

Integrability and chaos: the classical uncertainty

Jaume Masoliver¹ and Ana Ros²

¹ Departament de Física Fonamental, Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

² Department Algebra und Zahlentheorie, Universität Hamburg, Bundesstrasse 55, 20146 Hamburg, Germany

E-mail: jaume.masoliver@ub.edu and anaroscamacho@gmail.com

Received 18 November 2010, in final form 13 December 2010

Published 24 January 2011

Online at stacks.iop.org/EJP/32/431

Abstract

In recent years there has been a considerable increase in the publishing of textbooks and monographs covering what was formerly known as random or irregular deterministic motion, now referred to as deterministic chaos. There is still substantial interest in a matter that is included in many graduate and even undergraduate courses on classical mechanics. Based on the Hamiltonian formalism, the main objective of this paper is to provide, from the physicist's point of view, an overall and intuitive review of this broad subject (with some emphasis on the Kolmogorov–Arnold–Moser theorem and the stability of planetary motions) which may be useful to both students and instructors.

1. Introduction

At the beginning of the 20th century ‘mechanics had not yet lost its place as the central subject within physics, although it was on the verge of losing it’ [16]. Fifty years later classical mechanics was considered by the majority of physicists a closed field from which one could not expect new challenges, especially in fundamental issues. But from then on, fresh mathematical results, together with additional numerical data obtained by high-speed computers, revived a field of knowledge related to nonlinear dynamics and irregular behaviour of deterministic systems, a field that had begun at the end of the 19th century mainly by the works of Henri Poincaré in his attempt to develop a convergent perturbation theory of planetary orbits.

The Solar System, despite its complexity, shows extremely regular behaviour which can be predicted very accurately for short periods of time. This is due, in part, to the weakness of gravitational force, but also because Kepler's two-body problem is completely integrable, despite the fact that any gravitational system of three or more bodies is not (let us imagine for a moment the difficulty of guessing the law of gravity had the Earth been orbiting around a

double star). The Newtonian deduction of Kepler's laws is based precisely on the properties of the integrable system of two bodies. Nevertheless, the dynamical interactions of the many bodies that form the Solar System necessarily lead us to consider deviations to the predictions based on Kepler's laws. This makes us wonder: why does the Solar System behave in such a regular way? Or, as in the inquiry of Moser: is the Solar System stable [21]? That is, will it follow the order that we presently observe in the future? Even today these questions do not have a complete and satisfactory answer.

For more than 300 years, since the time of Newton, the evolution and stability of mechanical systems, and specially that of the Solar System, have been central to physics and mathematics. During the 18th century, Euler, Lagrange and Laplace made substantial developments by predicting changes in the planetary orbits due to small perturbations, establishing a framework for the study of global stability. All of this culminated in the 19th century works of Hamilton and Jacobi who reformulated the Lagrangian formalism of classical mechanics in terms of the phase space, a step which proved to be most fruitful for the developments of both statistical and quantum mechanics.

These successes consolidated the idea of classical determinism. However, at the turn of the 19th century, the works of Poincaré not only closed the door to an age but generated the first serious fracture in the philosophical conception of determinism. These works showed the impossibility of proving the convergence of perturbation series and, therefore, central questions, about the stability of the Solar System, remained unanswered. Poincaré was thus the first to study what much later has been called (apparently by J Yorke in 1975) *chaos*.

A plain, albeit not simplistic, definition of chaos is 'the complicated temporal evolution of simple systems' [26]. Thus, and contrary to common thinking, chaos is not spatial and static disorder but a characteristic of certain motions. It is essentially a dynamical concept, in which two initially close trajectories may be divergent after a finite time. Chaos may appear in a variety of fields: physics, chemical reactions, the spread of illnesses, Internet, economics and, of course, in planetary motions [26]. For contrary to intuition, chaotic behaviour is not an exclusive property of dissipative or random systems but of conservative and deterministic systems as well.

Focusing on conservative systems we will show that small denominators giving place to resonances are associated with the appearance of chaos, and that due to this irregular behaviour, it seems impossible to predict the long-term evolution of nonintegrable systems (the vast majority of mechanical systems) using perturbation techniques. Since the end of the 19th century there was no remarkable advance and this fundamental question was practically forgotten until 1954, when Kolmogorov gave a sketch of the proof that most trajectories of nonintegrable conservative systems are quasiperiodic and that one can obtain them through a convergent perturbation development. In the 1960s, Arnold and Moser gave a more formal and rigorous proof of this result, known as the Kolmogorov–Arnold–Moser (KAM) theorem.

In the coming sections we will explain and develop these ideas, stressing physical aspects, rather than mathematical concepts and technicalities, of which there are plenty in a field that was the starting point of modern mathematical developments such as topology. In this way the paper is intended as a comprehensive and intuitive introduction to deterministic chaos which, we hope, will be useful for both students and instructors.

2. Hamiltonian mechanics

The quintessential mechanical system, to which most physical systems are reduced, consists of a collection of mass points that interact. Experience shows that the state of the system is completely determined by the set of positions and velocities of all its particles. The

reference system chosen to describe position and velocity need not be Cartesian. Thus, in the Lagrangian formulation of mechanics, the representation of the state of the system is obtained through generalized coordinates q_1, \dots, q_n and velocities $\dot{q}_1, \dots, \dot{q}_n$. The minimum number of generalized coordinates needed to describe the state of the system is called the number of degrees of freedom. In what follows we will use bold letters to denote vectors. Accordingly, the set of all positions is represented by the vector $\mathbf{q} = (q_1, \dots, q_n)$ and the set of all velocities by $\dot{\mathbf{q}} = (\dot{q}_1, \dots, \dot{q}_n)$.

The laws of mechanics are those that determine the motion of the system by providing the time evolution of the positions, $\mathbf{q}(t)$, and the velocities, $\dot{\mathbf{q}}(t)$, of all its components. Therefore, the main problem is the determination of how the state of the system evolves with time. There have been several approaches to achieve this goal. The first one was based on Newton's laws which directly emanate from experience. This approach was subsequently refined and generalized by the Lagrangian and Hamiltonian formulations, the latter being the most appropriate for the present development.

In the Hamiltonian formulation, the description of the state of the system is also given by generalized coordinates $\mathbf{q} = (q_1, \dots, q_n)$ but instead of velocities by generalized momenta $\mathbf{p} = (p_1, \dots, p_n)$. The main problem is then finding the time evolution of these quantities, in other words, the knowledge of the functions $\mathbf{q}(t)$ and $\mathbf{p}(t)$ which give the temporal evolution of coordinates and momenta. This is achieved by solving the following set of $2n$ first-order differential equations known as *Hamilton equations* [6, 11, 18]:

$$\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}, \quad (1)$$

where the function $H(\mathbf{q}, \mathbf{p}, t)$ is the Hamiltonian which, for inertial reference frames, coincides with the total energy of the system [6]. In (1) we have used the notation

$$\frac{\partial H}{\partial \mathbf{q}} = \left(\frac{\partial H}{\partial q_1}, \dots, \frac{\partial H}{\partial q_n} \right)$$

to denote the gradient of H with respect to \mathbf{q} and analogously for $\partial H / \partial \mathbf{p}$.

For those readers not familiar with the Hamiltonian formulation, it may be useful to recall that for the three-dimensional motion of a particle of mass m inside a conservative field of potential energy $V(\mathbf{r})$, the energy (i.e. the Hamiltonian) is

$$H = \frac{p^2}{2m} + V(\mathbf{r}),$$

where $\mathbf{q} = \mathbf{r} = (x, y, z)$ and $p^2 = \mathbf{p} \cdot \mathbf{p} = p_x^2 + p_y^2 + p_z^2$. In this case Hamilton equations (1) read

$$\dot{\mathbf{r}} = \frac{\mathbf{p}}{m}, \quad \dot{\mathbf{p}} = -\frac{\partial V}{\partial \mathbf{r}},$$

which coincide with Newton's second law.

In the Hamiltonian formulation, the state of a system with n degrees of freedom is described by a single point $(\mathbf{q}, \mathbf{p}) = (q_1, \dots, q_n, p_1, \dots, p_n)$ of a space of dimension $2n$ called *phase space*. Hence, starting at $t = 0$ from an initial point $(\mathbf{q}_0, \mathbf{p}_0)$, the state of the system in a later time t will be given by the point $(\mathbf{q}(t), \mathbf{p}(t))$, where $\mathbf{q}(t)$ and $\mathbf{p}(t)$ are the equations of motion, that is, the solutions of Hamilton equations (1) with the initial conditions $\mathbf{q}(0) = \mathbf{q}_0$ and $\mathbf{p}(0) = \mathbf{p}_0$. The trajectory described by the point $(\mathbf{q}(t), \mathbf{p}(t))$ as time progresses is called the *phasespace trajectory* of the system.

One of the advantages of the Hamiltonian formulation is that we can evaluate the time evolution of any property of the system without having to know the form of the equations of motion, that is to say, without solving Hamilton equations which is usually quite involved.

Let us assume that a given property of the system (for instance, the energy or the angular momentum) can be represented by a function, $f(\mathbf{q}, \mathbf{p}, t)$, of the state of the system and time. How does f change when the state $(\mathbf{q}(t), \mathbf{p}(t))$ evolves with time? The answer is simple and reads [11, 18]

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + [f, H], \quad (2)$$

where $[f, H]$ is the *Poisson bracket* defined by

$$[f, H] = \sum_{i=1}^n \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right). \quad (3)$$

Observe that if f does not depend explicitly on time, $\partial f/\partial t = 0$ and f will be constant (i.e. $df/dt = 0$) if its Poisson bracket with the Hamiltonian vanishes: $[f, H] = 0$. In such a case $f(\mathbf{q}, \mathbf{p})$ is a *constant of motion*. Incidentally, for conservative systems the Hamiltonian is time independent; hence, $\partial H/\partial t = 0$ and, since $[H, H] = 0$, we see that H is a constant of motion, the energy.

The Poisson bracket may be extended to any pair of dynamical functions $f(\mathbf{q}, \mathbf{p}, t)$ and $g(\mathbf{q}, \mathbf{p}, t)$. A direct generalization of (3) gives

$$[f, g] = \sum_{i=1}^n \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right). \quad (4)$$

From this definition one easily obtains a series of properties satisfied by the Poisson bracket, properties that endow the set of dynamical functions with an algebraic structure called *Lie algebra*. We will not proceed here with this mathematical development and refer the interested reader to specialized texts (see, for instance, [10]).

For the special case that f and g are any of the qs or ps , definition (4) gives

$$[q_i, q_j] = [p_i, p_j] = 0, \quad [q_i, p_j] = \delta_{ij}. \quad (5)$$

This is the condition for any set of variables (\mathbf{p}, \mathbf{q}) to be a canonical set, i.e. they satisfy Hamilton equations with some Hamiltonian H [11].

2.1. Canonical transformations: the Hamilton–Jacobi equation

Perhaps the greatest advantage of the Hamiltonian formulation is that it allows for transformations of variables preserving the form of Hamilton equations. There are several ways, all of them equivalent, to define these kinds of transformations. We choose the following.

We say that the change of variables, $(\mathbf{q}, \mathbf{p}) \rightarrow (\mathbf{q}', \mathbf{p}')$, given by the equations

$$\mathbf{q} = \mathbf{q}(\mathbf{q}', \mathbf{p}', t), \quad \mathbf{p} = \mathbf{p}(\mathbf{q}', \mathbf{p}', t) \quad (6)$$

is a *canonical transformation* if the infinitesimal quantities $\mathbf{p}' \cdot d\mathbf{q}' = \sum p'_i dq'_i$ and $\mathbf{p} \cdot d\mathbf{q} = \sum p_i dq_i$ differ only in the total differential of a scalar function S :

$$\mathbf{p}' \cdot d\mathbf{q}' - \mathbf{p} \cdot d\mathbf{q} = dS. \quad (7)$$

The function S is called the *generating function* of the canonical transformation.

