Topological aspects of chaotic scattering in higher dimensions

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We investigate the topological properties of the chaotic invariant set associated with the dynamics of scattering systems with three or more degrees of freedom. We show that the separation of one degree of freedom from the rest in the asymptotic regime, a common property in a large class of scattering models, defines a gate which is a dynamical object with phase space separating invariant manifolds. The manifolds form an invariant set causing singularities in the scattering process. The codimension one property of the manifolds ensures that the fractal structure of the invariant set can be studied by scattering functions defined over simple one-dimensional families of initial conditions as usually done in two-degree-of-freedom scattering problems. It is found that the fractal dimension of the invariant set is not due to the gates but to interior hyperbolic periodic orbits.

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I. INTRODUCTION

Chaotic scattering in open Hamiltonian systems with two degrees of freedom (dof) has become a well understood phenomenon [1]. A central role is played in these processes by the *chaotic invariant set* which consists of all the bounded orbits, i.e., those without the simple incoming and outgoing asymptotic motions characteristic of the system. Scattering trajectories starting close to the stable manifold of the invariant set can show temporarily chaotic behavior in its vicinity before eventually escaping along the unstable manifold. For initial conditions exactly on a stable manifold branch, the trajectories may even become asymptotically trapped by bounded orbits; this leads to singularities on a fractal set in the scattering functions.

Our goal here is to try to extend the detailed comprehension that we have in 2 dof towards 3 dof. For dimensional reasons and topological reasons, the 3-dof case is vastly more difficult than the 2-dof one. This is explained in detail in Sec. II.

Some steps towards the comprehension of 3-dof dynamical systems exist in the literature, whether for transport in general [2], for systems nearby integrability [3], or for chemical systems [4,5]. It is the authors' opinion that phase space transport theory and chaotic scattering theory [1] are in a sufficiently advanced stage by now. Thus, some steps may be safely taken in the direction of a dynamical and geometrical analysis of chaotic scattering in higher dimensions, in the same way as has been undertaken for 20 years for 2-dof systems.

In this paper, we show that in a large class of common scattering problems the separation of one translational degree of freedom from the rest in the asymptotic region defines invariant subspaces. These invariant subspaces are dimension-wise large enough so that chaotic invariant sets may be defined with the help of their invariant manifolds. We will demonstrate these points using a simple planar three-body scattering problem as an illustrative example. This example bears some similarities to the example we used in the past for 2-dof scattering.

II. DIMENSIONS, SEPARATRICES, AND GATES

The vast majority of studies concerning Hamiltonian dynamics is concerned with 2-dof systems, at least as far as actual systems and applications are concerned. The main reason for that is of course the question of dimensionality. Since this is the main concern of this paper, let us discuss this point in some detail. Two facts facilitate the study of 2-dof Hamiltonians (see Table I). First, a Poincaré section that is transverse to the flow is a two-dimensional manifold, easily depicted on a sheet of paper or a computer screen. Second, and maybe more important, invariant objects that are codimension 1 in the energy level naturally arise in 2-dof systems, as stable/unstable manifolds of periodic orbits (Table I). These codimension 1 objects are especially important in scattering system: in the asymptotic region, they will determine the final outcome of a scattering experiment. Indeed, these invariant objects induce a division in the asymptotic phase

TABLE I. Dimensionalities of invariant objects arising in the energy level of a Hamiltonian flow. The codimension of the object in the energy level is indicated in parentheses, when relevant. The nature of the gate depends on the number of degrees of freedom, see text.

	Dimensions and codimensions		
Degrees of freedom	2	3	N
Phase space	4	6	$2N$
Energy level	3	5	$2N-1$
Poincaré section	2	4	$2N-2$
Periodic orbit	1 (2)	1 (4)	$1(2N-2)$
Gate	1 (2)	3 (2)	$2N-3(2)$
Stable/unstable manifolds of the gate	2 (**1**)	4 (**1**)	$2N-2$(**1**)

