general 3-dof system, there are lines along which the rank of the Jacobian matrix drops by 1, and there can also be points at which the rank drops by 2. For a good explanation of rainbow singularities, see chapter 5 in Ref. [34]. Note that generic rainbow singularities are of one over square root type, and therefore the integral over them is finite. At the points where the rank of the Jacobian matrix in Eq. (6) drops by 2, there might be singularities of another functional form, however also here the integral over the differential cross-section is always finite. There is no violation of flux conservation.

In the present system, most regions of continuity of the scattering function are stripes running around in \( \phi_i \) direction or annular shaped regions, see Fig.4. However, under a change of the energy, the processes of fusion of regions of continuity happen as explained in all details in subsection 3.1. In the rest of this subsection, we will study how the process of fusion shown in the Figs.4, 5, 6 shows up in the cross-section.

If we project the graph of the scattering function of one vertical stripe or also of one disc-shaped region of continuity into the plane \( \Delta E - \theta_f \) we can see a caustic like the one coming from the projection of a deformed semi-torus, this structure is characteristic of 3-dof systems with 1 open dof and 2 closed dofs [12], it is one normal form for these projection caustics. A more detailed explanation for this structure is the following.

First, let us consider the unperturbed case. In the inner part of a vertical stripe of continuity, the scattering function is flat in the \( \phi \) direction, and we have a kind of half semi-torus in the plot of the scattering function, remember that \( \phi \) is a periodic variable and that the vertical stripe closes to a ring. The projection of this graph on the plane \( \Delta E - \theta_f \) is a curvilinear rectangle, this being
due to the symmetry of the system. And it is a 4:1 projection. If we perturb the system, the rotational symmetry is lost, and the plot of the scattering function is deformed. The semi-torus is then deformed, and it is no longer of constant height; accordingly, the caustics change, and also, some regions are formed where we find a 2:1 projection. For the perturbed case, the caustics have the same qualitative structure for different values of the perturbation parameter as long as we are in the regime of weak perturbation. Analogous considerations hold for the contractible ring-shaped regions of continuity.

The complete caustic structure of the entire cross-section is a superposition of the various basic caustic structures coming from all the different regions of continuity. Of course, the various structures are shifted in their exact position, and they have different heights and different total strength. This total strength is proportional to the area of the corresponding interval of continuity because it must be proportional to the incoming flux falling into this particular interval of continuity.

The Fig. 8 shows a plot of the cross-section for $\theta_i = 80^\circ$ and for the 6 different values of the initial energy $E_0$, which also have been shown in Figs. 4, 5, 6. In the plots, the basic structure of the singularities of the projection of the plots of the disc-shaped regions of continuity of the scattering function is apparent.

First, let us look at part (a) of the Figs. 4, 5, 6 for $E_0 = 1.9$. Here the scattering function has 3 important regions of continuity. The first one, the outer region, which occupies the largest area in the domain and which accordingly causes the strongest structure in the cross-section. It is the strong structure reaching up to rather small values of $\theta_f$. It comes close to a rectangle, which is the result of a 4:1 projection of a semi torus. In addition, we see also strong structures coming from the two separate components of the region $R$ defined in subsection 3.1. Because we are mainly interested in the contributions from region $R$, we repeat in part (b) the cross-section again for $E_0 = 1.9$ where however, we have illuminated a neighborhood of the region $R$ only. Thereby the structures caused by region $R$ are clearly visible. They are two of the above mentioned deformed torus-shaped structures. The structures reaching up to smaller values of $\theta_f$ is the one coming from the left part of $R$ in Figs. 4, 5, 6.

Now let us proceed to $E_0 = 2.0125$. The cross-sections with complete and partial illumination of the domain of initial conditions is plotted in parts (c) and (d) of Fig.8. When we compare parts (b) and (d) of the figure, then we see the beginning of the fusion process in the upper right part of the main structure. Parts (e) and (f) show the complete and the partial cross-section for $E_0 = 2.1$. Here the fusion has proceeded to strong deviations compared to $E_0 = 1.9$. Parts (g) and (h) show the cross-sections for $E_0 = 2.16$ and parts (i) and (j) show it for $E_0 = 2.175$. Here the region $R$ has already turned into a single vertical stripe. However, as Fig.6 (e) shows there are still remnants of the additional det $J = 0$ curves which create the additional rainbow structures around $\theta_f \approx 7\pi/16$. Finally, the parts (k) and (l) show the cross-section for $E_0 = 2.45$, where the transformation process of the region $R$ is finished. Here the rainbow structure coming from $R$ is again just the projection of half a torus.