Observe that, because of (6), out of the four sets of variables: $\mathbf{q}, \mathbf{p}, \mathbf{q}'$ and \mathbf{p}' , involved in a canonical transformation, only two of them are actually independent. The generating function S will thus depend upon the two sets of variables chosen to be independent, and also on t in the case of a time-dependent canonical transformation. One convenient choice, among others, lies in assuming that the generating function depends on the original coordinates and

the transformed momenta, i.e. $S = S(\mathbf{q}, \mathbf{p}', t)$. Combining this assumption with condition (7) one can easily show that the equations of the canonical transformation are given by [11]

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}}, \quad \mathbf{q}' = \frac{\partial S}{\partial \mathbf{p}'}. \quad (8)$$

It can be shown [11, 18] that after a canonical transformation the Hamilton equations preserve the form

$$\dot{\mathbf{q}}' = \frac{\partial H'}{\partial \mathbf{p}'}, \quad \dot{\mathbf{p}}' = -\frac{\partial H'}{\partial \mathbf{q}'}, \quad (9)$$

where

$$H'(\mathbf{q}', \mathbf{p}', t) = H(\mathbf{q}, \mathbf{p}, t) + \frac{\partial S}{\partial t}, \quad (10)$$

is the transformed Hamiltonian. Note that for time-independent canonical transformations $\partial S/\partial t = 0$, and $H' = H$, so that the transformed Hamiltonian coincides with the original one (the latter being written in terms of the transformed variables).

Let us observe that *any* arbitrary function S generates *some* canonical transformation. This is quite remarkable, because it implies the freedom of writing Hamilton equations—that is, the laws of motion—in any convenient way only by the introduction of a given function S .

Following this line of reasoning we might look for a canonical transformation such that the equations of motion would be the simplest ones. In other words, what would be the generating function of the canonical transformation such that the transformed qs and ps are constants? Note that, if we could find this transformation, then we would have solved the problem of motion, for the equations of the transformation (6) (or, equivalently, (8)) given the equations of motion $\mathbf{q}(t) = \mathbf{q}(\alpha, \beta, t)$ and $\mathbf{p}(t) = \mathbf{p}(\alpha, \beta, t)$, where the new coordinates and momenta $\mathbf{q}' = \alpha$ and $\mathbf{p}' = \beta$ are constants determined by the initial conditions.

If the transformed variables are constant, their time derivatives are zero, and from (9) we see that $\partial H'/\partial \mathbf{p}' = \partial H'/\partial \mathbf{q}' = 0$. Accordingly, the transformed Hamiltonian H' must be independent of the coordinates and momenta and, at most, a function of time, which, for simplicity, we choose to be zero. Therefore, if in (10) we set $H' = 0$, and remembering that $\mathbf{p} = \partial S/\partial \mathbf{q}$ (cf (8)), we see that the generating function of the canonical transformation $(\mathbf{q}, \mathbf{p}) \rightarrow (\alpha, \beta)$ obeys the equation

$$\frac{\partial S}{\partial t} + H\left(\mathbf{q}, \frac{\partial S}{\partial \mathbf{q}}, t\right) = 0 \quad (11)$$

called the *Hamilton–Jacobi equation*. This is a first-order nonlinear partial differential equation and it provides an alternative procedure for finding the equations of motion [6, 11, 18].

3. Integrable Hamiltonians

In classical mechanics one of the most fundamental questions is the *integrability* of a given system. Here integrability does not mean whether or not the Hamilton equations can be solved in some particular way. In fact, as a set of $2n$ differential equations, they can always be solved (at least numerically) under very general conditions given by the Cauchy theorem [27].³

The concept of integrability refers to *the existence of constants of motion* (also called *integrals* and hence the name) which are responsible for the regular evolution of the phase space trajectories of the system in well-defined regions of phase space. Due to its importance, let

³ The same considerations apply to the alternative procedure provided by the Hamilton–Jacobi equation.

us recall that a constant of motion is any function of positions and momenta which does not change with time whereas the qs and ps do.

There are several equivalent definitions of integrability [11, 23, 25, 27], all of them underlying, in one way or another, the fact that *Hamilton equations (or the Hamilton–Jacobi equation) are integrated in terms of as many constants of motion as degrees of freedom*. One of these definitions, which turns out to be convenient for our purposes, is the following.

The Hamiltonian of a system with n degrees of freedom is integrable if there exist n independent constants, or integrals of motion, $I_i(\mathbf{q}, \mathbf{p}) = \alpha_i$ ($\alpha_i = \text{constant}$, $i = 1, \dots, n$), which are in ‘involution’, meaning that the quantities I_i satisfy

$$[I_i, I_j] = 0 \quad (i, j = 1, 2, \dots, n) \quad (12)$$

where $[I_i, I_j]$ is the Poisson bracket defined as in (4).

Let us remark that the mere existence of n independent constants of motions is not sufficient for integrability; to ensure that any system is integrable it is also necessary that the constants of motion satisfy the property of involution (12), a property that guarantees the existence of a canonical transformation for which the transformed momenta are precisely the integrals of motion $p'_i = I_i$ and, therefore, constants. For constant momenta the integration of Hamilton equations is immediate. This is essentially the content of a theorem attributed to Liouville [27] and what ultimately justifies the above definition of integrability (see appendix A for a more complete discussion).

Unfortunately, the existence of n integrals of motion in involution is the exception more than the rule. Poincaré proved, more than a century ago, that most mechanical systems only have the energy as a constant of motion. Therefore, *most systems with more than one degree of freedom are not integrable*.

A paradigmatic example is provided by a closed N -body system, i.e. a set of N point particles interacting with each other without external forces acting on them⁴. The N body system has $3N$ degrees of freedom (three for each particle) and only 10 integrals of motion. These are as follows.

- The three components of the total momentum

$$\mathbf{P} = \sum_{k=1}^N \mathbf{p}_k = \text{constant.}$$

- The three components of the motion of the centre of mass (M is the total mass of the system)

$$\mathbf{R}_{CM}(t) - \frac{1}{M} \mathbf{P}t = \text{constant.}$$

- The three components of the total angular momentum

$$\mathbf{L} = \sum_{k=1}^N \mathbf{l}_k = \mathbf{R}_{CM} \times \mathbf{P} + \mathbf{l} = \text{constant,}$$

where \mathbf{l} is the relative angular momentum.

⁴ This is the case, within certain approximation, of the Solar System, the Milky Way or even the system Moon–Earth–Sun among many others.

- The energy

$$E = \frac{1}{2M} \mathbf{P}^2 + T_{\text{rel}} + V = \text{constant},$$

where T_{rel} is the relative kinetic energy and V is the potential energy.

From these ten integrals *only six of them are independent and in involution*: the three components of the total momentum \mathbf{P} , the square of the relative angular momentum $|\mathbf{l}|^2$, the third component of the relative angular momentum l_3 and the total relative energy $T_{\text{rel}} + V$ [22].

When $N = 2$, *the two-body problem*, there are six degrees of freedom and the problem is integrable. However, when $N = 3$, *the three-body problem*, there are nine degrees of freedom but only six independent constants of motion in involution; from which, the three-body problem (for example, the system Sun–Earth–Moon) is not integrable.

3.1. Invariant tori

Let us first focus on integrable systems and postpone nonintegrable systems for later sections. The first and most important consequence of the existence of n involution constants I_i is that the trajectories of the system cannot pass through all points of the phase space. This is due to the fact that all trajectories are confined to move in an n -dimensional manifold M determined by the constants of motion and embedded in the phase space of dimension $2n$. Indeed, the manifold M is defined by the set of n algebraic equations:

$$I_1(\mathbf{q}, \mathbf{p}) = \alpha_1 \quad \dots \quad I_n(\mathbf{q}, \mathbf{p}) = \alpha_n, \quad (13)$$

where $\alpha_1, \dots, \alpha_n$ are arbitrary constants. Consequently, *the phasespace trajectories never leave M* because otherwise the conservation laws would be violated. Note that the manifold M depends on the particular value of the constants of motion and, since the latter depends on the choice of the initial state of the system, we see that M is fixed by the initial conditions.

In what follows we will assume that the motion of the system is bounded (recall, for instance, the planetary motion). As a consequence of this, the manifold M must be bounded as well. In fact, it can be shown that M is a compact (closed and bounded) manifold [23]. We will now see that in this case M has the topology of an n -dimensional torus.

In effect, let us define the following n velocity fields:

$$\mathbf{v}_i \equiv \left(\frac{\partial I_i}{\partial \mathbf{p}}, -\frac{\partial I_i}{\partial \mathbf{q}} \right) \quad (i = 1, 2, \dots, n). \quad (14)$$

Note that if, for example, $I_1 = H$, then (cf (1)) $\mathbf{v}_1 = (\dot{\mathbf{q}}, \dot{\mathbf{p}})$. Accordingly, in (14) is included the Hamiltonian flux of the phasespace trajectories which, due to the existence of n independent integrals in involution, must be completely contained in the manifold M .

In order to visualize that M has the topology of an n -dimensional torus, let us first show that the fields \mathbf{v}_i ($i = 1, 2, \dots, n$) are independent and tangential to M . The property of independence immediately follows from the independence of the integrals I_i . We next observe that the $2n$ -dimensional gradients:

$$\nabla I_j = \left(\frac{\partial I_j}{\partial \mathbf{q}}, \frac{\partial I_j}{\partial \mathbf{p}} \right) \quad (j = 1, \dots, n),$$

are orthogonal to every surface $I_j(\mathbf{p}, \mathbf{q}) = \alpha_j$.

On the other hand, the scalar product of the fields \mathbf{v}_i with these gradients is

$$\mathbf{v}_i \cdot \nabla I_j = \frac{\partial I_i}{\partial \mathbf{p}} \cdot \frac{\partial I_j}{\partial \mathbf{q}} - \frac{\partial I_i}{\partial \mathbf{q}} \cdot \frac{\partial I_j}{\partial \mathbf{p}} = \sum_{k=1}^n \left(\frac{\partial I_i}{\partial q_k} \frac{\partial I_j}{\partial p_k} - \frac{\partial I_i}{\partial p_k} \frac{\partial I_j}{\partial q_k} \right)$$

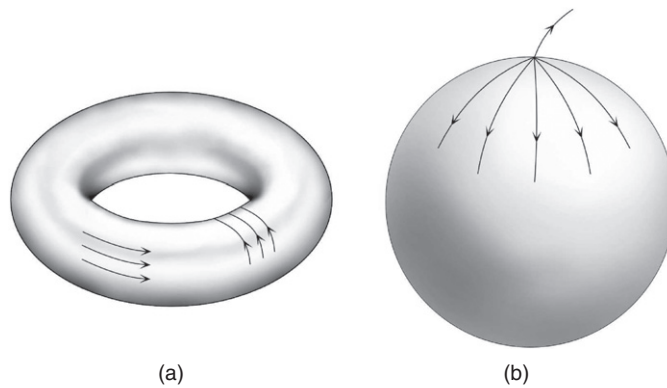


Figure 1. The ‘hairy ball theorem’. (a) Vector fields smoothly ‘combed’ on a two-dimensional torus. (b) Singular point of a vector field on a two-dimensional sphere.

and, by virtue of the involution property, we obtain

$$\mathbf{v}_i \cdot \nabla I_j = [I_i, I_j] = 0$$

($i, j = 1, 2, \dots, n$). Hence, the fields \mathbf{v}_i are orthogonal to ∇I_j and, since the gradients ∇I_j are orthogonal to M , we conclude that *the fields \mathbf{v}_i are tangential to the manifold M .*

There is a theorem in topology—the Poincaré–Hopf theorem, jokingly known as the ‘hairy ball theorem’—which states that if in a compact manifold M of dimension n , one can define n independent vector fields tangential to M , then M has necessarily the topology of an n -dimensional torus [2, 23, 25].