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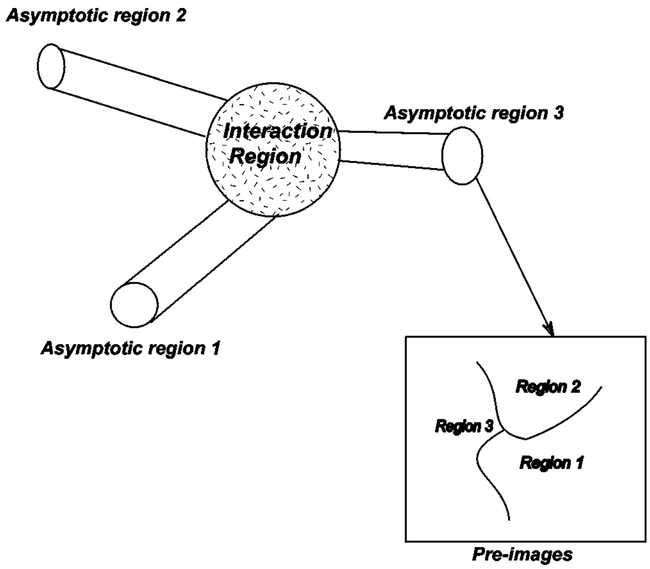

FIG. 1. A very schematic view of the scattering event, with three channels displayed. In asymptotic region 1, three regions are displayed: they correspond to the three preimages of the three asymptotic regions. Any trajectory originating in preimage i will eventually be transported by the flow towards region i. The regions are separated by separatrices, which, in reality, are much more complicated.

space between the different channels of the scattering event. That is, the Hamiltonian flow connects the different outgoing asymptotic regions to the incoming asymptotic regions. The limit of those regions is given by the condimension 1 invariant objects; these manifolds act as effective boundaries (see Fig. 1).

Inspection of Table I shows that for a 2-dof system, codimension 1 invariant manifolds naturally arise. They are the stable and unstable manifolds associated with very well known objects: periodic orbits and equilibrium points having invariant stable and unstable manifolds. The relevant periodic orbits are the unstable ones (their associated linearized map have a pair of real eigenvalues), whose invariant manifolds extend smoothly towards the asymptotic regions. The relevant equilibrium points are of the stable/unstable type (their linearized map have one pair of real eigenvalue and one pair of purely imaginary eigenvalues). The stable unstable manifold may also extend smoothly towards the asymptotic regions. Since these objects (the periodic orbit and the equilibrium points) give structure to the whole phase space, they are called *the gates* of the scattering event. A lengthy discussion of their role have been put forward in our earlier work, for 2-dof scattering [6–8].

Finally, it must be underlined that the stable/unstable manifolds under discussion intersect generically, both being of codimension 1. Thus, a chaotic invariant set is readily found by forming these intersections, which appear as a fractal set of points on a Poincaré section.

With three degrees of freedom, the nature of the problem changes. Periodic orbits, even if always present, are no more the main dynamical objects, as far as boundaries and invariant objects are concerned. Indeed, depending on the specific case at hand, their invariant stable/unstable manifolds may have a codimension 3 in the energy level, meaning that they would cross the four-dimensional Poincaré section as an object of codimension 3 (a line) and of codimension $1+3$ in the energy level. By no means may this be considered as an effective boundary.

Table I show that there exist invariant objects which are candidates for generating separatrices, and hence possibly act as gates. As has been pointed out by Wiggins [2,9] that there may exist large invariant objects in phase space, whose stable/unstable manifolds may act as separatrices. In the three-dimensional configuration space of a three degrees of freedom system, such an object could be a two-dimensional invariant subset. It would be hyperbolic in the perpendicular (noninvariant) direction. Consequently, both the stable and unstable manifolds would be invariant manifolds, of codimension 1 in the energy level. Intersection of these stable/unstable manifolds with Poincaré section yields again a codimension 1 object. This is very convenient, since a two-dimension cut of the four-dimensional section will display generically the stable or unstable manifolds as simple curves, even if these lines may be very complicated, due to the folding and stretching mechanism associated with the Hamiltonian flow.

Also, stable/unstable manifolds, should intersect generically, yielding a codimension 2 invariant chaotic set. Finally, such objects can act as gates to a scattering process, provided their location in phase space makes it possible. We shall describe such gates in detail (Sec. IV), after having described our simple model (Sec. III). Some conclusion will be drawn afterwards, and an Appendix describes in detail the equations of motion, since these are not very well known outside of the chemical physics community.

III. A SIMPLE MODEL

A typical scattering problem appearing in many contexts is a single particle interacting with a two-body system; the most common examples are from chemical physics (reactive collisions) and celestial mechanics (planetary motion). Models of this type have been studied in several varieties, including ones restricted to 2 dof. In fact, reactive collisions in collinear or T-shape configurations [6,10] or the interaction of satellites in coplanar circular orbits (Hill's problem) [11] are well-known representatives of chaotic scattering. However, a more general treatment involving more than 2 dof in these systems and similar ones is clearly necessary.