The sequence of changes we have just seen is the typical one for any fusion of regions of continuity of the scattering functions. It is the 3-dof generalization of the 2-dof fusion events explained in Ref. [29].
Figure 8: Scattering cross-section for $\theta_i = 80^\circ$ and for the 6 values $E_0 = 1.9$, 2.0125, 2.1, 2.16, 2.175 and 2.45 in the parts (a) and (b), (c) and (d), (e) and (f), (g) and (h), (i) and (j), (k) and (l) respectively. The parts (a), (c), (e), (g), (i) and (k) in the left column show the cross section for a constant illumination of the whole $b - \varphi_i$ plane. The parts (b), (d), (f), (h), (j), (l) show it for partial illumination of a neighbourhood of the region $R$ only.
Figure 8: Continuation

(g) $E_0 = 2.16$

(h) $E_0 = 2.16$

(i) $E_0 = 2.175$

(j) $E_0 = 2.45$

(k) $E_0 = 2.45$

(l) $E_0 = 2.45$
4 Remarks and conclusions

We studied the chaotic scattering in a 3-dof Hamiltonian model with one open and 2 closed dof. To start the study of the 3-dof system, it is convenient to consider the family of 2-dof systems parametrized by the initial energy of the particle $E_0$ associated with the elastic system, the scattering functions, and its set of singularities. The set of singularities reflects the structure of the stable and unstable manifolds that divide the constant energy manifold of the total system and direct the dynamics. When the surface oscillates, the particle exchanges energy with the surface, but these invariant manifolds are robust under small perturbations.

The natural scattering function for this system gives the change of the energy and the final scattering angle as a function of the initial impact parameter and the initial phase of the oscillation of the surface $(\Delta E_0(b, \phi_i), \theta_f(b, \phi_i))$. The double differential cross-section is the projection of the graph of the scattering function on the range of the scattering function, the singularities of the projection are the caustics.

The structures of the caustics are related to the regions of continuity of the scattering function and the curves where the Jacobian determinant of the scattering function is zero, $\det J = 0$. The regions of continuity generate characteristic types of structures on the cross-section; it is like a projection of a semitorus in the $\Delta E_0 - \theta_f$ plane. An increment in the value of the initial particle energy creates changes in the regions of continuity of the scattering functions and in the set of curves $\det J = 0$, and we can see clearly how those changes are reflected in the fusion of the caustics on the cross-section.

The present system helps to clarify the elementary transitions in the scattering functions and the corresponding transitions in the cross-section in other systems with qualitatively similar changes in the scattering function, for example 3-dof systems with a perturbation of partial integrability [11], [12], [35], a perturbed magnetic dipole [14], and a realistic molecular system treated in [36]. The considerations of subsections 3.1 and 3.3 hold for all the above mentioned system in an analogous form. Note that Ref. [36] is a system with 2 open degrees of freedom, and accordingly, the structure of the vertical $\det J = 0$ lines is more complicated. The scattering function oscillates in the interior of regions of continuity, and this leads to a sequence of vertical $\det J = 0$ lines in each region of continuity. Otherwise, the basic phenomena are the same.

For any scattering system, there is always the interesting question of the inverse scattering problem. For chaotic scattering, one considers this problem as the problem to reconstruct information on the chaotic invariant set from scattering data, in particular from cross-section data. So far, for 3-dof systems, there is a general strategy to do this job only for the uniformly hyperbolic case, see Ref. [28]. However, these hyperbolic cases are always far away from any stack construction; they are a kind of opposite extremal case to the partially integrable case. Therefore they do not provide any clue for our present case, which is a case of mixed-phase space close to partial integrability.

Finally, we offer some remarks about the implications of the classical scattering results for the quantum scattering problem in the semiclassical regime. Classically the cross-section is a sum over contributions from all preimages, see Eq.6. Semiclassically, the scattering amplitude is a corresponding sum over the square roots of the classical contributions where each contribution gets, in ad-
dition, a phase which is the complex exponential function of the reduced action along the corresponding path. And the semiclassical cross-section is the absolute square of the semiclassical scattering amplitude, and thereby it is a double sum. Accordingly, the semiclassical cross-section is a sum of the classical cross-section coming from the diagonal terms of the double sum and a double sum of the nondiagonal interference terms. Thereby the resulting cross-section contains interference oscillations superimposed over the classical cross-section.

In addition, a semiclassical approach should uniformize the rainbow singularities and remove, thereby, the infinities. In a generic rainbow line, 2 classical contributing paths coincide and disappear. Then the uniformized semiclassical contribution of these 2 classical paths to the semiclassical scattering amplitude can be modeled by an Airy function, which is the normal form of a wave rainbow contribution. The contribution of a point where the rank of the Jacobian determinant of the scattering function drops by 2 should be described by some other appropriate catastrophe function. For more detailed information on the semiclassical treatment of chaotic scattering see Refs. [37], [38], [39], [40].

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