Without getting into technical details, we can intuitively imagine this result as follows. Among the several possibilities for a manifold M to be compact, and hence bounded, the simplest ones are either M is an n -dimensional sphere (or a surface with the same topology, like an apple) or it has the topology of an n -dimensional torus. However, it is impossible to define a vector field on a sphere in all its points while it is perfectly possible to define a vector field on the surface of a torus. This is easily visualized if we compare the act of combing down hair on a torus and on a sphere—for the latter case, a hair always sticks up at the pole and, hence, it is not tangential to the sphere—see figure 1.

4. Action-angle variables

We have just seen that, for the bounded motion of integrable systems with n degrees of freedom, the phase space trajectories lie on n -dimensional tori embedded in the $2n$ -dimensional phase space. We will now see that the existence of these invariant tori⁵ provides a way of defining a new set of canonical variables, the action-angle variables, which are crucial for the further development of the subject.

Indeed, any n -dimensional torus is a periodic object which can be considered as the product of n independent periodicities. In other words, we can define n topologically independent closed curves, $\Gamma_1, \dots, \Gamma_n$, on a given torus, where none of the Γ_i can be deformed continuously into each other or shrunk to zero [23, 25]. In figure 2 we represent a two-dimensional torus for which Γ_1 turns around through the longest path while Γ_2 does it through

⁵ The tori defined in (13) are often called ‘invariant tori’ because they are constructed by giving different values to the integral invariants I_i .

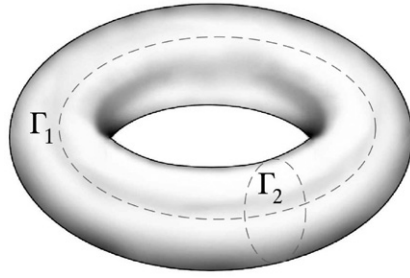


Figure 2. The two topological independent curves Γ_1 and Γ_2 on a two-dimensional torus.

the shortest path. Note that neither Γ_1 nor Γ_2 can be converted into each other by continuous transformations.

Having this set of closed curves at our disposal, we define the *action variables* by means of the line integrals:

$$J_i = \frac{1}{2\pi} \oint_{\Gamma_i} \sum_{k=1}^n p_k dq_k, \quad (15)$$

where

$$p_k = p_k(\mathbf{q}, \boldsymbol{\alpha}) \quad (16)$$

are the momenta written in terms of the coordinates $\mathbf{q} = (q_1, \dots, q_n)$ and the constants of motion $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)$. Note that (16) is obtained by solving for the p s the set of algebraic equations (13) provided by the existence of n independent integrals.

Since in (15) we integrate with respect to the generalized coordinates, the action variables only depend on the integral invariants:

$$J_i = J_i(\alpha_1, \dots, \alpha_n) \quad (i = 1, \dots, n), \quad (17)$$

and are themselves constants of motion.

We now define a canonical transformation from the original variables (\mathbf{q}, \mathbf{p}) to a new set of variables $(\boldsymbol{\theta}, \mathbf{J})$ where the actions are the transformed momenta. A generating function for this transformation is given by the indefinite integral

$$S(\mathbf{q}, \mathbf{J}) = \int \sum_{k=1}^n p_k(\mathbf{q}, \mathbf{J}) dq_k, \quad (18)$$

where $p_k(\mathbf{q}, \mathbf{J})$ is given by (16) in which the α s have been written in terms of the J s after solving (17).

We see below that the new coordinates, defined by

$$\boldsymbol{\theta} = \frac{\partial S}{\partial \mathbf{J}}, \quad (19)$$

play the role of angles, increasing by 2π when the phasespace trajectory undergoes a complete turn around Γ_i , while momenta (i.e. the actions) are the radii of the invariant tori (see figure 3).

In action-angle variables, Hamilton equations read

$$\dot{\boldsymbol{\theta}} = \frac{\partial H'}{\partial \mathbf{J}}, \quad \dot{\mathbf{J}} = -\frac{\partial H'}{\partial \boldsymbol{\theta}}, \quad (20)$$

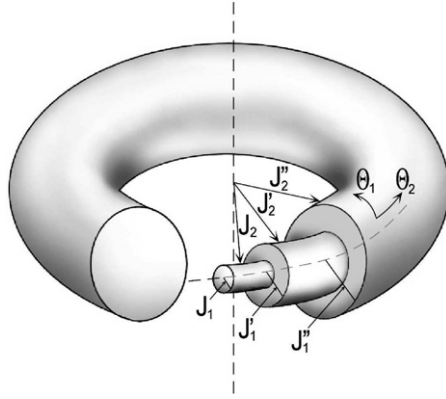


Figure 3. Nested tori for several values of the actions in two degrees of freedom. The vectors $\mathbf{J} = (J_1, J_2)$, $\mathbf{J}' = (J'_1, J'_2)$ and $\mathbf{J}'' = (J''_1, J''_2)$ label the different tori and correspond to different initial conditions. (θ_1, θ_2) are the angle coordinates on a given torus.

where $H' = H$ is the transformed Hamiltonian which coincides with the original one since we are dealing with a time-independent canonical transformation.

However, $\dot{\mathbf{J}} = 0$, because the J 's are constants of motion. Hence, $\partial H'/\partial \theta = 0$, and the transformed Hamiltonian only depends on the actions:

$$H' = H(\mathbf{J}),$$

whence

$$\dot{\theta} = \frac{\partial H(\mathbf{J})}{\partial \mathbf{J}} \equiv \boldsymbol{\omega}(\mathbf{J}) = \text{constant}. \quad (21)$$

The solution of the Hamilton equations (20) thus reads

$$J_i = \text{constant}, \quad \theta_i(t) = \omega_i t + \beta_i, \quad (22)$$

where $\beta_i = \theta_i(0)$ ($i = 1, \dots, n$).

In action-angle variables, the equations of motion are, therefore, very simple: the actions (transformed momenta) are constants and the angle variables (transformed coordinates) are linear functions of time. In the original variables, (\mathbf{q}, \mathbf{p}) , the equations of motion are obtained by introducing (22) into the equations of the canonical transformation $(\mathbf{q}, \mathbf{p}) \rightarrow (\boldsymbol{\theta}, \mathbf{J})$ which gives the original variables in terms of action-angle variables.

Before proceeding further let us note that the transformation to action-angle variables is global. That is, the entire phase space is filled with tori (see figure 3) and a given trajectory will forever reside on the surface of the particular torus fixed by the initial conditions $(\mathbf{q}(0), \mathbf{p}(0))$. Indeed, the choice of any invariant torus depends on the value of the constants $\alpha_i = I_i(\mathbf{q}(0), \mathbf{p}(0))$. The set of constants α_i determines the torus where the trajectory stays and the value of the angle variable θ_i , at a given time, determines the position of the trajectory on that torus.

We will see next that *the ω s are the angular frequencies of the multiply periodic motion of the system*. To this end we first show that when the state of the system performs a complete oscillation along a closed curve Γ_i , the corresponding angle variable varies in 2π . In effect, let us denote by $\Delta_i \theta_j$ the change of the angle variable θ_j when the coordinate q_i realizes a complete oscillation (also known by the astronomical name of ‘libration’). In appendix B we show that

$$\Delta_i \theta_j = 2\pi \delta_{ij}. \quad (23)$$

In other words, the angle variable θ_i changes in 2π only when the system executes a complete oscillation along the curve Γ_i and no change otherwise.

On the other hand, let T_i ($i = 1, \dots, n$) be the different periods of each libration motion. We see from (22) that the change in θ_i after a period T_i is

$$\Delta_i \theta_i = \theta_i(t + T_i) - \theta_i(t) = \omega_i T_i,$$

and equating it with (23) we obtain

$$T_i = \frac{2\pi}{\omega_i}.$$

Therefore, the quantities ω_i —defined in (21) as derivatives of the Hamiltonian with respect to the actions—are the angular frequencies of the (multi-periodic) motion of the system. This is quite remarkable since, for integrable Hamiltonians described by action-angle variables, to obtain the frequencies of the motion it is not necessary to integrate Hamilton equations, it suffices to take the derivative of the Hamiltonian with respect to the actions, a much easier task indeed.

4.1. Periodic and multiply periodic motion

Recall that the original variables, (\mathbf{q}, \mathbf{p}) , and the action-angle variables, $(\boldsymbol{\theta}, \mathbf{J})$, are related by a canonical transformation with the generating function (18). This obviously implies that the relationship between these two sets of canonical variables is known. Let us denote this relationship by

$$\mathbf{q} = \mathbf{q}(\boldsymbol{\theta}, \mathbf{J}), \quad \mathbf{p} = \mathbf{p}(\boldsymbol{\theta}, \mathbf{J}). \quad (24)$$

Owing to the periodic nature of the angle variables, as expressed in equation (23), we see from (24) that the q s and p s are multiply periodic functions of the θ s with periods 2π , and the same is true for any dynamical function $f(\boldsymbol{\theta}, \mathbf{J})$.

As is well known from analysis, any multiple periodic function can be represented by a multiple Fourier series. Thus, for instance, q_j would appear as

$$q_j = \sum_{k_1=-\infty}^{\infty} \cdots \sum_{k_n=-\infty}^{\infty} c_{k_1, \dots, k_n}^{(j)} \exp\{i(k_1\theta_1 + \cdots + k_n\theta_n)\},$$

where the k_i s are integer indices running from $-\infty$ to ∞ . By treating the set of k_i s also as an n -dimensional vector, $\mathbf{k} = (k_1, \dots, k_n)$, the expansion can be written in a more compact form:

$$q_j = \sum_{\mathbf{k}} c_{\mathbf{k}}^{(j)} e^{i\mathbf{k} \cdot \boldsymbol{\theta}},$$

where we use the abbreviated notation:

$$\sum_{\mathbf{k}} = \sum_{k_1=-\infty}^{\infty} \cdots \sum_{k_n=-\infty}^{\infty}.$$

The Fourier coefficients $c_{\mathbf{k}}^{(j)}$, which depend on the actions, are given by

$$c_{\mathbf{k}}^{(j)}(\mathbf{J}) = \frac{1}{(2\pi)^n} \int_0^{2\pi} d\theta_1 \cdots \int_0^{2\pi} d\theta_n e^{-i\mathbf{k} \cdot \boldsymbol{\theta}} q_j(\boldsymbol{\theta}, \mathbf{J}).$$

If we also write the time dependence of the angle variables—given in (22)—as a vector equation

$$\boldsymbol{\theta} = \boldsymbol{\omega}t + \boldsymbol{\beta},$$

then the time dependence of q_j appears in the form

$$q_j(t) = \sum_{\mathbf{k}} a_{\mathbf{k}}^{(j)}(\mathbf{J}) e^{i\mathbf{k} \cdot \boldsymbol{\omega} t}, \quad (25)$$

where $a_{\mathbf{k}}^{(j)} = c_{\mathbf{k}}^{(j)} e^{i\mathbf{k} \cdot \boldsymbol{\beta}}$. We easily convince ourselves that a similar expression holds for any momentum:

$$p_j(t) = \sum_{\mathbf{k}} b_{\mathbf{k}}^{(j)}(\mathbf{J}) e^{i\mathbf{k} \cdot \boldsymbol{\omega} t}. \quad (26)$$

Note that the right-hand sides of equations (25) and (26) correspond to a superposition of the equations of motion of n linear oscillators. Therefore,

the coordinates and momenta of integrable systems can be represented as a sum of n -dimensional harmonic oscillators with angular frequencies given by the fundamental ones, $\boldsymbol{\omega} = (\omega_1, \dots, \omega_n)$, and their harmonics $\mathbf{k} \cdot \boldsymbol{\omega} = k_1\omega_1 + \dots + k_n\omega_n$, ($k_j = 0, \pm 1, \pm 2, \dots$).