For this purpose, we have chosen a planar atom-diatom collision of total angular momentum $J=0$ with pairwise Morse potentials between the atoms, at a total energy E below the complete dissociation threshold so that scattering consists of an exchange reaction. There are three qualitatively different channels corresponding to which of the three atoms escapes after the decay of the transient complex. Since we are more interested in the general topological properties of chaotic scattering rather than in accurate modeling of particular chemical reactions, we have chosen

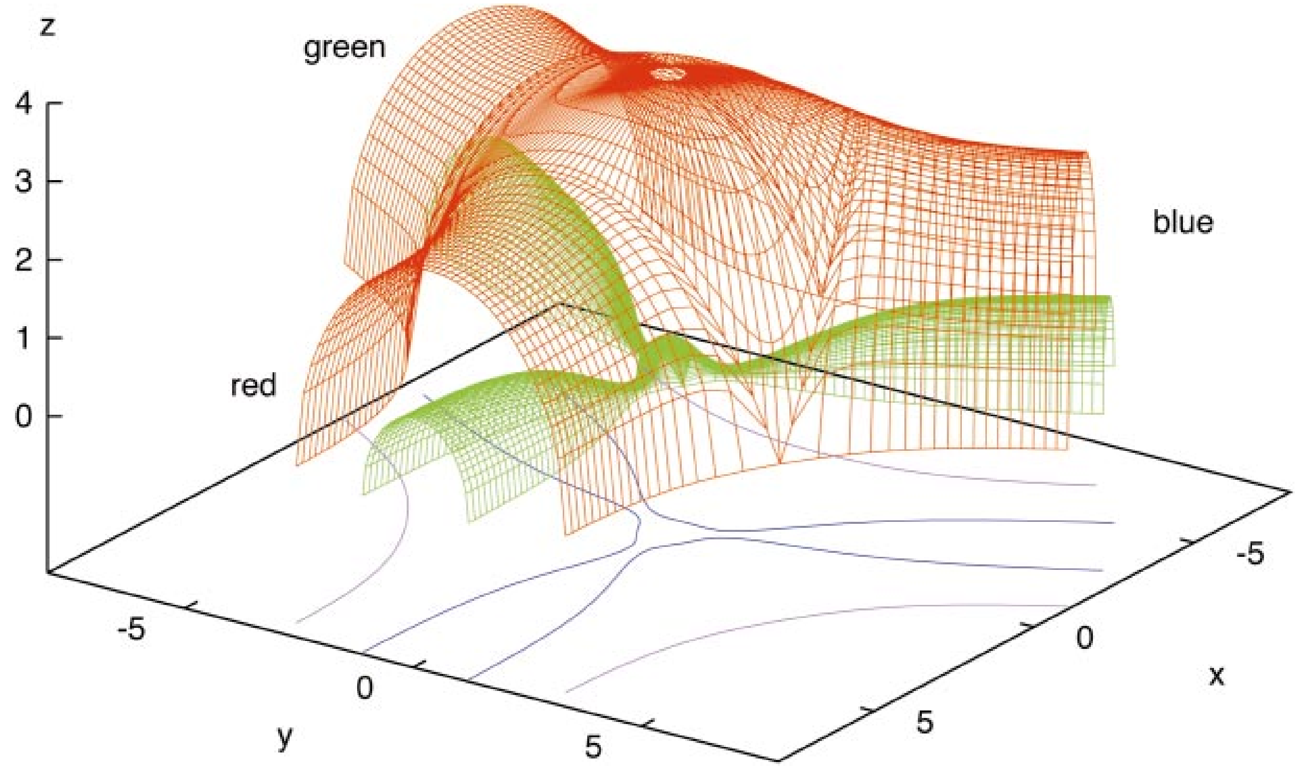

FIG. 2. (Color) Zero-kinetic energy surfaces in the abstract representation for $E=2.4$. Because of the mirror symmetry of the potential, only the $z\geqslant 0$ halves are shown. Trajectories must stay between the red and green surfaces. The $z=0$ contours on the base are $K=0$ curves for collinear configurations. The labels next to the exit channels give the color coding used in Fig. 3 for the outcome of the scattering process.

identical atomic masses and Morse potential parameters for simplicity.

