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Can the integrability of Hamiltonian systems be decided by the knowledge of scattering data?

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Abstract. A method is proposed to show how scattering data of a classical Hamiltonian system can be used to decide whether the Hamiltonian function is completely integrable or not. An appropriate infinite set of scattering trajectories is linked together at infinity and the intersection of this sequence of trajectories with a surface in the set of all asymptotes is studied. The plot of these intersections provides the same information as the plots of the usual Poincaré sections for bound states do. Numerical examples are given for the scattering of a spinning top, for collisional excitation of an oscillator and a rotator and for potential scattering under the additional influence of an electromagnetic field.

1. Introduction

It is one of the interesting problems in classical mechanics to find methods to decide whether or not a given Hamiltonian function is completely integrable. Up to now it is not known how this question can be answered by the sole knowledge of the functional form of the Hamiltonian. So far integrability can be demonstrated rigorously only by the explicit construction of additional integrals of motion. In all other cases we have to rely on hints given by the evaluation of numerical data, in particular by constructing plots of Poincaré sections (Poincaré 1892). (For the construction of Poincaré sections see § 7.1 in Abraham and Marsden (1978). For many examples of the utility of Poincaré plots in the investigation of physical systems see Lichtenberg and Lieberman (1983).) For these plots we need a knowledge of bound-state trajectories of the system.

What can we do if only scattering trajectories are known? Or if even less information is available, namely if we only know which incoming asymptotic scattering state will develop into which outgoing asymptotic scattering state during a scattering event? Poincaré's original idea does not work in these cases. Regardless of whether the Hamiltonian is completely integrable or not, any generic scattering trajectory γ pierces any surface of section S a finite number of times only. Therefore the points of intersection between γ and S can never be dense in any part of S and accordingly a scattering trajectory can never be chaotic. This also holds for scattering states of non-integrable systems with chaotic bound trajectories. The different behaviour between scattering and bound states arises because a generic scattering trajectory stays in the interaction region only for a finite time and it never comes back infinitely often and arbitrarily close to the same point, in contrast to bound trajectories.

On the other hand, the totality of all scattering events probes the structure of the interaction in the whole space. Therefore the information, whether the Hamiltonian is completely integrable or not, must be hidden somehow in the scattering data. The aim of the present paper is to construct a map out of the knowledge of the scattering events, which reveals this hidden information.

To obtain a scattering analogue of the Poincaré sections we can try to link together an infinite number of scattering trajectories at infinity in an appropriate way and let this sequence of trajectories pierce some surface in the set of asymptotic states. How such a construction can be done in detail for pure potential scattering has been shown in a recent paper (Jung 1986).

The asymptotes of the scattering trajectories (incoming ones as well as outgoing ones) are labelled by the values of the impact parameter b and the direction of the momentum given by the angle α . For scattering in a two-dimensional configuration space b and α are one-component quantities and for scattering in a three-dimensional configuration space b and α are two-component quantities. The scattering dynamics connects each incoming asymptote with an outgoing asymptote by following the exact scattering trajectory. This defines a map M , which maps (b, α) values of incoming asymptotes on the (b, α) values of the corresponding outgoing asymptotes. If we do not care whether the (b, α) values belong to in or out asymptotes, then we simply obtain a map from the (b, α) space on itself. The iteration of M produces a plot which looks like a Poincaré section for bound trajectories. For some initial (b, α) values the iteration gives smooth closed invariant lines, other values lead to stochastically scattered layers of points and some particular (b, α) values are periodic points which are encircled by invariant lines and secondary islands. The structure of the plot depends on the potential parameters. For some potentials there are exceptional parameter values, for which the plot of the iterated map consists of invariant lines only. This happens exactly for those parameter values, for which there is a second conserved quantity K in closed form, independent of the Hamiltonian H , such that $\{H, K\} = 0$ on the whole phase space.

In the present paper this construction is generalised to inelastic scattering, where in the scattering process unbound translational degrees of freedom interact and exchange energy either with internal bound degrees of freedom or with an external field.