The coordinates and momenta of integrable systems are multiply periodic functions of time with n independent (angular) frequencies $\omega_1, \dots, \omega_n$. However, this property *does not imply that, in general, the q s and p s are (simply) periodic functions of time*; for it would be necessary that there exists a single period T_0 for which all q s and p s are periodic:

$$\mathbf{q}(t + T_0) = \mathbf{q}(t) \quad \text{and} \quad \mathbf{p}(t + T_0) = \mathbf{p}(t).$$

In appendix C we show that this is the case if, and only if, the frequencies $\omega_1, \dots, \omega_n$ are integer multiples of a single frequency ω_0 :

$$\omega_j = l_j \omega_0, \quad (27)$$

($j = 1, \dots, n$), where $l_j = 0, \pm 1, \pm 2, \dots$ are integer numbers, and

$$\omega_0 = \frac{2\pi}{T_0}.$$

Equation (27) means that in order to have periodic motion, the frequencies must be *commensurable*. From (27) we immediately see that this is equivalent to assuming that all frequencies are rational multiples of each other:

$$\frac{\omega_i}{\omega_j} = \frac{l_i}{l_j} = \text{a rational number}. \quad (28)$$

If the frequencies are *incommensurable*, in other words, if they are not rationally related, then the motion is termed multiply periodic or quasiperiodic or conditionally periodic, according to different terminologies in use, and never repeats itself.

A formal condition for the frequencies to be commensurable is the existence of $n - 1$ relationships of the form

$$\sum_{j=1}^n l_{kj} \omega_j = 0 \quad (k = 1, \dots, n - 1), \quad (29)$$

where $l_{kj} = 0 \pm 1 \pm 2 \pm \dots$ are integers. Indeed, if (29) holds, then we have a homogeneous system of $n - 1$ algebraic equations (with integer coefficients) for n unknowns, the frequencies, which means that we can solve (29) by writing all frequencies in terms of one of them, say ω_1 . In other words, we obtain $\omega_j = (m_j/m_1)\omega_1$, where m_1 and m_j are integers. Therefore, $\omega_j/\omega_1 = m_j/m_1$ is a rational number, and all frequencies are commensurable.

Let us remember that the phase-space trajectories lie on the invariant tori defined by equation (22), and since these curves are mathematically described by functions of coordinates

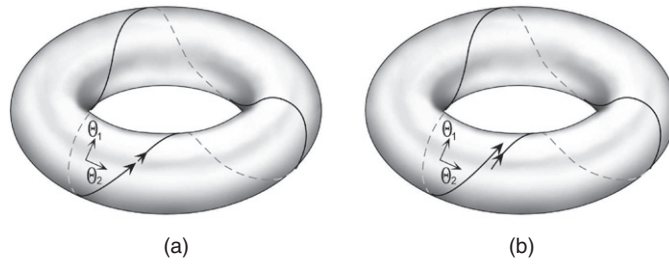


Figure 4. Comparison of phasespace trajectories on two-dimensional tori. The torus in (a) is a rational surface (resonant torus) where $\omega_1/\omega_2 = 3$, that is, the trajectory closes over itself after three turns around Γ_1 and one turn around Γ_2 . The torus in (b) is an irrational surface (nonresonant torus) where the frequencies are not commensurable. In (b) the phasespace trajectory will eventually cover the surface of the torus densely.

and momenta, the above considerations on single or multiple periodicity apply to phasespace trajectories as well. We can, therefore, conclude that *on a given torus, the phasespace trajectory will be a closed curve (i.e. the motion of the system will be periodic) if and only if the frequencies of the motion are commensurable. When frequencies are incommensurable the trajectory will densely cover the torus, never closing on itself.* In the first case, we call it *rational, or resonant, torus*, while in the latter *irrational, or nonresonant, torus* (figure 4).

4.2. The Kepler problem

A classic example of an integrable Hamiltonian is provided by the Kepler problem. Consider the relative motion of a planet of mass m orbiting around a star of mass M . The Hamiltonian of the system in polar coordinates, (r, ϕ) , is

$$H_0 = \frac{p_r^2}{2\mu} + \frac{p_\phi^2}{2\mu r^2} - \frac{k}{r}, \quad (30)$$

where (p_r, p_ϕ) is the relative momentum of the two bodies, $\mu = mM/(m+M)$ is the reduced mass and $k = GmM$ (G is the gravitational constant).

Both the energy, $H_0 = E$, and the angular momentum, \mathbf{L} , of the two-body system are constants of the motion. The latter implies that the motion takes place on the plane perpendicular to the direction of \mathbf{L} .

After a canonical transformation from the original variables (p_r, p_ϕ, r, ϕ) to the action-angle variables $(J_1, J_2, \theta_1, \theta_2)$, the Hamiltonian is only a function of the actions [6, 11, 18]:

$$H_0 = \frac{-\mu k^2}{2(J_1 + J_2)^2}. \quad (31)$$

The equations of motion in the original variables are quite complicated (elliptic orbits), but in terms of action-angle variables they are very simple:

$$J_i = \alpha_i, \quad \theta_i(t) = \omega_i t + \beta_i \quad (i = 1, 2) \quad (32)$$

where α_i and β_i are constants determined by the initial conditions.

The motion of the system in the phase space (i.e. the phasespace trajectory) lies on a two-dimensional torus embedded in the three-dimensional manifold of constant energy. The torus has two angular coordinates θ_1 and θ_2 and two constant radii $J_1 = \alpha_1$ and $J_2 = \alpha_2$ which are fixed by the initial conditions.

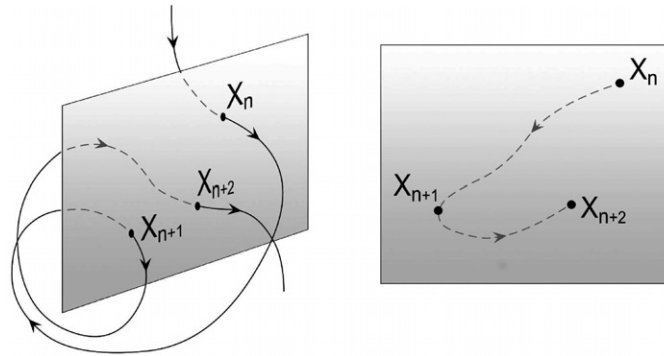


Figure 5. Intersections of a phasespace trajectory with a Poincaré surface of section.

There are two frequencies, ω_1 and ω_2 , associated with the motion; If they are commensurable, that is if $l_1\omega_1 = l_2\omega_2$, where l_1 and l_2 are integers, the trajectory is closed and the motion is periodic (the trajectory closes on itself after l_1 turns around Γ_1 and l_2 turns around Γ_2). If the frequencies are incommensurable the trajectory will never repeat itself and will eventually cover the entire surface of the torus.

For the Kepler problem the frequencies are (recall that $\omega_i = \dot{\theta}_i = \partial H_0 / \partial J_i$)

$$\omega_1 = \omega_2 = \frac{1}{k} \sqrt{-\frac{2H_0^3}{\mu}},$$

which is Kepler's third law. The frequencies are commensurable (in fact, equal) and hence the phasespace trajectory is always closed. In other words, the motion is periodic.

5. Nonintegrable Hamiltonians

We know that the existence of as many constants of motion in involution as degrees of freedom determines integrability and regular motion. On the other hand, conservative systems with one degree of freedom always have one integral of motion, the energy, and they are, therefore, integrable. The following question then arises: can we know whether or not a conservative system with $n > 1$ degrees of freedom is integrable? Unfortunately there is no general answer to this problem. In most situations, integrability is guessed, but not proved, by constructing a *Poincaré surface of section* which we can define as any bidimensional surface, contained in the phase space, where one can conveniently analyse the successive intersections of the phasespace trajectory (figure 5).

To see how this concept works, let us suppose a conservative system with two degrees of freedom. The Hamiltonian is a constant of motion and we write

$$H(q_1, q_2; p_1, p_2) = E. \quad (33)$$

This restricts phasespace trajectories to evolve inside a three-dimensional manifold—the surface of constant energy or ‘energy shell’ represented by (33)—embedded in the phase space which has dimension 4. Suppose the system has a second integral (for instance, the angular momentum):

$$I(q_1, q_2; p_1, p_2) = \alpha, \quad (34)$$

where α is an arbitrary constant; then this integral also defines another three-dimensional manifold in the four-dimensional phase space and any trajectory must also evolve in it.

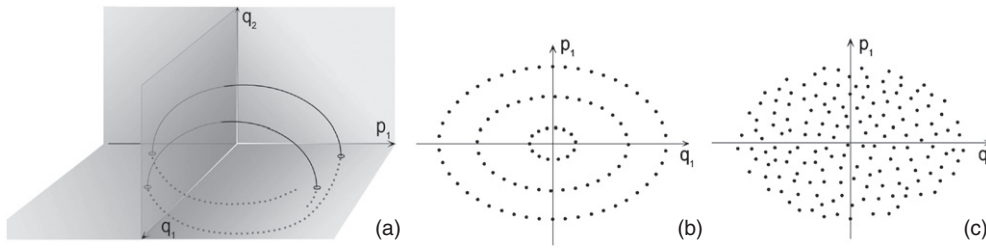


Figure 6. Construction of a Poincaré surface of section for a system with two degrees of freedom. (a) We can obtain a Poincaré section plotting a point each time $q_2 = 0$, i.e. each time the trajectory passes through the plane (q_1, p_1) . (b) If there are two integrals of motion in involution, the trajectory will remain along one-dimensional curves, $p_1 = \phi(q_1, 0; E, \alpha)$, in the plane (q_1, p_1) . (c) If only one constant of motion exists (the energy), the trajectory will disperse over a region of the (q_1, p_1) plane.

The coordinates and momenta of the system cannot take arbitrary values because they must satisfy the conservation laws (33) and (34). From a geometrical point of view, this means that any phase space trajectory is bounded to move on a two-dimensional surface which is the intersection of two three-dimensional manifolds $H = E$ and $I = \alpha$. Indeed, from the conservation of energy (33), we can write, for instance, p_2 as a function of p_1, q_1, q_2 and the energy E , that is, $p_2 = p_2(q_1, q_2, p_1; E)$. Substituting this expression into the second conservation law (34) we can obtain p_1 in terms of q_1 and q_2 and the constants E and α :

$$p_1 = \phi(q_1, q_2; E, \alpha). \quad (35)$$

This is the equation of a two-dimensional surface within the four-dimensional phase space. Such a surface is determined by the specific values of the constants E and α , which, in turn, depend on the initial conditions.

If we now consider the section $q_2 = 0$ of the surface (35)—and this is an example of a Poincaré surface of section—we see that the successive intersections of the phase space trajectory with this Poincaré section are along the curve

$$p_1 = \phi(q_1, 0; E, \alpha)$$

on the plane (q_1, p_1) .

In general, for a given conservative Hamiltonian, we do not know whether or not a second integral of motion exists. We can guess, nonetheless, its existence by solving Hamilton equations numerically and then drawing p_1 and q_1 each time $q_2 = 0$ (figure 6(a)). If the system is integrable, the intersections of the trajectory in the Poincaré section $q_2 = 0$ will appear as a collection of points regularly distributed on the curve $p_1 = \phi(q_1, 0; E, \alpha)$ (figure 6(b)). On the other hand, if the system is not integrable the intersections of the phase space trajectory will appear randomly—that is, chaotically—scattered over a region only limited by the conservation of energy (figure 6(c)).

This was the method used by Henon and Heiles [15] to determine the possible existence of a third integral which, as the observations showed, constrained the motion of a star in a galaxy with an axis of symmetry. This system has three degrees of freedom and two known constants of motion, the energy and the component of the angular momentum along the direction of the symmetry axis. For a long time it was believed that there was no third integral of motion because it had not been found analytically.