In a center-of-mass coordinate system, the total number of dof for this process is four, with E and J conserved. By choosing suitable new coordinates, the angle variable conjugate to J can be separated from the other three which still contain all the information on the relative distances of the atoms; thus we obtain a reduced model with only three dof. For our purposes, the most appropriate choice is an abstract representation of the configuration by Cartesian coordinates (x,y,z) based on hyperspherical coordinates widely used for three-body problems [12–14]. The new variables and their time derivatives can then be used to express the kinetic energy K [13] and the interatomic distances r_{12}, r_{13}, and r_{23} [14]. The actual expressions are rather complicated and not reproduced here for lack of space. We refer the interested reader to the literature on these coordinate systems, especially the references given above. The Hamiltonian takes the (dimensionless) form

$$H(x,y,z,p_x,p_y,p_z)=K+V_M(r_{12})+V_M(r_{13})+V_M(r_{23}), \tag{1}$$

where $V_M(r)=(1-e^{-r})^2$ is the Morse potential. The explicit Hamiltonian and the equations of motion can be found in Eqs. (60)–(66) of Ref. [13].

Important symmetries and special cases are reflected in these coordinates. The potential is mirror symmetric with respect to the plane $z=0$, containing collinear configurations, while the plane $y=0$ and its two images obtained by rotation around the z axis by $\pm 2\pi/3$ correspond to symmetric T-shape configurations. For a given energy E below the total dissociation threshold $E_{\rm tot}=3$, z is confined to a range $[-z_{\rm max},z_{\rm max}]$, but x and y can be arbitrarily large. The three channels corresponding to possible outcomes of the reaction extend to infinity along the intersection lines of the T-shape planes with the collinear one. The boundaries of the three-dimensional energy surface, defined by $K=0$, are plotted in Fig. 2 as level surfaces in the abstract (x,y,z) space for a typical scattering energy.

Far from the origin, the escape channels have an asymptotic axial symmetry due to the separation of the translational motion of the outgoing single atom from the bound rotation/vibration of the molecule (a two-dimensional Morse oscillator). This observation provides us the key point concerning the topological properties of the system.

IV. THE GATE AND ITS INVARIANT SET

In scattering systems like ours that asymptotically separate into a subsystem with $n-1=2$ dof plus 1 translational dof, a two-dimensional (2D) invariant object naturally exists: it consists of the 2-dof subsystem plus the free particle resting infinitely far away from it. In fact, it has been shown by Toda [15] that in a planar atom-diatom collision the dynamics of the molecule and the third atom at rest defines an object in the four-dimensional Poincaré section with three-dimensional stable and unstable manifolds.