2. Construction of asymptotic variables

The map to be constructed operates on the set of all possible asymptotic scattering states. At first we have to label asymptotes in an appropriate way. Let us assume that the Hamiltonian function of the system has the following form:

$$H(\mathbf{q}, \mathbf{p}, \mathbf{I}, \boldsymbol{\varphi}, t) = \frac{\mathbf{p}^2}{2m} + H_{\text{int}}(\mathbf{I}) + V(\mathbf{q}, \mathbf{p}, \mathbf{I}, \boldsymbol{\varphi}, t) \quad (1)$$

with

$$\lim_{|\mathbf{q}| \rightarrow \infty} (|\mathbf{q}| \cdot V(\mathbf{q}, \mathbf{p}, \mathbf{I}, \boldsymbol{\varphi}, t)) = 0 \quad (2)$$

\mathbf{q} is the relative position vector between target and projectile with cartesian components q_1, q_2, q_3 . \mathbf{p} is the momentum conjugate to \mathbf{q} with cartesian components p_1, p_2, p_3 . m is the reduced mass of the target-projectile system. \mathbf{I} are the action variables of

the internal degrees of freedom of the target and the projectile, φ are the angles conjugate to \mathbf{I} with $\varphi_i \in [-\pi, +\pi)$, k is the number of internal degrees of freedom, i.e. \mathbf{I} and φ are vectors with k components, t is the time and H_{int} is the Hamiltonian for the motion of the internal degrees of freedom in the asymptotic region, where they are decoupled from the other degrees of freedom. Note that the assumption (1) implies that H in the asymptotic region

$$H_{\text{as}} = \lim_{|q| \rightarrow \infty} H = \mathbf{p}^2/2m + H_{\text{int}}(\mathbf{I}) \quad (3)$$

depends on the momenta and actions only and H_{as} is completely integrable trivially.

If V depends on time explicitly, then we use the formalism of the extended phase space. For the treatment of mechanics in the extended phase space we follow section E.V. in Sygne (1960). t becomes an additional position variable and its conjugate momentum is $-E$, minus the energy. The generator of the dynamics is

$$\Omega(\mathbf{q}, \mathbf{p}, \mathbf{I}, \varphi, t, -E) = H(\mathbf{q}, \mathbf{p}, \mathbf{I}, \varphi, t) - E. \quad (4)$$

In the asymptotic region ($|q| \rightarrow \infty$) we find

$$\Omega_{\text{as}} = \mathbf{p}^2/2m + H_{\text{int}}(\mathbf{I}) - E. \quad (5)$$

How can we label asymptotes? First, we observe, that \mathbf{p} , \mathbf{I} and E are constant in the asymptotic region. The orbital motion of asymptotes can be given by the values of the kinetic energy, the direction of the momentum given by the angle α and the impact parameter \mathbf{b} (as in the case of pure potential scattering). For the internal motion we have the constant values of \mathbf{I} . But what do we do with the angles? Along asymptotes they move with the asymptotic angular velocity

$$\dot{\varphi}_i = \omega_{\text{as},i}(\mathbf{I}) = \frac{\partial}{\partial I_i} H_{\text{int}}(\mathbf{I}). \quad (6)$$

If $\omega_{\text{as},i}$ would be zero for all i , then the angles would stand still in the asymptotic region and could be used to determine the asymptotes further. But what can we do if $\omega_{\text{as}} \neq 0$? At which point of the asymptote do we measure the angles against which reference angle?

To solve this problem, we apply a canonical transformation, such that in the new coordinates $\bar{\omega}_{\text{as}} = 0$ and the new angle $\bar{\varphi}$ can be measured at any point in the asymptotic region. Transformations which remove the internal motion in the asymptotic region have been used by Wong and Marcus (1971) and Miller (1970) for semiclassical calculations of inelastic molecular scattering.

Because Ω_{as} depends on the momenta only, the transformation can be defined by a point transformation in the extended momentum space and then supplemented easily to a canonical transformation in the extended phase space. The new coordinates are denoted by letters with an overbar. We construct the transformation such that $\Omega_{\text{as}} = \bar{p}_1$, $\bar{E} = E$, $\bar{I} = \mathbf{I}$ and \bar{p}_2, \bar{p}_3 are some convenient functions of \mathbf{p} . We give the transformation by a generator G which is a function of the old (momentum, action, energy) variables and the new (position, angle, time) variables:

$$G(\bar{\mathbf{q}}, \bar{\varphi}, \bar{t}, \mathbf{p}, \mathbf{I}, E) = -\bar{q}_1 \left(\frac{\mathbf{p}^2}{2m} + H_{\text{int}}(\mathbf{I}) - E \right) - \bar{q}_2 f_2(\mathbf{p}) - \bar{q}_3 f_3(\mathbf{p}) + \bar{t} E - \sum_{i=1}^k \bar{\varphi}_i I_i. \quad (7)$$