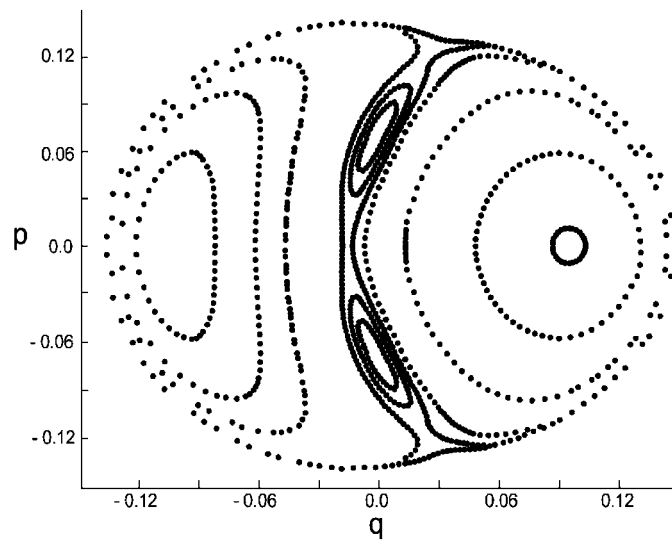


Figure 7. Poincaré section for the Henon–Heiles Hamiltonian at low energy $E = 0.01$.

Henon and Heiles proposed the following Hamiltonian—without any known symmetries leading to a third integral—that could model the basic traits of the problem [15, 19]:

$$H = \frac{1}{2} (p_1^2 + p_2^2) + \frac{1}{2} (q_1^2 + q_2^2 + 2q_1^2 q_2 - \frac{2}{3} q_2^3) = E,$$

and numerically studied the behaviour of the equations of motion. The Hamilton equations are

$$\dot{q}_i = p_i, \quad \dot{p}_1 = -q_1 - 2q_1 q_2, \quad \dot{p}_2 = -q_2 - 2q_1^2 - 2q_2^2$$

($i = 1, 2$). Observe the occurrence of nonlinear quadratic terms in these equations of motion which are a consequence of the cubic terms in the potential energy. Note also that the magnitude of these nonlinear terms increases with the energy. The representation of the intersections of the phase space trajectory on the Poincaré section $q_2 = 0$ is given in figures 7 and 8. For low energies (figure 7), the distribution of points is apparently regular, which seems to suggest the existence of a third integral, at least to the accuracy of the plotting. As the energy increases (which increases the effect of the nonlinear terms) the third integral appears to be destroyed, at least partially, but there still remain some ‘islands’ where the motion is regular (figure 8). For even higher energies the hypothetical third integral is completely destroyed. The scattered points appearing in figure 8 correspond to a single phase space trajectory that, for obvious reasons, we will call chaotic, and which implies a highly sensitive dependence on initial conditions that makes the long-time evolution of the system totally unpredictable.

6. Canonical perturbation theory: resonances

As stated in previous sections, most mechanical systems are not integrable, having only the energy as a constant of motion. However, in many situations, integrable and nonintegrable Hamiltonians differ very little. In such cases we can obtain approximate solutions of the equations of motion by means of the canonical perturbation theory. We will outline this theory because it provides the clue to the appearance of chaos in deterministic systems, for it shows that chaotic behaviour is a direct consequence of the occurrence of resonances, i.e. of small denominators leading to infinities.

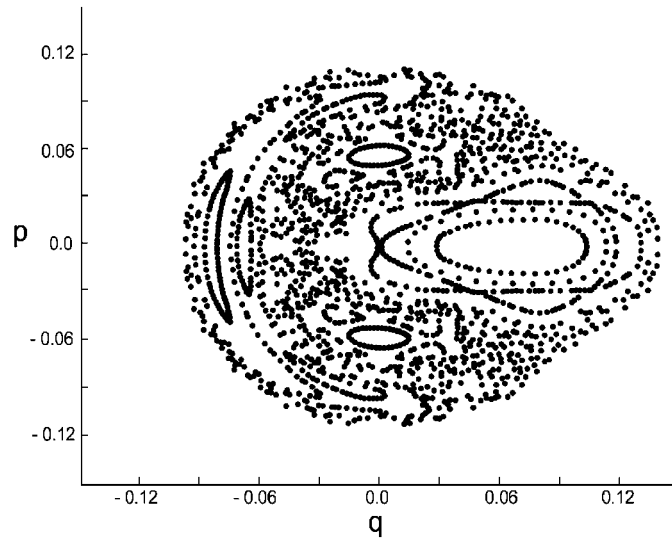


Figure 8. Poincaré section for the Henon–Heiles Hamiltonian at high energy $E = 0.12$.

In order to fix ideas, let us return to the Kepler problem discussed in section 4.2 and suppose that, in addition to the planet orbiting the Sun, there is another celestial body which perturbs the motion of the two-body system. We assume that the effect of this perturbation is small (because, for instance, the third body is small or more distant), so that the total Hamiltonian can be written in the form

$$H = H_0(J_1, J_2) + \epsilon H_1(J_1, J_2, \theta_1, \theta_2), \quad (36)$$

where $\epsilon \ll 1$ is a small parameter and H_0 is the unperturbed Hamiltonian of the Kepler problem as given in (31).

According to our previous discussions, we know that the unperturbed motion, represented by H_0 , takes place on a bidimensional torus of radii $J_i = \alpha_i$ ($i = 1, 2$). We want now to find the corrections to the unperturbed motion due to the presence of a third body. As we generally cannot obtain an exact solution to the equations of motion, we search for approximations via perturbation expansions in powers of ϵ .

Observe that the motion generated by the Hamiltonian (36) is bounded. This allows us to expand the perturbation as a Fourier series in the angular variables. Therefore, following the notation of section 4.1, we see that (36) can be written as⁶

$$H(\boldsymbol{\theta}, \mathbf{J}) = H_0(\mathbf{J}) + \epsilon \sum_{\mathbf{k}} H_{\mathbf{k}}^{(1)}(\mathbf{J}) \cos(\mathbf{k} \cdot \boldsymbol{\theta}), \quad (37)$$

where $\boldsymbol{\theta} = (\theta_1, \dots, \theta_n)$, $\mathbf{J} = (J_1, \dots, J_n)$ and $\mathbf{k} = (k_1, \dots, k_n)$ ($k_i = 0, \pm 1, \pm 2, \dots$). The Fourier coefficients, $H_{\mathbf{k}}^{(1)}(\mathbf{J})$, are defined by

$$H_{\mathbf{k}}^{(1)}(\mathbf{J}) = \frac{1}{(2\pi)^n} \int_0^{2\pi} d\theta_1 \cdots \int_0^{2\pi} d\theta_n H_1(\mathbf{J}, \boldsymbol{\theta}) \cos(\mathbf{k} \cdot \boldsymbol{\theta}). \quad (38)$$

Let us note that we have generalized (36) to include multiply periodic systems with n degrees of freedom.

⁶ It is more convenient for the following development on perturbation theory to work with real Fourier series of sines and cosines instead of complex exponential series as in section 4.1.

The main idea behind canonical perturbation theory is simple and consists in finding, by means of a power series in ϵ , a canonical transformation,

$$(\boldsymbol{\theta}, \mathbf{J}) \longrightarrow (\boldsymbol{\theta}', \mathbf{J}'), \quad (39)$$

to a new set of action-angle variables such that *the transformed Hamiltonian $H'(\mathbf{J}')$ is only a function of the new actions \mathbf{J}'* . If we could achieve this, then the Hamiltonian (36) would become completely integrable and its equations of motion would be easily obtained; that is, the J 's would be constants and the θ 's linear functions of time.

Unfortunately, this procedure cannot be done exactly. However, we may proceed by perturbation expansions since ϵ is small. We take this path and introduce the following generating function for the canonical transformation (39):

$$S(\boldsymbol{\theta}, \mathbf{J}') = \boldsymbol{\theta} \cdot \mathbf{J}' + \epsilon \sum_{\mathbf{k}} S_{\mathbf{k}}(\mathbf{J}') \sin(\mathbf{k} \cdot \boldsymbol{\theta}) + O(\epsilon^2), \quad (40)$$

which is defined by a perturbation series up to first order in ϵ with the unknown Fourier coefficients $S_{\mathbf{k}}(\mathbf{J}')$ to be determined later. In terms of the generating function, the canonical transformation is obtained by (cf (8))

$$\mathbf{J} = \frac{\partial S}{\partial \boldsymbol{\theta}}, \quad \boldsymbol{\theta}' = \frac{\partial S}{\partial \mathbf{J}'}$$

That is

$$\mathbf{J} = \mathbf{J}' + \epsilon \sum_{\mathbf{k}} \mathbf{k} S_{\mathbf{k}}(\mathbf{J}') \cos(\mathbf{k} \cdot \boldsymbol{\theta}) + O(\epsilon^2), \quad (41)$$

$$\boldsymbol{\theta}' = \boldsymbol{\theta} + \epsilon \sum_{\mathbf{k}} \frac{\partial S_{\mathbf{k}}(\mathbf{J}')}{\partial \mathbf{J}'} \sin(\mathbf{k} \cdot \boldsymbol{\theta}) + O(\epsilon^2). \quad (42)$$

Since we are dealing with a time-independent canonical transformation, the transformed Hamiltonian, $H' = H$, coincides with the original one. Therefore, the new Hamiltonian is found from (37) by solving equations (41) and (42) for $(\boldsymbol{\theta}, \mathbf{J})$ as a function of $(\boldsymbol{\theta}', \mathbf{J}')$. We detail this procedure in appendix D where we show that

$$H'(\boldsymbol{\theta}', \mathbf{J}') = H_0(\mathbf{J}') + \epsilon H_0^{(1)}(\mathbf{J}') + \epsilon \sum_{\mathbf{k} \neq \mathbf{0}} [H_{\mathbf{k}}^{(1)}(\mathbf{J}') + \mathbf{k} \cdot \boldsymbol{\omega} S_{\mathbf{k}}(\mathbf{J}')] \cos(\mathbf{k} \cdot \boldsymbol{\theta}') + O(\epsilon^2). \quad (43)$$

In these expressions $\boldsymbol{\omega} = \boldsymbol{\omega}(\mathbf{J}')$ are the (known) frequencies of the unperturbed motion:

$$\boldsymbol{\omega} = \frac{\partial H_0}{\partial \mathbf{J}'}, \quad (44)$$

whereas $H_0^{(1)}(\mathbf{J}')$ is the Fourier coefficient of the perturbation corresponding to $\mathbf{k} = \mathbf{0}$ and reads (see (38))

$$H_0^{(1)}(\mathbf{J}') = \frac{1}{(2\pi)^n} \int_0^{2\pi} d\theta_1 \cdots \int_0^{2\pi} d\theta_n H_1(\mathbf{J}', \boldsymbol{\theta}). \quad (45)$$

In other words, $H_0^{(1)}$ is the average of the perturbation H_1 with respect to the original angle variables.

Recall that the Fourier coefficients $S_{\mathbf{k}}(\mathbf{J}')$ of the generating function (40) are still unknown and we are, therefore, free to choose them in the most convenient way. Let us take

$$S_{\mathbf{k}}(\mathbf{J}') = -\frac{H_{\mathbf{k}}^{(1)}(\mathbf{J}')}{\mathbf{k} \cdot \boldsymbol{\omega}}, \quad (46)$$

($\mathbf{k} \neq \mathbf{0}$), so that the term inside the sum in equation (43) vanishes; we obtain

$$H' = H_0(\mathbf{J}') + \epsilon H_0^{(1)}(\mathbf{J}') + O(\epsilon^2). \quad (47)$$

In such a case, and to the first order in ϵ , *the transformed Hamiltonian H' is only a function of the new action variables and is, therefore, integrable (up to first order).*

Moreover, the perturbed frequencies ω' (given by the derivatives of the transformed Hamiltonian H' with respect to the actions) read

$$\omega' = \omega + \epsilon \frac{\partial}{\partial \mathbf{J}} H_0^{(1)}(\mathbf{J}') + O(\epsilon^2), \quad (48)$$

where $H_0^{(1)}(\mathbf{J}')$ is the average of the perturbation H_1 (cf (46)) and ω are the unperturbed frequencies given by (44).