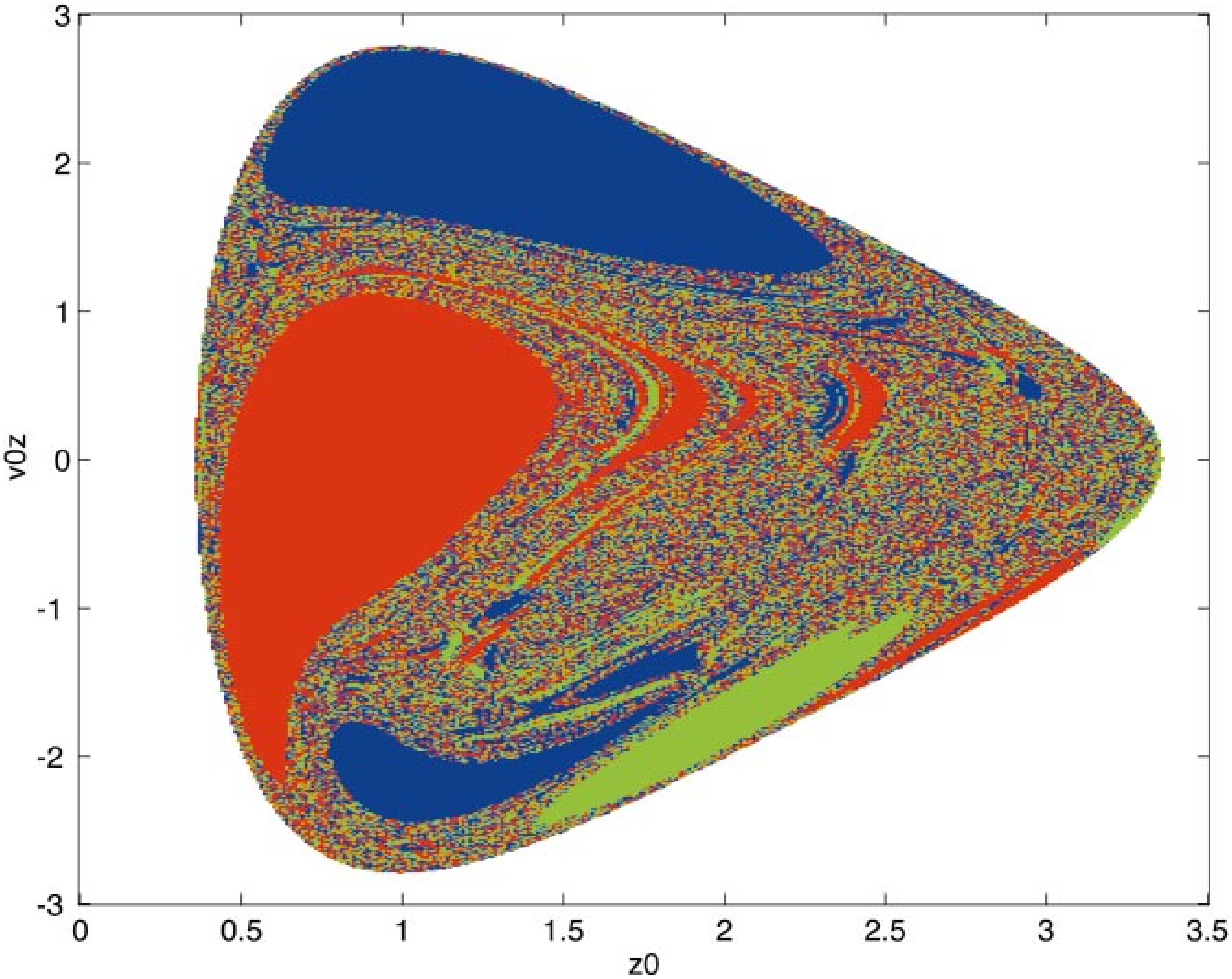

FIG. 3. (Color) Initial conditions from the 2D subspace of the Poincaré section colored according to the corresponding exit channels. The boundary curves of single-color regions are the slices of the stable manifold of the gate object.

By definition, the intersection points of the stable and unstable manifolds of an invariant object define an invariant set for the dynamics. In our scattering model, the gate objects in configuration space are two-dimensional subsets (annuli) at the ''end'' of the outgoing channels. In the Poincaré section, such a gate appears as a two-dimensional, too. In the remaining two dimensions in its vicinity, one can draw a curve from each point of the gate so that initial conditions on the curve will lead to asymptotic convergence to the orbit started from the point on the gate. The stable manifold of the gate is then the collection of these curves forming locally a three-dimensional object.

Because of the global stretching and folding generated by the nonlinear dynamics of the system, this stable manifold also has a fractal structure in the direction perpendicular to it, so globally it has a total dimension $d_g = 3+\delta$ with $0<\delta<1$ being the partial fractal dimension in the perpendicular direction. Because of time reversal symmetry, the unstable manifold must have the same dimension. Their intersections define an invariant set with a dimension

$$d_s = 2d_g - D = 2 + 2\delta, \tag{2}$$

where $D=4$ is the dimension of the Poincaré section. This set contains all the bounded orbits of the system and is responsible for the chaotic properties of the scattering.

Following the approach of Chen *et al.* [16], we represent the stable and unstable manifolds and the invariant set on a planar (two-dimensional) cut of the four-dimensional Poincaré section by choosing initial conditions with two fixed restrictions and two free parameters. Our Poincaré section for the triple Morse system is defined by $y=0$ (with $v_y>0$) while the restrictions in the initial conditions are $x_0+z_0=0$ and $v_{0x}+v_{0z}=0$. In Fig. 3, we plotted initial points in the (z_0, v_{0z}) plane in colors depending on the exit channel eventually taken by the corresponding trajectories (cf. Fig. 2). The most important point is that in this picture, all three colors form (locally) compact regions with smooth boundaries. The boundary of a single-colored region consists of trajectories with vanishing translational kinetic energy at the ''end'' of the channel, i.e., asymptotic to the corresponding gate object. In other words, the boundary curves of regions of a given color are just the planar sections of the stable manifold of the gate closing the channel associated with that color. On the outer side of these curves, smaller, differently colored regions can be found, accumulating on the boundaries in a fractal manner. Similar pictures have been presented [17] for the gravitational three-body problem.

In fact, the stable manifold curves in Fig. 3 are an example of Wada boundaries [18], i.e., fractal boundary sets where all three colors are present in any neighborhood of boundary points. It is worth noting that in chaotic scattering processes with more than two outgoing channels, Wada boundaries are typical [19,20], but such objects can also appear, e.g., as physical boundaries between dyes of different color poured into open hydrodynamical flows [21]. It must be also noted that these manifolds may have other types of topologies, if energy level boundaries have other topologies and/or symmetries [22]. It is not so much the properties of the boundaries that the very existance of regions of one color (basins) that is of importance, on the physical point of view. Indeed, since the basins are of non zero measure, the result of actual experiments are not totally unpredictable, but simply depend on which basin the initial conditions fall. As basins exist at all scales, the characterictic behavior of chaotic scattering in two degrees of freedom is maintained in three degrees of freedom, as boundaries of Wada type exist.