This leads to the transformation formulae

$$\bar{p}_1 = -\frac{\partial G}{\partial \bar{q}_1} = \frac{\mathbf{p}^2}{2m} + H_{\text{int}}(\mathbf{I}) - E \quad (8a)$$

$$\bar{p}_i = -\frac{\partial G}{\partial \bar{q}_i} = f_i(\mathbf{p}) \quad \text{for } i = 2, 3 \quad (8b)$$

$$\bar{E} = \frac{\partial G}{\partial \bar{t}} = E \quad (8c)$$

$$\bar{I}_i = -\frac{\partial G}{\partial \bar{\varphi}_i} = I_i \quad \text{for } i = 1, \dots, k \quad (8d)$$

$$q_i = -\frac{\partial G}{\partial p_i} = \bar{q}_1 \frac{p_i}{m} + \bar{q}_2 \frac{\partial f_2(\mathbf{p})}{\partial p_i} + \bar{q}_3 \frac{\partial f_3(\mathbf{p})}{\partial p_i} \quad \text{for } i = 1, 2, 3 \quad (8e)$$

$$t = \frac{\partial G}{\partial E} = \bar{t} + \bar{q}_1 \quad (8f)$$

$$\varphi_i = -\frac{\partial G}{\partial I_i} = \bar{\varphi}_i + \omega_{\text{as},i}(\mathbf{I}) \bar{q}_i \quad \text{for } i = 1, \dots, k. \quad (8g)$$

f_2, f_3 will be chosen such that

$$\sum_{i=1}^3 p_i \frac{\partial}{\partial p_i} f_j(\mathbf{p}) = 0 \quad \text{for } j = 2, 3. \quad (9)$$

One possible choice is

$$f_2(\mathbf{p}) = \tan^{-1}(p_2/p_1) \quad (10a)$$

$$f_3(\mathbf{p}) = \tan^{-1}[(p_1^2 + p_2^2)^{1/2}/p_3]. \quad (10b)$$

Then f_2 and f_3 give the direction of the momentum. Equations (10) are particularly useful if V depends on \mathbf{q}^2 only, i.e. if the potential is rotationally symmetric in the position space. Equations (8) and (9) give

$$\bar{q}_1 = m\mathbf{q} \cdot \mathbf{p}/p^2 \quad (11)$$

i.e. \bar{q}_1 is the time of flight of the system along the asymptote. Equations (11), (8f) and (8g) show that

$$\bar{t} = t - \bar{q}_1 \quad (12)$$

and

$$\bar{\varphi}_i = \varphi_i - \omega_{\text{as},i}(\mathbf{I}) \bar{q}_1 \quad (13)$$

are constant in the asymptotic region and can be read off at any arbitrary point along the asymptote.

We label asymptotes by giving the values of the quantities $(E, \bar{p}_2, \bar{p}_3, \mathbf{I}, \bar{t}, \bar{q}_2, \bar{q}_3, \bar{\varphi})$. Trajectories starting in the hypersurface $\Omega = 0$ always stay in this hypersurface and only those trajectories are physically relevant. Therefore \bar{p}_1 is fixed on the numerical value zero automatically. \bar{q}_1 is the only new coordinate, which is not constant along asymptotes and it can be used to parametrise trajectories.

If V does not depend on t explicitly, then we can leave out the coordinates E and t from the phase space as uninteresting and leave out the terms containing E in (7).

The set of all possible $(E, \bar{p}_2, \bar{p}_3, I, \bar{i}, \bar{q}_2, \bar{q}_3, \bar{\varphi})$ values is the space on which the iterated scattering map will act. We call this space of asymptotes Λ and in the next section x is a $(2k+6)$ -component vector out of the space Λ .

The choice of the canonical transformation is not unique. Besides the generator (7) there are many other reasonable possibilities. Another choice would mean other coordinates in Λ or another choice for the space Λ itself. This freedom in choosing Λ and the coordinates in Λ corresponds exactly to the freedom in choosing the surface of section and the coordinates in this surface for the usual Poincaré sections for bound trajectories.

3. The iteration process

Each incoming asymptote can be labelled by its value $x_{in} \in \Lambda$. Following the exact scattering trajectory, which develops from this incoming asymptote, the system finally ends at some outgoing asymptote with the value $x_{out} \in \Lambda$. We define the scattering map M by

$$M(x_{in}) = x_{out}. \quad (14)$$

M acts on incoming asymptotes and turns them into outgoing asymptotes. In order to construct an iteration, we need in addition a feedback map F , which turns outgoing asymptotes back into incoming asymptotes. Then an iteration can consist in applying M and F alternately on some starting point $x \in \Lambda$. In order to make a particular choice for F we use the following two reasonable restrictions.