Finally, the relationship between the original actions and the new variables is given by (see (41) and (42))

$$\mathbf{J} = \mathbf{J}' - \epsilon \sum_{\mathbf{k} \neq \mathbf{0}} \mathbf{k} \frac{H_{\mathbf{k}}^{(1)}(\mathbf{J}')}{\mathbf{k} \cdot \omega} \cos(\mathbf{k} \cdot \theta') + O(\epsilon^2). \quad (49)$$

Equation (49) is, to the lowest order in ϵ , the solution to our problem. We have obtained the new action variables \mathbf{J}' which contain the first-order correction due to the perturbation. To first order in ϵ the \mathbf{J}' are constants and the new angles θ' are linear functions of time.

Unfortunately, expressions (46) and (49) suffer a serious illness for both $S_{\mathbf{k}}$ and \mathbf{J} diverge if

$$\mathbf{k} \cdot \omega = k_1 \omega_1 + \dots + k_n \omega_n = 0. \quad (50)$$

In other words, *the perturbation method breaks down when internal resonances occur inducing perturbation expansions to diverge.*

Let us observe that if the unperturbed motion takes place on a rational (resonant) torus, i.e. if the frequencies of the unperturbed Hamiltonian H_0 are commensurable, there always exists a set of integers such that condition (50) holds (see (29)). At first sight, this would imply the restriction of canonical perturbations to the motion on irrational (nonresonant) tori. However, the problem is worse because, even if the frequencies are incommensurable (and recalling that any irrational number can be approximated, within any degree of accuracy, by a sequence of rational numbers) there will always be integers k_1, \dots, k_n that generate denominators $\mathbf{k} \cdot \omega$ as small as desired, with the result of convergence failure⁷. Hence we obtain two series whose convergence is uncertain. On one hand, we have Fourier series that cannot converge due to internal resonances which lead to the famous problem of ‘small denominators’. On the other hand, far from resonant frequencies and also because of small divisors, it is quite unclear that the perturbation series in ϵ converge. In fact, Poincaré proved that all these series do not lead to a convergent representation of the perturbed problem [27]. Consequently, fundamental questions, such as the long-time stability of planetary orbits in the Solar System, could not be answered in a satisfactory way. Let us remind ourselves of Moser’s query and ask again: Is the Solar System stable?

7. The KAM theorem: stability and chaos

At the end of the 19th century, the general consensus was that the addition of even the smallest perturbation would render any conservative system nonintegrable, and that any phase space

⁷ In the perturbed Kepler problem, as given in (36), the term $k_1 \omega_1 + k_2 \omega_2$ which appears in the denominator of the perturbation series, albeit never zero, can be arbitrarily small for k_1 and k_2 covering all integer numbers except 0. Thus, for instance, Jupiter and Saturn, in their motion around the Sun cover 299 and 1205 s of arc in a day and the denominator $5\omega_{\text{Sat}} - 2\omega_{\text{Jup}}$ is very small compared with each frequency.

trajectory would densely explore the energy shell in a chaotic manner.⁸ This was the first crack in classical certainty and a severe blow to classical thinking.

All efforts and attempts by some of the finest mathematicians and physicists of the time failed to solve the small divisor problem. Poincaré called it the ‘fundamental problem of classical mechanics’ and seemed to be an insurmountable obstacle. Thus, around the beginning of the 20th century, this field of research dropped off and questions concerning long-time planetary stability were almost forgotten in mainstream research.

The breakthrough came in 1954, when Kolmogorov [17] devised a way of obtaining a theory of canonical perturbations which is rapidly convergent and appropriate to nonresonant tori. Kolmogorov’s new idea was rigorously proved by Arnold in 1961 [1] and, independently, by Moser in 1962 [20]. The complete result is known as the KAM theorem.

Following Arnold ([1, 2], see also [25]) suppose that an integrable Hamiltonian H_0 is perturbed by a function H_1 , so that the total Hamiltonian is

$$H = H_0(\mathbf{J}) + \epsilon H_1(\mathbf{J}, \boldsymbol{\theta}) \quad (\epsilon \ll 1) \quad (51)$$

where the perturbation H_1 is assumed to be periodic in the angular variables:

$$H_1(\mathbf{J}, \theta_1 + 2\pi, \dots, \theta_n + 2\pi) = H_1(\mathbf{J}, \theta_1, \dots, \theta_n).$$

Hamilton equations read

$$\dot{J}_i = -\epsilon \frac{\partial H_1}{\partial \theta_i}, \quad \dot{\theta}_i = \omega_i(\mathbf{J}) + \epsilon \frac{\partial H_1}{\partial J_i} \quad (i = 1, 2, \dots, n) \quad (52)$$

where $\omega_i = \partial H_0 / \partial J_i$ are the frequencies of the unperturbed motion.

Kolmogorov’s idea was that, far from resonant frequencies, it is possible to construct a perturbation series *in even powers of ϵ* . This leads to a fast convergent (‘superconvergent’) perturbation series with the overall result that, for most initial conditions, the motion generated by the Hamiltonian (51) remains quasiperiodic, that is, confined to reside on certain surfaces which resemble slightly deformed tori, while the complement of this regular motion—that is, the chaotic motion—has a small Lebesgue measure if ϵ is small. In other words, the set of chaotic trajectories is negligible as $\epsilon \rightarrow 0$.

In order to be more precise in the formulation of the theorem, one has to assume that H is an analytic function and that the unperturbed motion generated by H_0 is nondegenerate. The last statement implies that the Hessian of H_0 is different from zero:

$$\det \left| \frac{\partial^2 H_0}{\partial J_i \partial J_j} \right| \neq 0.$$

The next step consists in identifying, for the unperturbed system, a particular torus, $T_0(\boldsymbol{\omega}^*)$, defined by a set of frequencies, $\boldsymbol{\omega}^* = (\omega_1^*, \dots, \omega_n^*)$, which are incommensurable, that is

$$k_1 \omega_1^* + \dots + k_n \omega_n^* \neq 0$$

for all the integers $k_i \neq 0$. The KAM theorem can then be stated as [1, 2, 25] follows.

If ϵH_1 is small enough, then for almost all nonresonant frequencies $\boldsymbol{\omega}^*$ there exists an invariant surface $T(\boldsymbol{\omega}^*)$ of the perturbed system such that $T(\boldsymbol{\omega}^*)$ is close to $T_0(\boldsymbol{\omega}^*)$.

In other words, the trajectories of the perturbed Hamiltonian will evolve on surfaces $T^* = T(\boldsymbol{\omega}^*)$ which are ‘close to’ tori T_0 of the integrable system. This means that, for almost all (but *not* all) nonresonant frequencies, the phase space trajectories are regular and not chaotic as far as ϵ is small enough (the theorem does not tell how small ϵ has to be).

⁸ When this occurs the system is termed ‘ergodic’, a key concept in statistical mechanics because it implies that time averages are equivalent to phase space averages.

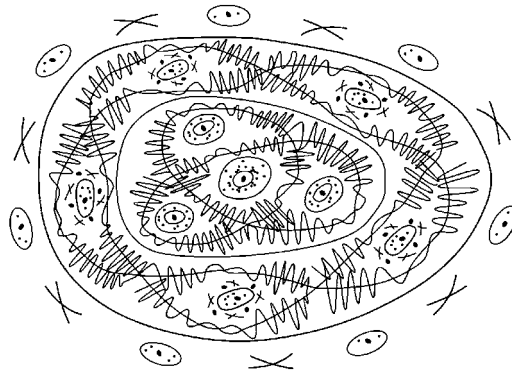


Figure 9. Schematic representation of Poincaré sections for nonintegrable systems stressing the complex mixture of regular and chaotic trajectories.

Moreover, the theorem also proves that the measure of the set of points in phase space which do not lie on any surface T^* tends to zero when $\epsilon \rightarrow 0$. That is to say, the probability of randomly choosing initial conditions not leading to motion on stable surfaces T^* is vanishingly small as $\epsilon \rightarrow 0$. This has momentous consequences for the stability of planetary orbits because it is extremely unlikely (though not impossible) that a given celestial body is located in some unstable (i.e. resonant) region (see, nonetheless, the next section).

Therefore, we see that, under the conditions of the theorem, small perturbations do not destroy invariant tori T_0 but only deform them. On these deformed tori, called *KAM surfaces*, the motion is regular and not chaotic.

The rigorous proof of the theorem is highly technical and we will not give it here. There are, however, more accessible derivations, for instance that of Barrar [3] to which we refer the interested reader (see also [24]). As mentioned above, the clue of the proof discovered by Kolmogorov, is a superconvergent perturbation method similar to the old Newton–Raphson technique for solving algebraic equations [25].

KAM tori T^* are determined by nonresonant frequencies ω^* and on these deformed tori the motion is not chaotic. But, what about resonant tori? What happens to them? In other words, what is the fate, when a perturbation is added, of those tori defined by a rational relationship of frequencies? It can be shown that resonances completely destroy resonant tori [19]. Consequently the trajectories on these tori—which, remember, in the absence of perturbation follow well-defined closed and periodic curves on them—lose their bounds and wander through the phase space (in fact, only through the subspace given by the surface of constant energy). Therefore, motion on resonant tori becomes completely irregular and unstable. This is an example of the so-called *hard chaos*, as opposed to *soft chaos* which relates to the motion near KAM surfaces [12] (see also the next section).

Fortunately, as KAM theorem proves, the set of resonant tori, on which regular motion is destroyed, has a vanishingly small measure as long as the perturbation is small. Equivalently, the remaining slightly deformed tori, where the motion is still regular, have a measure close to 1 if ϵ is small. This means that most tori are not destroyed for small perturbations and KAM surfaces almost densely fill the energy shell and between them there appear ‘islands’ with chaotic motion. This results in Poincaré sections which are extraordinarily complex and that some authors picture as in figure 9.

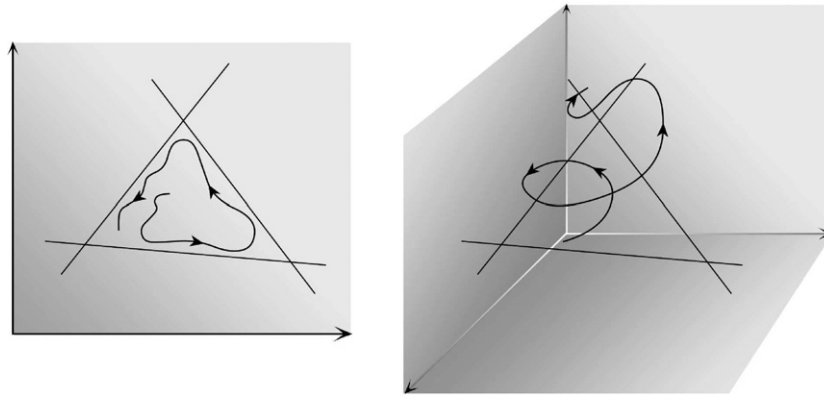


Figure 10. Phasespace trajectories are confined by lines (KAM surfaces) in a two-dimensional space but not in three dimensions.

8. Miscellaneous results

In this closing section we briefly outline some additional developments and applications of the theory.