Due to the special symmetries of the section chosen for Fig. 3, the unstable manifold curves in that plane can be obtained by simply mirroring the stable manifold curves with respect to the z_0 axis. Then we can plot an approximation of the gate invariant set by considering a color pixel as a cross section point of the stable and unstable manifold if both itself and its mirror image on the other side of the z_0 axis have at least one neighbor cell of different color. The result is shown on Fig. 4; the fractal nature of the plot is indicated by a blowup. Since the invariant set is of dimension $d_s = 2 + 2\delta$, each point in this plot represents a smooth two-dimensional object in the total invariant set embedded in the four-dimensional Poincaré map. In other words, our plot captures the fractal part of the gate invariant set; its fractal dimension is 2δ.

V. LINEAR SECTIONS AND SCALING PROPERTIES

One of the convenient characteristics of two dof chaotic scattering is that its scaling properties can be studied through one-dimensional sets of initial conditions. However, this property may or may not be true in general hyperbolic chaotic scattering with 3 dof, depending on the fractal dimension of the invariant set and its stable manifold [16]. In this paper, we provided evidence that in three dof scattering systems with the asymptotic separation of 1 dof, the feasibility of the one-dimensional description is restored. The reason for this is that the crossing of three-dimensional stable manifolds with a line in a four-dimensional space is a generic property. Thus, typically any one-dimensional family of initial conditions would yield scattering function plots with a fractal set of singularities, as in 2-dof chaotic scattering. These singularities are the fingerprints of the fractal structure of the stable manifold of the gate, so their fractal dimension is just δ.

We have checked this point by plotting the scattering time for various linear sets of initial conditions in our triple Morse model. They all showed the typical singular behavior well known from two dof chaotic scattering examples. We also determined for the set of singularities the *uncertainty exponent* α_u, related to the (partial) fractal dimension as $\delta = 1 - \alpha_u$ [23]. One can measure α_u by choosing pairs of initial conditions with a separation of ε along the line: the rate $p(\varepsilon)$ of pairs where the two orbits escape along different channels scales as $p(\varepsilon) \sim \varepsilon^{\alpha_u}$. We have obtained $\alpha_u = 0.12$, which gives a fractal dimension $\delta = 0.88$ for the stable manifold of the gates. As in our earlier work [6], this result holds only for an intermediate (although broad) range of scattering times, due to the fact that the dynamics is not fully hyperbolic.

It is worth noting that although we measured the fractal dimension of the stable manifold of the gates, this scaling behavior cannot originate from the gates themselves since they are only marginally unstable due to the behavior of the Morse potential: The marginal instability of the gates should lead to an asymptotic fractal dimension value of 1. However, if our statistics is based on moderately long scattering orbits, we can still observe a scaling region associated with an apparent fractal dimension which is lower than 1 as if there were only hyperbolic orbits in the system. In our model, the only hyperbolic orbits are the inner (three-body) periodic orbits, so the observed scaling can only be produced by them. This indicates that they can dictate the fractal scaling properties of the invariant set as in two dof problems in spite of the fact that now the gate is not a periodic orbit.

VI. CONCLUSIONS

We have shown in a simple example that for a large class of 3-dof chaotic scattering systems, the asymptotic separation of a translational dof leads to gate objects with codimension one invariant manifolds capable of controlling the escape process. The intersections of these manifolds form an invariant set with two smooth and two fractal directions in the four-dimensional Poincaré map. The stable manifold of the gate defines disjunct smooth regions for asymptotic initial conditions containing topological different trajectories. Thus, fractal properties of the scattering can be captured in one-dimensional cuts of phase space as in 2-dof systems.