- (i) F is allowed to depend on x_{out} only and it must not depend on any other variables or parameters and not on the particular interaction V .
- (ii) If $V \equiv 0$ then the composition of M and F should be the identity map on the whole space Λ .

With these restrictions there remains only the following choice for the feedback map F : F applied to the outgoing trajectory labelled by x gives that incoming trajectory, which has the same values for all $2k+6$ components of x . This gives a one-to-one connection, because to any set of values of x there exists exactly one incoming and one outgoing asymptote. Therefore, in the space Λ the map F acts like the identity and the iterated scattering map is just the iteration by the map M only.

The action of the feedback map F can be understood as a compactification of the position space. In the q space we cut out a ball B_R of radius R , with R chosen such that V is negligible outside B_R . In the extended phase space we thereby cut out a $(2k+7)$ -dimensional cylinder out of the hypersurface $\Omega = 0$. The space Λ is half of the surface of this cylinder. Parts of the surface of the cylinder are glued together by identification of the in and out asymptotes with the same values of x . Thereby a trajectory leaving the cylinder in a point p_1 of its surface is fed back automatically into the cylinder at the other point p_2 where $p_2 = F(p_1)$. The iterated scattering map can be understood as a Poincaré return map on the surface of this cylinder.

4. Numerical examples

In this section we give a few simple examples for the iterated map constructed in the previous sections. In order to be able to show plots of the map we must restrict the

examples to systems with two essential degrees of freedom. For all numerical examples the reduced mass m is set to the value 1 and all quantities are measured in arbitrary dimensionless units.

4.1. Example 1

Scattering of a spinning top

$$H(\mathbf{p}, \mathbf{q}, I, \varphi) = \mathbf{p}^2/2 + [(1 - D\mathbf{q}^2)I + \cos \varphi(1 - I^2)^{1/2}] \exp(-\mathbf{q}^2) \tag{15}$$

$$H_{as} = \mathbf{p}^2/2. \tag{16}$$

The projectile is a spinning top with total internal angular momentum 1 and I is the 3-component of the internal angular momentum. $(1 - D\mathbf{q}^2) \exp(-\mathbf{q}^2)$ is a potential, which causes an energy split between the various inclinations of the axis of the top. D is a free parameter. $\cos \varphi(1 - I^2)^{1/2} \exp(-\mathbf{q}^2)$ is an interaction, which causes the inclination of the axis to change.

This system may be viewed as a classical spin-dependent scattering. For the possibility of classical spin models of similar structure see Schiller (1962). The classical quantities I and $\cos \varphi(1 - I^2)^{1/2}$ correspond to the operators σ_3 and σ_1 in quantum mechanics. $\partial H_{as}/\partial I = 0$ and the angle φ stands still outside the interaction region and we do not need to transform to new coordinates. The \mathbf{q} dependence of H is in \mathbf{q}^2 only and only the radial variable $r = |\mathbf{q}|$ and its conjugate momentum p_r are essential for the orbital motion. Together with the internal degree of freedom we have two essential degrees of freedom and for Λ we can use the (I, φ) plane. The orbital angular momentum L is a conserved quantity throughout the interaction process and its value appears only as a parameter in the equations of motion. In the essential variables the H function is

$$H(p_r, r, I, \varphi) = p_r^2/2 + L^2/2r^2 + [(1 - Dr^2)I + \cos \varphi(1 - I^2)^{1/2}] \exp(-r^2). \tag{17}$$

In figure 1 we have fixed L on the value 1, E on the value 0.5, have chosen several initial points in the (I, φ) plane (marked by a cross) and plotted the next 700 iterates of these initial points under the map M . For the value $D = 0$ we obtain invariant lines only. This should be correlated with the fact that the square bracket in (17) is a conserved quantity for $D = 0$.

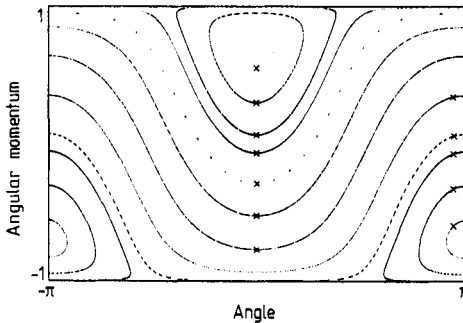


Figure 1. Iterated scattering map to the Hamiltonian (17) for $D = 0, E = 0.5, L = 1.0$. The vertical axis gives I , the 3-component of the internal angular momentum of the projectile. The horizontal axis gives the angle φ , canonically conjugate to I . Each initial point is marked by a cross.