8.1. Arnold diffusion

As KAM theorem proves, the energy shell of a conservative and nonintegrable Hamiltonian of the form $H = H_0 + \epsilon H_1$, where H_0 is integrable and ϵ is small, is densely filled with KAM surfaces on which phasespace trajectories are fairly regular. However, outside KAM tori trajectories are random. In order to analyse these chaotic trajectories we must distinguish between the cases of two and more than two degrees of freedom.

Let us recall that, for integrable conservative systems with n degrees of freedom, the phase space is $2n$ dimensional, the energy shell is $(2n - 1)$ dimensional and invariant tori are n dimensional. Hence, for $n = 2$, the two-dimensional tori are embedded in the three-dimensional energy surface. This means that any closed surface, such as a torus, divides the energy shell into an inner region and an outer region. The same applies to KAM tori of conservative nonintegrable systems with two degrees of freedom. Accordingly, any chaotic trajectory, located in the interspace between two tori, cannot escape from it. No matter how complicated its motion is, the trajectory never leaves the region and the action variables remain close to their initial values. This is another aspect of the soft chaos mentioned above, for there exists a certain stability of motion because KAM surfaces densely populate the energy shell and are, therefore, very close to each other.

However, for $n \geq 3$ chaotic trajectories located in regions between tori can escape to other regions of the energy shell (see figure 10). Thus, for instance, if $n = 3$ the energy shell is five dimensional, KAM surfaces three dimensional and chaotic trajectories have two additional dimensions to wander through. Hence, for $n \geq 3$ the existence of KAM surfaces does not guarantee the stability of motion, as two trajectories which are initially very close to each other can be very distant after a finite period of time. This phenomenon, that exists for arbitrarily small perturbations, is known as *Arnold diffusion* and only appears in systems with more than two degrees of freedom.

The set of wandering trajectories resulting from it constitute the so-called *Arnold web*. There have been several attempts to determine the average speed of the spreading of trajectories defined as $|\Delta\mathbf{J}/\Delta t|$, where $\Delta\mathbf{J} = \mathbf{J}(t) - \mathbf{J}(0)$. Several theoretical models and numerical studies seem to indicate that this velocity is very small. Some models predict that [19]

$$|\Delta\mathbf{J}| < \epsilon^{1/2} \quad \text{for} \quad t < \epsilon^{-1} \exp(\epsilon^{-1/2}),$$

which means, that for small ϵ , the action at time t , $\mathbf{J}(t)$, remains close to its initial value, $\mathbf{J}(0)$, for a very long time $t \sim \exp(\epsilon^{-1/2})$. In other words, the average diffusion velocity is of the order

$$\left| \frac{\Delta\mathbf{J}}{\Delta t} \right| \sim e^{-1/\sqrt{\epsilon}},$$

which is exponentially small and practically undetectable if $\epsilon \ll 1$.

8.2. Planetary motion

Let us return to the problem of the long-time stability of the Solar System, one of the major challenges of mechanics for more than three centuries. As we know, the Solar System is a nonintegrable many-body problem which, to first approximation, can be considered conservative. The key point is whether planetary motions are quasiperiodic or random. The Solar System is too complicated and a direct application of the KAM theorem does not bring practical results. On the other hand, planet orbits exhibit great regularity and until recently it was thought that the Solar System evolves quasiperiodically. In spite of this, there seems to be some evidence that this may not be the case.

In 1857 the American astronomer D Kirkwood discovered a series of discontinuities in the distribution of main-belt asteroids which circle the Sun and lie between Mars and Jupiter. There are regions where there is a depletion in the number of asteroids. These regions are called *Kirkwood gaps*. One of the most plausible explanation for them has been given by Dermott and Murray [8], who in 1983 proposed that the gaps are due to resonances in the three-body problem of the Sun, Jupiter, and the individual asteroids [8, 24]. That is, Jupiter perturbs the asteroid's almost Keplerian orbit around the Sun and creates resonances in the asteroid's phase space. The location of the observed gaps is found to be very close to the resonant surfaces of Jupiter and the asteroids, which would agree with KAM theory about the destruction of resonant tori. It has also been argued that the mechanism of Arnold diffusion might be responsible for removing asteroids from the gap regions and force some of them to collide with Mars [19].

Let us finally mention that there seems to be some numerical evidence that the long-term motion of the former planet Pluto is chaotic and also that of some of the main planets of the Solar System [24]. All these results seem to indicate that the long-time motion of the Solar System may be chaotic and, to some extent, unpredictable.

8.3. Quantum chaos

Let us finish this exposition by giving a very brief view on the possible manifestation of chaotic behaviour in quantum systems.

If one naively tries to extend, in a direct manner, the concepts of regular and chaotic trajectories to quantum systems, one is immediately faced with an insurmountable difficulty: due to Heisenberg's uncertainty principle, between canonically conjugated variables, it makes no sense to define trajectories in the quantum phase space.

In fact, the phase space of any system of n degrees of freedom is divided into cells of volume h^n (h is Planck's constant) and one cannot determine at which point inside a given cell the system is. This renders the construction of phase space trajectories meaningless. Therefore, the notion of invariant tori, over which the trajectories of integrable systems stay, also loses its meaning in the quantum world.

The problem of the quantization of nonintegrable Hamiltonians can be traced back to the early days of the old quantum theory [12] (see [4] for a thorough review). However, strictly speaking, there is no such thing as 'quantum chaos', although there have been detected some peculiar effects in quantum systems whose classical counterparts correspond to chaotic systems. Quoting Gutzwiller: 'the term 'quantum chaos' serves more to describe a conundrum than to define a well-posed problem' [13].

What is understood by quantum chaos is essentially the relationship between classical chaotic systems and their quantum counterparts. Let us recall that in quantum mechanics, the state of the system is not specified by a point (\mathbf{q}, \mathbf{p}) of the phase space but by a wavefunction $\psi(\mathbf{q}, t)$ giving the probability of finding the system at a position \mathbf{q} in time t . However, this wave-like character of quantum systems implies a smooth nature. How can the irregular character of classical chaos be reconciled with the smooth and wave-like nature of phenomena on the atomic scale governed by quantum mechanics? [13]. What are, therefore, the quantum manifestations of chaos?

There are several places and situations where one can look for the 'quantum signatures' of chaos [14], and substantial research has been done along this direction in the last three decades. We can single out one aspect where quantum chaos is quite significant. The first place to look is in the energy levels, not a particular level but the distribution of them. Thus, and somewhat paradoxically, in nonchaotic quantum systems (i.e. those quantum systems whose classical counterparts are integrable) the energy levels are completely random without any correlation, while in chaotic systems the energy levels show strong correlations between them, which implies a lower degree of randomness. There are other situations in which quantum manifestations of chaos appear as, for example, in the distribution of stationary states and in electron scattering, among others. We refer the interested reader to more specialized literature for further information (see, for instance, [12, 14, 24]).

9. Closing words

There is a line of thought, among some philosophers and scientists, affirming that science is a construction, that scientists are designers who fit as much data as possible within consistent frames. Opposite to that, others believe, and this is the traditional thinking, that science is discovery and the scientist is like a detective struggling to unveil the hidden truth [9], 'the secret of the Old One', as Einstein put it [7]. Obviously, mainstream scientists lie somewhere in between these two extremes.

Whatever the interpretation one may support, it is beyond any doubt that classical mechanics is one of the finest and most creative works that scientific endeavour can yield. In its most sophisticated form, the Hamiltonian approach, classical mechanics even forecasts its own limitation: the long-time unpredictable behaviour of nonintegrable systems which, as mechanics also proves, are ubiquitous in nature. The Solar System, galaxies, galaxy clusters, perhaps atoms and beyond, all of them are nonintegrable.

In this paper we have tried to report on this striking consequence of classical mechanics. In a world of uncertainties—it all began with quantum mechanics [5]—we can add, as Poincaré envisaged, another one: the classical uncertainty.

Acknowledgments

Partial financial support from the Ministerio de Ciencia e Innovación under contract no FIS 2009-09689 is acknowledged. We thank Miquel Montero, Josep Perelló and Nitin Rughoonauth for a careful reading of the manuscript. We are indebted to Professor Luis Navarro for useful discussions and suggestions.

Appendix A. Integrability and the involution property

We know that, by definition, a system is integrable when there exist n integrals of motion $I_i(\mathbf{q}, \mathbf{p}) = \alpha_i$ that are independent and in involution:

$$[I_i, I_j] = 0.$$

This property allows us to use the I s as the transformed momenta of some canonical transformation. Indeed, let us recall from (5) that any set of n variables $\mathbf{p}' = (p'_1, \dots, p'_n)$ can be considered as the momenta associated with some Hamiltonian if $[p'_i, p'_j] = 0$. Accordingly, we make the canonical transformation

$$(\mathbf{q}, \mathbf{p}) \longrightarrow (\mathbf{q}', \mathbf{p}' = \boldsymbol{\alpha}),$$

in which the integrals of motion are the transformed momenta because the involution property grants it. The generating function of this canonical transformation is given by the indefinite integral

$$S(\mathbf{q}, \boldsymbol{\alpha}) = \int \sum_{k=1}^n p_k(\mathbf{q}, \boldsymbol{\alpha}) dq_k,$$

where $p_k(\mathbf{q}, \boldsymbol{\alpha})$ are the momenta written in terms of the coordinates and the constants of motion.

The equations of the canonical transformation are

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}}, \quad \mathbf{q}' = \frac{\partial S}{\partial \boldsymbol{\alpha}},$$

and, since we deal with a time-independent transformation, the transformed Hamiltonian, $H' = H(\mathbf{q}', \boldsymbol{\alpha})$, coincides with the original one written in terms of the new coordinates and momenta.

In the new variables, Hamilton equations read

$$\dot{\mathbf{q}}' = \frac{\partial H}{\partial \boldsymbol{\alpha}}, \quad \dot{\boldsymbol{\alpha}} = \frac{\partial H}{\partial \mathbf{q}'}$$

But $\dot{\boldsymbol{\alpha}} = 0$, hence $\partial H / \partial \mathbf{q}' = 0$ and H is independent of the coordinates depending only upon the constants of motion:

$$H = H(\alpha_1, \dots, \alpha_n) = E.$$

Therefore, from the first group of Hamilton equations, we see that

$$\dot{\mathbf{q}}' = \frac{\partial H(\boldsymbol{\alpha})}{\partial \boldsymbol{\alpha}} \equiv \boldsymbol{\nu}(\boldsymbol{\alpha}) = \text{constant}$$

and the equations of motion read

$$\mathbf{q}'(t) = \boldsymbol{\nu}(\boldsymbol{\alpha})t + \text{constant} \quad \text{and} \quad \mathbf{p}'(t) = \boldsymbol{\alpha} = \text{constant}. \quad (\text{A.1})$$

In this way we have completely integrated Hamilton equations for the motion of the system. Hence, the existence of n independent integrals in involution leads to the complete integration of Hamilton equations.

Appendix B. Periodicity of the angle variables

The variation, $\Delta_i\theta_j$, of the angle θ_j when the coordinate q_i performs a complete oscillation is defined by

$$\Delta_i\theta_j \equiv \sum_{k=1}^n \oint_{\Gamma_i} \frac{\partial\theta_j}{\partial q_k} dq_k,$$

which, recalling that $\theta_j = \partial S/\partial J_j$ (see (19)), we write as

$$\Delta_i\theta_j = \sum_{k=1}^n \oint_{\Gamma_i} \frac{\partial^2 S}{\partial q_k \partial J_j} dq_k = \frac{\partial}{\partial J_j} \oint_{\Gamma_i} \sum_{k=1}^n \frac{\partial S}{\partial q_k} dq_k.$$

But from (18) we have $\partial S/\partial q_k = p_k$; hence

$$\Delta_i\theta_j = \frac{\partial}{\partial J_j} \oint_{\Gamma_i} \sum_{k=1}^n p_k dq_k.$$

Using definition (15) we obtain

$$\Delta_i\theta_j = 2\pi \frac{\partial J_i}{\partial J_j}$$

and, since (J_1, \dots, J_n) are independent variables, we finally obtain

$$\Delta_i\theta_j = 2\pi \delta_{ij},$$

which is equation (23).