We have also shown that the inner periodic orbits can affect scaling properties of the gate invariant set. In this context, it is important to notice that periodic orbits do not have codimension one invariant manifolds. This leaves open the question whether another invariant set defined as the closure of the set of all three-body periodic orbits would coincide with the gate invariant set (this is true for 2-dof problems). If yes, then the locally two-dimensional manifolds of inner periodic orbits must conspire to form smooth surfaces along the gate manifolds; otherwise we arrive at the equally nontrivial

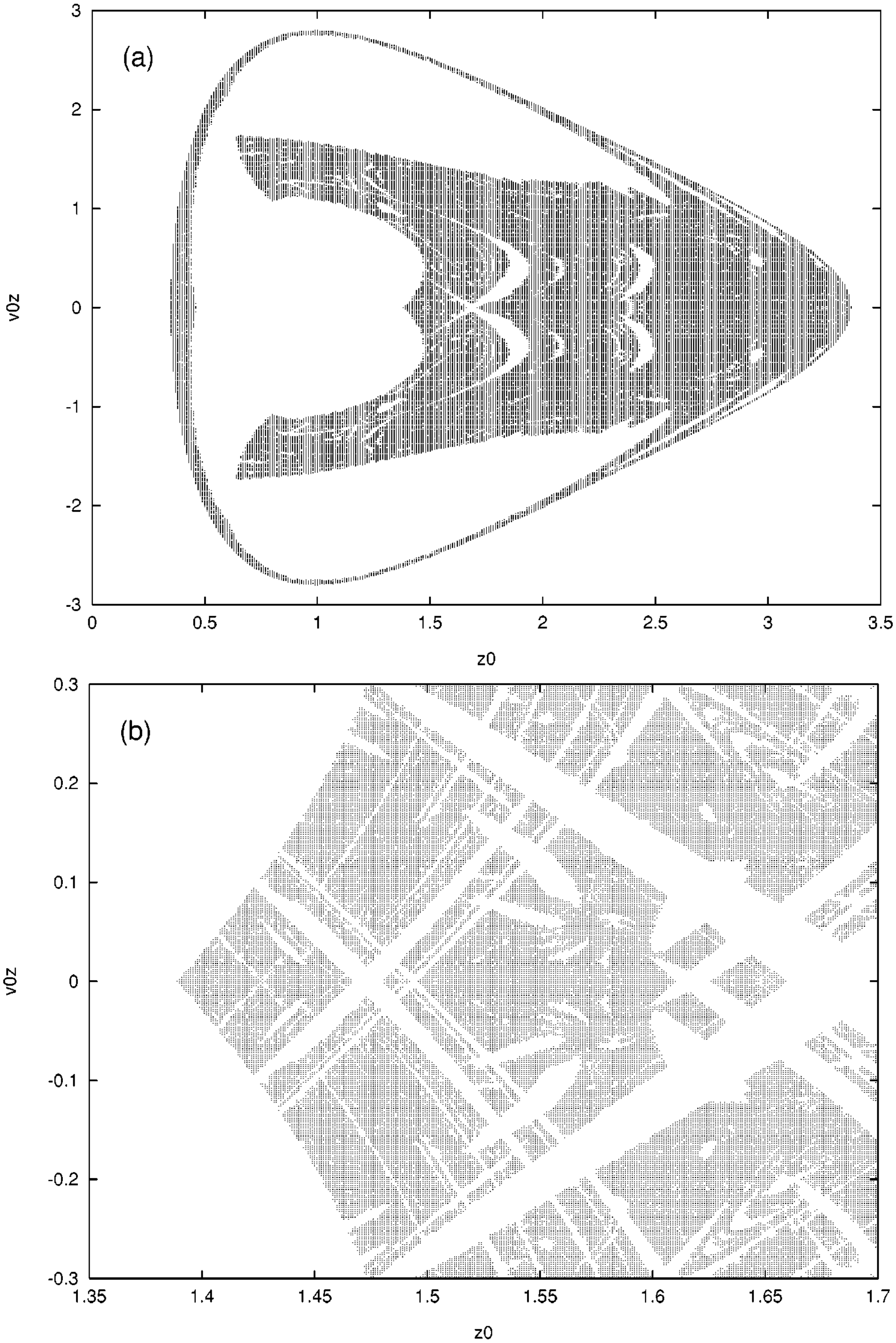

FIG. 4. Approximation of the planar section of the gate invariant set (a). The fractal structure of the picture is indicated by the blowup (b) of a small region looking homogeneous at a lower resolution.

conclusion that these periodic orbits are nowhere dense in the gate invariant set. Further efforts to clarify this question are underway.

Although we treated only one example in three dof chaotic scattering, our findings can be generalized to any Hamiltonian problem described by a four-dimensional Poincaré map with a suitable two-dimensional invariant subspace. Another possible extension is considering systems with more than 3 dof: if there is an asymptotic separation of only one dof from the rest, then, in principle, gate objects can be defined in an analogous way, and the topological consequences can be similar too. An obvious example is the full spatial dynamics of a three-body collision that can be reduced to four nontrivial degrees of freedom.