In figure 2 the value $D = 1$ has been chosen. We see a layer in the (I, φ) plane covered by stochastically distributed points, which are iterates of a single initial point. Besides there are invariant lines and islands around periodic points. For $D \neq 0$ there seems to be no second conserved quantity in closed form on the whole phase space for Hamiltonian (17).

4.2. Example 2

This is an example to demonstrate the method; it is not considered to describe any common system.

$$H(p, q, I, \varphi) = p^2/2 + I^2/2 + (I \sin \varphi + Ap \cos \varphi) \exp(-q) + 2 \exp(-2q). \tag{18}$$

The potential goes to infinity for $q \rightarrow -\infty$. So we interpret q as $\ln r$ where r is a radial variable of a three-dimensional orbital motion. The limit for asymptotes is the limit $q \rightarrow +\infty$:

$$H_{as} = p^2/2 + I^2/2 \tag{19}$$

$$\omega_{as} = I. \tag{20}$$

A is a free parameter.

We apply the canonical transformation given by the generator

$$G(p, I, \bar{q}, \bar{\varphi}) = -\bar{q}(p^2 + I^2)/2 - \bar{\varphi}I \tag{21}$$

and obtain

$$\bar{p} = p^2/2 + I^2/2 = H_{as} \tag{22a}$$

$$\bar{I} = I \tag{22b}$$

$$\bar{q} = q/p \tag{22c}$$

$$\bar{\varphi} = \varphi - Iq/p = \varphi - \omega_{as}(I)q/p. \tag{22d}$$

In new coordinates $\bar{H}_{as} = \bar{p}$, $\bar{\omega}_{as} = 0$ and $\bar{\varphi}$ is constant in the asymptotic region. The iterated scattering map acts in the $(I, \bar{\varphi})$ plane.

Now we show the plots of the iterated map for several values of A all for the value 1 of the energy E . The H function is invariant under the transformation $(I, \varphi) \rightarrow (-I, -\varphi)$. This symmetry also shows up in the plots of the iterated map M .

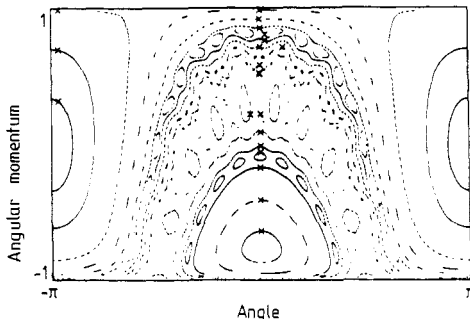


Figure 2. As figure 1 for $D = 1.0$, $E = 0.5$, $L = 1.0$.

For $A = 1.5$ in figure 3 we see three large regions of chaotic points and some islands of invariant lines surrounded by secondary structures. For $A = 1.25$ in figure 4 the chaos has diminished to small strips and we observe mainly invariant lines. For $A = 1.05$ in figure 5 there is no chaos of visible size left. We see a few large islands and many invariant lines going around all values of $\bar{\varphi}$. For $A = 1$ (not shown in a figure) the plot consists of horizontal invariant lines only. For A decreasing below 1 resonance islands show up again and for small or negative values of A chaotic strips can be found again.

What is special for the value $A = 1$? For $A = 1$ there is the second conserved quantity

$$K = I + \sin \varphi \exp(-q). \tag{23}$$

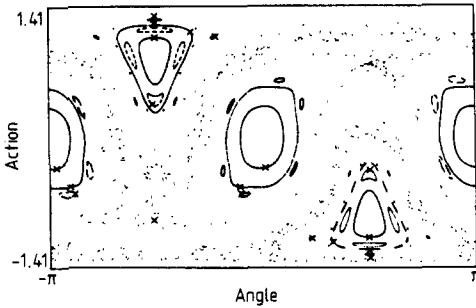


Figure 3. Iterated scattering map to the Hamiltonian (18) for $A = 1.5$, $E = 1.0$. The vertical axis gives I , the action of the internal degree of freedom. The horizontal axis gives the transformed angle $\bar{\varphi}$, canonically conjugate to I . Each initial point is marked by a cross.

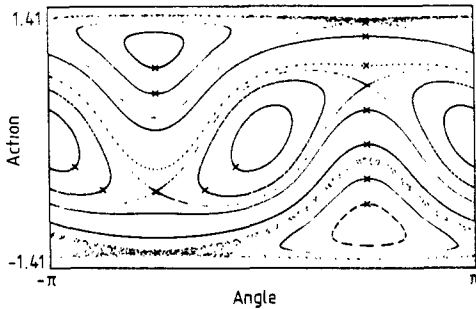


Figure 4. As figure 3 for $A = 1.25$, $E = 1.0$.