Appendix C. Commensurable frequencies

From (25) we have

$$q_j(t) = \sum_{\mathbf{k}} a_{\mathbf{k}}^{(j)} e^{i\mathbf{k}\cdot\boldsymbol{\omega}t},$$

whence

$$q_j(t + T_0) = \sum_{\mathbf{k}} a_{\mathbf{k}}^{(j)} e^{i\mathbf{k}\cdot\boldsymbol{\omega}t} e^{i\mathbf{k}\cdot\boldsymbol{\omega}T_0},$$

and $q_j(t + T_0) = q_j(t)$ if and only if $e^{i\mathbf{k}\cdot\boldsymbol{\omega}T_0} = 1$, which implies

$$\mathbf{k} \cdot \boldsymbol{\omega}T_0 = 2\pi l, \tag{C.1}$$

where $l = 0, \pm 1, \pm 2, \dots$ is an arbitrary integer. This condition is equivalent to

$$\boldsymbol{\omega}T_0 = 2\pi \mathbf{l},$$

where

$$\mathbf{l} = (l_1, \dots, l_n)$$

($l_j = 0, \pm 1, \pm 2, \dots$) is an arbitrary integer vector. In effect, if, as (C.1) demands, the scalar product of *any* integer vector \mathbf{k} with the real vector $(1/2\pi)\boldsymbol{\omega}T_0$ has to be an integer number, then necessarily $(1/2\pi)\boldsymbol{\omega}T_0$ has to be an integer vector.

Therefore, any coordinate (and the same applies to momenta) will be a periodic function of time, that is to say, there will exist a single period T_0 for the entire system, if all frequencies $\boldsymbol{\omega} = (\omega_1, \dots, \omega_n)$ are integer multiples of a single frequency $\omega_0 = 2\pi/T_0$. That is

$$\boldsymbol{\omega} = \omega_0 \mathbf{l}, \tag{C.2}$$

which is equation (27) of the main text.

Appendix D. Canonical perturbations

In order to prove equation (43) we have to obtain the transformed Hamiltonian H' under the canonical transformation (39). Since we are dealing with a time-independent transformation $H' = H$, and from (37) we write

$$H'(\boldsymbol{\theta}', \mathbf{J}') = H_0(\mathbf{J}(\epsilon)) + \epsilon \sum_{\mathbf{k}} H_{\mathbf{k}}^{(1)}(\mathbf{J}(\epsilon)) \cos[\mathbf{k} \cdot \boldsymbol{\theta}(\epsilon)], \quad (\text{D.1})$$

where $\mathbf{J}(\epsilon)$ and $\boldsymbol{\theta}(\epsilon)$ are given (implicitly) in terms of \mathbf{J}' and $\boldsymbol{\theta}'$ by (41)–(42):

$$\mathbf{J}(\epsilon) = \mathbf{J}' + \epsilon \sum_{\mathbf{k}} \mathbf{k} S_{\mathbf{k}}(\mathbf{J}') \cos[\mathbf{k} \cdot \boldsymbol{\theta}(\epsilon)] + O(\epsilon^2), \quad (\text{D.2})$$

$$\boldsymbol{\theta}' = \boldsymbol{\theta}(\epsilon) + \epsilon \sum_{\mathbf{k}} \frac{\partial S_{\mathbf{k}}(\mathbf{J}')}{\partial \mathbf{J}'} \sin[\mathbf{k} \cdot \boldsymbol{\theta}(\epsilon)] + O(\epsilon^2). \quad (\text{D.3})$$

We will expand the right-hand side of (D.1) in powers of ϵ . Let us first observe, as trivially seen from (D.2) and (D.3), that

$$\mathbf{J}(\epsilon) = \mathbf{J}' + O(\epsilon), \quad \boldsymbol{\theta}(\epsilon) = \boldsymbol{\theta}' + O(\epsilon); \quad (\text{D.4})$$

hence,

$$H_{\mathbf{k}}^{(1)}(\mathbf{J}(\epsilon)) = H_{\mathbf{k}}^{(1)}(\mathbf{J}') + O(\epsilon), \quad \cos[\mathbf{k} \cdot \boldsymbol{\theta}(\epsilon)] = \cos(\mathbf{k} \cdot \boldsymbol{\theta}') + O(\epsilon).$$

Therefore, (D.1) reads

$$H'(\boldsymbol{\theta}', \mathbf{J}') = H_0(\mathbf{J}(\epsilon)) + \epsilon \sum_{\mathbf{k}} H_{\mathbf{k}}^{(1)}(\mathbf{J}') \cos(\mathbf{k} \cdot \boldsymbol{\theta}') + O(\epsilon^2). \quad (\text{D.5})$$

We next develop the unperturbed Hamiltonian $H_0(\mathbf{J}(\epsilon))$ in powers of ϵ up to first order; by Taylor expansion we have

$$H_0(\mathbf{J}(\epsilon)) = H_0(\mathbf{J}(0)) + \epsilon \left. \frac{d}{d\epsilon} H_0(\mathbf{J}(\epsilon)) \right|_{\epsilon=0} + O(\epsilon^2), \quad (\text{D.6})$$

where $\mathbf{J}(0) = \mathbf{J}'$ (see (D.4)). On the other hand, using the chain rule, we write

$$\left. \frac{d}{d\epsilon} H_0(\mathbf{J}(\epsilon)) \right|_{\epsilon=0} = \frac{\partial H_0}{\partial \mathbf{J}(\epsilon)} \cdot \left. \frac{d\mathbf{J}(\epsilon)}{d\epsilon} \right|_{\epsilon=0},$$

where the dot means the scalar product; but from (D.2) we obtain

$$\left. \frac{d\mathbf{J}(\epsilon)}{d\epsilon} \right|_{\epsilon=0} = \sum_{\mathbf{k}} \mathbf{k} S_{\mathbf{k}}(\mathbf{J}') \cos[\mathbf{k} \cdot \boldsymbol{\theta}(\epsilon)] + O(\epsilon);$$

hence,

$$\left. \frac{d}{d\epsilon} H_0(\mathbf{J}(\epsilon)) \right|_{\epsilon=0} = \left. \frac{\partial H_0}{\partial \mathbf{J}(\epsilon)} \right|_{\epsilon=0} \cdot \sum_{\mathbf{k}} \mathbf{k} S_{\mathbf{k}}(\mathbf{J}') \cos(\mathbf{k} \cdot \boldsymbol{\theta}'),$$

since $\boldsymbol{\theta}(0) = \boldsymbol{\theta}'$.

Recalling that $\partial H_0 / \partial \mathbf{J} = \boldsymbol{\omega}$ are the frequencies of the unperturbed Hamiltonian, we have

$$\left. \frac{\partial H_0}{\partial \mathbf{J}(\epsilon)} \right|_{\epsilon=0} = \boldsymbol{\omega}(\mathbf{J}(0)) = \boldsymbol{\omega}(\mathbf{J}').$$

Therefore,

$$\left. \frac{d}{d\epsilon} H_0(\mathbf{J}(\epsilon)) \right|_{\epsilon=0} = \sum_{\mathbf{k}} \mathbf{k} \cdot \boldsymbol{\omega}(\mathbf{J}') S_{\mathbf{k}}(\mathbf{J}') \cos(\mathbf{k} \cdot \boldsymbol{\theta}'),$$

which substituted into expansion (D.6) yields

$$H_0(\mathbf{J}(\epsilon)) = H_0(\mathbf{J}') + \epsilon \sum_{\mathbf{k}} \mathbf{k} \cdot \boldsymbol{\omega}(\mathbf{J}') S_{\mathbf{k}}(\mathbf{J}') \cos(\mathbf{k} \cdot \boldsymbol{\theta}') + O(\epsilon^2);$$

plugging this expression into (D.5) we obtain

$$H'(\boldsymbol{\theta}', \mathbf{J}') = H_0(\mathbf{J}') + \epsilon \sum_{\mathbf{k}} [H_{\mathbf{k}}^{(1)}(\mathbf{J}') + \mathbf{k} \cdot \boldsymbol{\omega}(\mathbf{J}') S_{\mathbf{k}}(\mathbf{J}')] \cos(\mathbf{k} \cdot \boldsymbol{\theta}') + O(\epsilon^2),$$

and removing from the sum the term with $k_1 = \dots = k_n = 0$, we finally have

$$H'(\boldsymbol{\theta}', \mathbf{J}') = H_0(\mathbf{J}') + \epsilon H_0^{(1)}(\mathbf{J}') + \epsilon \sum_{\mathbf{k} \neq \mathbf{0}} [H_{\mathbf{k}}^{(1)}(\mathbf{J}') + \mathbf{k} \cdot \boldsymbol{\omega}(\mathbf{J}') S_{\mathbf{k}}(\mathbf{J}')] \cos(\mathbf{k} \cdot \boldsymbol{\theta}') + O(\epsilon^2),$$

which is equation (43).

References

- [1] Arnold V I 1961 *Sov. Math. Dokl.* **2** 501
- [2] Arnold V I 1979 *Mathematical Methods of Classical Mechanics* (Berlin: Springer)
- [3] Barrar R 1970 *Celest. Mech.* **2** 494
- [4] Bergia S and Navarro L 2000 *Archives Internationales d'Histoire des Sciences* **50** 321
- [5] Bohm D 1989 *Quantum Theory* (New York: Dover) (first edition, 1951)
- [6] Born M 1960 *The Mechanics of the Atom* (New York: Ungar) (original German version, 1924)
- [7] Born M 2005 *The Born–Einstein Letters* (New York: Macmillan) p 88
- [8] Dermott S F and Murray C D 1983 *Nature* **301** 201
- [9] d'Espagnat B 1989 *Reality and the Physicist* (Cambridge: Cambridge University Press)
- [10] Fuchs J and Schweigert C 2003 *Symmetries Lie Algebras and Representations* (Cambridge: Cambridge University Press)
- [11] Goldstein H 1981 *Classical Mechanics* 2nd edn (Reading, MA: Addison-Wesley)
- [12] Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (Berlin: Springer)
- [13] Gutzwiller M C 1992 *Scientific American* January p 11
- [14] Haake F 2010 *Quantum Signatures of Chaos* (Berlin: Springer)
- [15] Henon M and Heiles C 1964 *Astron. J.* **69** 73
- [16] Klein M J 1970 *Paul Ehrenfest* (Amsterdam: North-Holland) p 54
- [17] Kolmogorov A N 1954 *Dokl. Akad. Nauk* **98** 527
- [18] Landau L D and Lifshitz E M 1976 *Mechanics* 3rd edn (Amsterdam: Butterworth-Heinemann)
- [19] Lichtenberg A and Lieberman M 1992 *Regular and Chaotic Dynamics* 2nd edn (Berlin: Springer)
- [20] Moser J K 1962 *Nachr. Akad. Wiss. Gött. II. Math.-Phys. Kl.* **1** 1
- [21] Moser J K 1975 *Neue Zürcher Zeitung*, 14 May p 24
- [22] Scheck F 1990 *Mechanics* (Berlin: Springer)
- [23] Rasband S N 1983 *Dynamics* (New York: Wiley)
- [24] Reichl L E 2004 *The Transition to Chaos* 2nd edn (Berlin: Springer)
- [25] Tabor M 1989 *Chaos and Integrability in Nonlinear Dynamics* (New York: Wiley)
- [26] Tél T and Gruiz M 2006 *Chaotic Dynamics* (Cambridge: Cambridge University Press)
- [27] Whittaker E T 1993 *A Treatise on Analytical Dynamics of Particles and Rigid Bodies* (Cambridge: Cambridge University Press) (first edition, 1904)