APPENDIX A: COORDINATES AND HAMILTONIANS

While the equations of motion have been published at several instances, we recall here the form of the Hamiltonian equations, as well as the connection between physical interparticle distances and abstract Cartesian coordinates. While this derivation could also be performed for a nonzero total angular momentum J (see Ref. [24]), we prefer keeping $J=0$ for simplicity. Everything can be found in the literature, see, for example Refs. [12] and [13].

A.1 Coordinates

In order to properly define the Hamiltonian, one has to go through a series of transformations, from natural interparticle distances, to Jacobi mass-scaled coordinates and eventually to the Cartesian coordinates used in this paper. Let us call the three particles A, B, C, and again for simplicity, let their masses be $m_{A,B,C}=1$, distances $R_{A,B}$. The plane formed by the three atoms Π is invariant. Let μ be the reduced mass ($M=3$, total mass):

$$\mu=\sqrt{\frac{m_A m_B m_C}{M}}=\frac{\sqrt{3}}{3}.$$

We define next the mass reduction factor

$$d_A^2=\frac{m_A}{\mu}\left(1-\frac{m_A}{M}\right)=\frac{2\sqrt{3}}{3}.$$

Let $\mathbf{x}_A$ be the coordinates in the Π plane of atom A. The two Jacobi coordinates are

$$\mathbf{r}_A=d_A^{-1}(\mathbf{x}_B-\mathbf{x}_C), \tag{3}$$

$$\mathbf{R}_A\mp d_A\left(\mathbf{x}_A-\frac{m_C\mathbf{x}_C+m_B\mathbf{x}_B}{m_B+m_C}\right). \tag{4}$$

It must be underlined that the Jacobi coordinates are not ‘‘democratic,’’ since atom A is singled out. This will be taken care of with the help of the hyperspherical coordinates.

The spherical hyperradius ρ is defined as the overall size of the system. Everything has an A index, but we leave it out for the ease of the notation:

$$\rho^2=r^2+R^2. \tag{5}$$

The shape of the ABC triangle is described by two angles θ, ϕ.

$$|r|^2-|R|^2=\rho^2\sin\theta\cos\phi,$$

$$2\mathbf{r}\cdot\mathbf{R}=\rho^2\sin\theta\sin\phi, \tag{6}$$

$$2|\mathbf{r}\wedge\mathbf{R}|=\rho^2\cos\theta.$$

From ρ, θ, ϕ, we may construct Cartesian coordinates x,y,z, defined as usually

$$x=\rho\sin\theta\cos\phi,$$

$$y=\rho\sin\theta\sin\phi,$$

$$z=\rho\cos\theta.$$

There is an easy connection between these Cartesian coordinates and the original interatomic distances. In order to find this, we define the three so-called kinematic angles

$$\epsilon^A=0,$$

$$\epsilon^B=+2\arctan\frac{m_C}{\mu}=2\pi/3,$$

$$\epsilon^C=-2\arctan\frac{m_B}{\mu}=-2\pi/3.$$

Then

$$x_i-x_j=\frac{d^k\rho}{\sqrt{2}}[1+\sin\theta\sin(\phi-\epsilon^k)] \tag{7}$$

or else

$$x_i-x_j=\frac{d^k}{\sqrt{2}}[\rho^2+\rho y\cos\epsilon^k-\rho x\sin\epsilon^k]^{1/2} \tag{8}$$

These coordinates are extremely useful for two reasons. Firstly, all three channels are on the same footing, and the shape of the asymptotic part is simple (see Fig. 2) Secondly, as next section shows, the Hamiltonian is particularly simple and economic, for $J=0$.

A.2 EQUATION OF MOTION

The equation of motion in the Cartesian coordinates have been derived several times. If total angular momentum is zero $(J=0)$, then they take a particularly simple from. Let T be the kinetic energy.

$$T=\frac{1}{\mu}(p^2-3p_\rho^2), \tag{9}$$

where

$$p^2=p_x^2+p_y^2+p_z^2,$$

$$p_\rho^2=\frac{1}{\rho^2}(xp_x+yp_y+zp_z)^2. \tag{10}$$

Hence, the Hamilton equation take the following form ($s=x,y,z$):

$$\begin{cases}\dot{s}=\dfrac{1}{\mu}(4\rho_s-3sW)\\[2ex] \dot{p}_s=\dfrac{3W}{\mu}(p_s-sW)-\dfrac{\partial V}{\partial s},\end{cases} \tag{11}$$

with

$$W=\frac{\Sigma s p_s}{\rho^2},$$

This defines completely the dynamics for $J=0$.

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