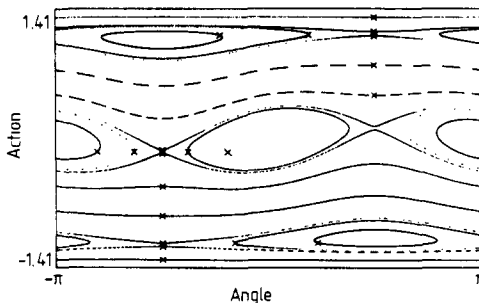


Figure 5. As figure 3 for $A = 1.05$, $E = 1.0$.

A direct calculation shows that $\{K, H\} = 0$. There seems to be no second conserved quantity on the whole phase space for $A \neq 1$. In the asymptotic region $K = I$ and therefore I is a conserved quantity for the map M if K is constant along exact trajectories. I may change inside the interaction region. But in the outgoing asymptotic state I must have the same value again as in the incoming asymptotic state.

Accordingly, for $A = 1$ the iterated scattering map is a pure twist map and for A deviating from 1 it is a perturbed twist map with $A - 1$ acting as perturbation parameter. In figures 3-5 we see all the phenomena, which are to be expected for perturbed twist maps (see Chirikov 1979, Greene 1979). For A close to 1 the differences in I between incoming and outgoing states are small and the first images of lines $I = \text{constant}$ under the map M are slightly bent curves. In addition the difference $\varphi_{\text{in}} - \varphi_{\text{out}}$ is nearly constant on these curves. However, for A far away from 1 the images of curves $I = \text{constant}$ can have a very complicated structure with long tendrils and very small changes in φ_{in} cause enormous changes in I and in $\varphi_{\text{in}} - \varphi_{\text{out}}$. Figure 6 shows an example for $A = 2$. There is the curve $I = \text{constant} = -0.6$ and its image under M . This figure indicates that the plot of the iterated map shows mainly chaos for $A = 2$. According to MacKay and Percival (1985) a perturbed twist map does not have invariant curves going around all values of the angle in those regions of the action variable, where the images of horizontal lines become steeper than some limit value.

Another hint on the complicated structure of the scattering process and on the sensitivity of the scattering trajectory on the initial angle φ_{in} gives figure 7. Here the

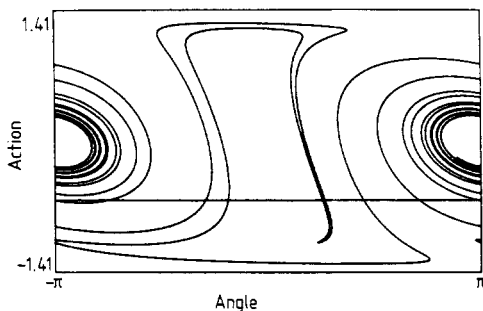


Figure 6. The line $I = \text{constant} = -0.6$ and its image under the scattering map M for the model system (18). The vertical axis gives I , the action of the internal degree of freedom. The horizontal axis gives the angle φ , canonically conjugate to I . $A = 2.0$, $E = 1.0$.

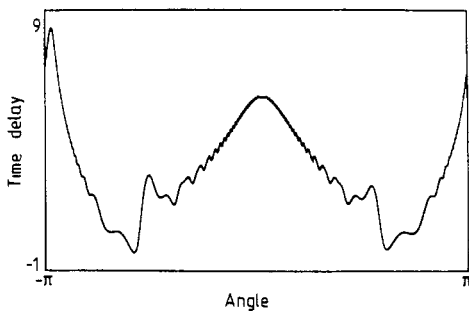


Figure 7. Time delay of the scattering trajectory as a function of the angle φ for the model system (18) for fixed values of the energy $E = 1$ and the action $I = 0.2$, $A = 2.0$.

initial action I_{in} is fixed on $I = 0.2$. The angle φ_{in} is scanned from $-\pi$ to $+\pi$ and for each value of φ_{in} the time delay of the scattering trajectory is plotted. We see very fine and rapid oscillations. In contrast, for $A = 1$ the time delay is a constant function of φ_{in} .

4.3. Example 3

Collisional excitation of an oscillator

$$H = p^2/2 + I + [1 - Bq^2 + A \sin \varphi (2I)^{1/2}] \exp(-q^2) \tag{24}$$

p and q are momentum and position of a projectile, which hits an oscillator with action I , angle φ and frequency 1 sitting at the origin. A and B are free parameters. V depends on q^2 only. Therefore the orbital angular momentum is conserved and the orbital motion lies in a plane. Accordingly, we can assume that p and q are two-dimensional vectors right from the beginning.

Applying the canonical transformation with the generator

$$G = -\bar{q}_1(p^2/2 + I) - \bar{q}_2 \tan^{-1}(p_2/p_1) - \bar{\varphi}I \tag{25}$$

gives

$$\bar{H}_{as} = \bar{p}_1 \tag{26}$$

$$\bar{q}_1 = \mathbf{q} \cdot \mathbf{p} / p^2 \tag{27a}$$

$$\bar{q}_2 = -q_1 p_2 + q_2 p_1 = -L \tag{27b}$$

$$\bar{\varphi} = \varphi - \bar{q}_1 \tag{27c}$$

\bar{q}_2 is minus the orbital angular momentum and it is a conserved quantity. For $A = 0$, H does not depend on φ . Then I is conserved and M is a pure twist map. For $A \neq 0$ there is no obvious third conserved quantity and M is a perturbed twist map. For L fixed the space Λ is the $(I, \bar{\varphi})$ plane.

In figure 8 we show an example of a plot of the iterated scattering map for the value $E = 1$ of the energy and $L = 1$ of the orbital angular momentum. We see stochastic regions, invariant lines and chains of islands in a pattern, which is common for perturbed twist maps and which occurs in qualitatively similar form in Poincaré plots of bound trajectories.

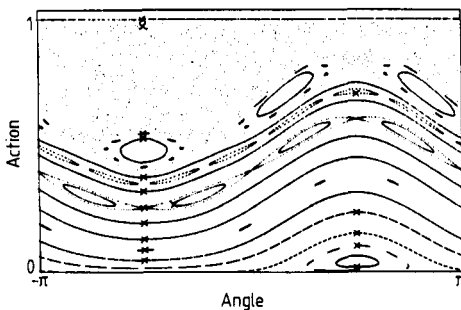


Figure 8. Iterated scattering map to the Hamiltonian (24) for the parameter values indicated. The vertical axis gives I , the action of the oscillator. The horizontal axis gives the transformed angle $\bar{\varphi}$, canonically conjugate to I . Each initial point is marked by a cross. $A = 0.5$, $B = 5.0$, $E = 1.0$, $L = 1.0$.

4.4. Example 4

Collisional excitation of a rotator

$$H = \mathbf{p}^2/2 + I^2/2 + (Aq_2 \sin \varphi + Aq_1 \cos \varphi + B) \exp(-q^2). \quad (28)$$

We assume that the orbital motion of the projectile is in a plane and \mathbf{p} and \mathbf{q} are two-dimensional momentum and position vectors. The projectile hits a rigid rotator sitting in the origin with internal angular momentum I and angle φ . A and B are free parameters. Applying the canonical transformation with generator

$$G = -\bar{q}_1(p_1^2 + p_2^2 + I^2)/2 - (I - \bar{q}_2) \tan^{-1}(p_2/p_1) - \bar{\varphi} I \quad (29)$$

gives

$$\bar{H}_{as} = \bar{p}_1 \quad (30)$$

$$\bar{q}_1 = \mathbf{q} \cdot \mathbf{p} / \mathbf{p}^2 \quad (31a)$$

$$\bar{q}_2 = q_1 p_2 - q_2 p_1 + I \quad (31b)$$

$$\bar{\varphi} = \varphi - \tan^{-1}(p_2/p_1) - I\bar{q}_1. \quad (31c)$$

\bar{q}_2 is the total angular momentum J and is a conserved quantity. For fixed J the space Λ is the $(I, \bar{\varphi})$ plane. For $A=0$, H does not depend on φ . Then I is conserved and M is a pure twist map. For $A \neq 0$ there is no obvious third conserved quantity and M is a perturbed twist map. Figure 9 shows an example of a plot of the iterated scattering map for the values $E=1$ of the energy and $J=0.5$ of the total angular momentum.

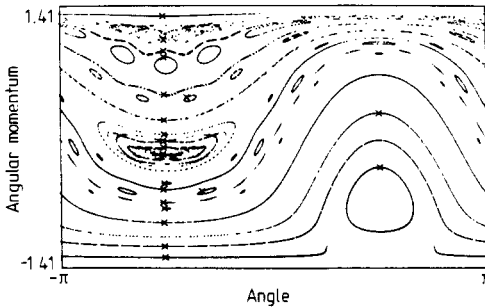


Figure 9. Iterated scattering map to the Hamiltonian (28) for $A=1.0$, $B=0.50$, $E=1.0$, $J=0.5$. The vertical axis gives I , the angular momentum of the rotator. The horizontal axis gives the transformed angle $\bar{\varphi}$, canonically conjugate to I . Each initial point is marked by a cross.

4.5. Example 5

Field modified scattering

$$H = [p - AU(q) \cos(\omega t)]^2/2 - \exp(-q^2) \quad (32)$$

where

$$u(q) = \{\exp[-(2q+20)^2] - \exp[-(2q-20)^2]\}2/\sqrt{\pi} \quad (33)$$

$$U(q) = \int_{-\infty}^q u(s) ds. \quad (34)$$

This describes the scattering of a projectile in one dimension off a local potential $-\exp(-q^2)$ under the additional influence of an electromagnetic field in dipole approximation. A is the amplitude and ω is the frequency of the field. $U(q)$ is a cutoff function for the field in position space

$$\Omega = H - E \quad \Omega_{as} = p^2/2 - E. \tag{35}$$

The canonical transformation with the generator

$$G = -\bar{q}(p^2/2 - E) + \bar{t}E \tag{36}$$

gives

$$\bar{q} = q/p \tag{37a}$$

$$\bar{t} = t - \bar{q}. \tag{37b}$$

According to § 2 the space Λ is the (E, \bar{t}) plane. However, it is more convenient to use in the plots the transformed field phase $\omega\bar{t} \bmod 2\pi$ instead of \bar{t} itself. In contrast to the other four examples there is no upper limit for the momentum variable E in this case. For the amplitude $A=0$, M is a pure twist map. It becomes perturbed as soon as $A \neq 0$. Figure 10 is an example for a plot of the iterated scattering map. Here we see surprisingly many islands around points of period 1 in an arrangement, which is unusual in Poincaré plots for bound systems and also unusual for scattering maps of time-independent systems. The basic structure of the plot seems to repeat itself for increasing energy on an increasing vertical scale. The relative fraction of the area filled by stochastic points decreases with increasing energy. The repetition of the basic pattern has been checked up to an energy value of $E = 1000$.

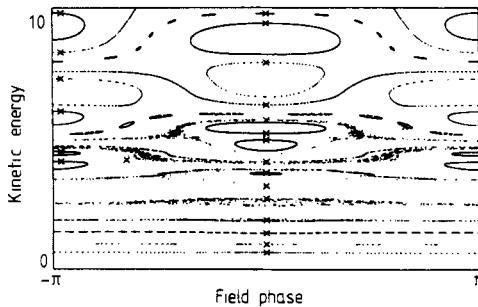


Figure 10. Iterated scattering map to the model system (32) for $A=0.1$, $\omega=10.0$. The vertical axis gives E , the asymptotic kinetic energy of the projectile. The horizontal axis gives $\omega\bar{t} \bmod 2\pi$, the transformed phase of the external field. Each initial point is marked by a cross.

5. Conclusions

For scattering systems a map M has been constructed from the set of asymptotes onto itself. This construction works if the H function has the form of equation (1). It is essential that the internal motion is completely integrable in the asymptotic region. In this case we can find a canonical transformation to new coordinates in the extended

phase space, such that all coordinates except \bar{q}_1 are constant along asymptotes. \bar{p}_1 has the value zero anyway in the formalism of the extended phase space. So the new coordinates beside (\bar{q}_1, \bar{p}_1) can be used to label asymptotes. \bar{q}_1 is the time parameter along the asymptotes. If the motion of the internal degrees of freedom would be chaotic in the asymptotic region, then such a canonical transformation could not be found and the whole method of this paper would fail.

The essential idea for the iteration procedure is to link together an infinite set of scattering trajectories into a single object and to treat this new object in the same way as a bound trajectory is treated in the usual Poincaré construction.

The iteration of M shows chaotic behaviour in most cases. Only for a few exceptional systems does the iterated map give invariant lines only. These exceptional cases are exactly the ones in which a second conserved quantity exists on the whole phase space. Therefore the construction given in this paper solves the problem raised in the introduction. It gives a numerical indication whether the Hamiltonian is integrable or not. As input information we need only the knowledge of which incoming asymptote is turned into which outgoing asymptote during the scattering process. This is interesting because many systems of practical interest are investigated in scattering experiments, giving the connection between in- and outgoing asymptotes.

So far we did not consider that in classical systems there can be exceptional trajectories at positive energy, which have no incoming or no outgoing asymptotes. (For the occurrence of such orbiting trajectories see § 5.4 in Newton (1982).) However, these exceptional trajectories do not cause serious problems, because they form a set of measure zero and they do not prevent the numerical construction of the scattering map.

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