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Linda Reichl

The Transition to Chaos

Conservative Classical and Quantum Systems

Third Edition

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Acknowledgements

The first edition of *The Transition to Chaos* appeared in 1992. It was based on a series of lectures on classical and quantum chaos that I gave at the University of California, San Diego, in 1987, and then at the Guangxi Normal University in Guilin China in 1990. The first edition focused on the classical chaos theory and the manifestations of chaos in bounded quantum systems. The second edition was published in 2004 and included the manifestations of chaos in open quantum systems with a strong emphasis on random matrix theory.

This third edition contains selected material from the previous editions but focuses on topics that have become important to modern research, including the influence of chaos on molecular scattering processes, lattice dynamics, gravitational structures, radiation-matter interactions, and the thermalization and control of quantum systems.

The book has been influenced, over the years, by discussions and collaborations with numerous colleagues. I particularly wish to thank Katya Lindenberg of UCSD who, years ago, invited me to write this series on chaos theory. I also wish to thank Christof Jung for our collaborations on classical scattering theory. This third edition has benefited from funding by the Robert A. Welch Foundation of Texas. Their support has enabled a number of students to work on aspects of the research reported here.

The University of Texas at Austin — Linda Reichl
Austin, TX, USA
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Contents

Chapter 1
Overview

Abstract The dynamical evolution of conservative chaotic systems is not deterministic because it is not possible to follow their dynamical evolution with any precision for more than a short time. In quantum systems, signatures of chaos emerge when classical chaos occupies phase space volumes greater than $\hbar^d$ ($\hbar$ is Planck's constant and d is number of degrees of freedom).

The phase space of most conservative nonlinear systems with three or more degrees of freedom (with a few exceptions) is permeated by an Arnol'd web consisting of a fractal set of nonlinear resonances that fill the phase space. The Arnol'd web is the source of the chaos that causes thermalization of both classical and quantum systems.

The publication of Newton's Principia in 1686 and the success and power of Newton's laws led to the huge growth in science that we see today. Belief that Newtonian mechanics is deterministic was shaken by the work of Poincaré who showed that perturbation expansions must diverge due to nonlinear resonances, making it impossible to make long-time predictions. When chaos manifests itself in quantum systems, the information content of a quantum system is extremized (minimized). In this book, we examine in more detail the mechanisms by which chaos emerges in conservative classical and quantum systems.

Keywords Classical chaos · Quantum manifestations of chaos · Determinism · History of dynamics · Symmetries · Perturbation theory divergence · KAM tori · Nonlinear resonance · Renormalization theory · Random matrix theory · Path integrals

1.1 Introduction

The existence of chaos in a conservative classical system means that the dynamical evolution of the system is no longer deterministic. Most classical systems with three or more degrees of freedom are either fully chaotic or have fractal regions of chaos distributed throughout the phase space. For example, the solar system appears to have regions where planetary motion is chaotic. Classical models of molecular

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motion often show large regions of chaos. Hard sphere gases are rigorously chaotic. The foundations of statistical mechanics (and thermodynamics) are based on the assumption that the underlying dynamics is chaotic.

The term *quantum chaos* refers to the signatures of classical chaos in the quantum dynamics of particles whose classical limit is chaotic. The *quantum signatures of chaos* appear wherever the classically chaotic regions have a size equal to $\hbar^d$ in phase space, where $\hbar$ is Planck's constant and d is the number of degrees of freedom. Signatures of chaos occur, for some parameter ranges, in most quantum systems and determine if a quantum system can thermalize. The signatures of chaos can be used to control quantum transitions. They can also destabilize quantum systems. In fact, the deeper we look into the fundamental dynamics governing the world, the more we see the profound impact of chaotic behavior.

The phase space of all conservative nonlinear systems with three or more degrees of freedom (with a few exceptions) forms an Arnol'd web (Arnol'd 1963). An Arnol'd web consists of a fractal set of resonances and chaos that fill the phase space. Depending on the degree of development of the web, an initial condition (one that is not known to infinite precision), may evolve deterministically for a long but finite period of time, or may begin to exhibit random behavior after a short time. The ubiquitous Arnol'd web, in conservative dynamical systems, provides the mechanism to thermalize the world.

In this regard, one of the important discoveries in quantum physics in recent years is that the information content of conservative quantum systems is extremized (minimized) when the underlying classical system undergoes a transition to chaos. The information content of the conservative quantum system approaches that of a system whose dynamics is governed by a random Hamiltonian matrix that is chosen to minimize information content.

In subsequent, sections we will first give a brief historical overview of the history of conservative dynamics and chaos theory. Then we will describe the content of the remaining chapters of this book.

1.2 Historical Overview

On April 28, 1686 the first of the three books that comprise Newton's Principia was formally presented to the Royal Society and, by July 1687 the complete first edition (consisting of perhaps 300 copies) was published Newton (1686). The publication of this work was probably the most important single event in the history of science because it formulated the science of mechanics in terms of just three basic laws:

- *A body maintains its state of rest or uniform velocity unless a net force acts on it.*
- *The time rate of change of momentum,* $\mathbf{p}$*, is equal to the net force,* $\mathbf{F}$*, acting on it.*
- *To every action there is an equal and opposite reaction.*

In the Principia, Newton not only wrote the three laws but also gave a systematic mathematical framework for exploring the implications of these laws. In addition, in the Principia Newton proposed his universal inverse square law of gravitation. He then used it to derive Kepler's empirical laws of planetary motion, to account for the motion of the moon and the phenomenon of tides, to explain the precession of the equinoxes, and to account for the behavior of falling bodies in Earth's gravitational field.

The success and power of Newton's laws led to a great optimism about our ability to predict the behavior of mechanical objects and, as a consequence, led to the huge growth in science that we see today. In addition, it was accompanied by a deterministic view of nature that is perhaps best exemplified in the writings of Laplace. In his Philosophical Essay on Probabilities, Laplace states (Laplace 1951): *Given for one instant an intelligence which could comprehend all the forces by which nature is animated and the respective situation of the beings who compose it—an intelligence sufficiently vast to submit these data to analysis—it would embrace in the same formula the movements of the greatest bodies of the universe and those of the lightest atom. For it, nothing would be uncertain and the future, as the past, would be present before its eyes.*

This deterministic view of nature was completely natural, given the success of Newtonian mechanics, and it persists up until the present day. Newton's three laws of motion led to a description of the motion of point masses in terms of a set of coupled second-order differential equations. The theory of extended objects can be derived from Newton's laws by treating them as collections of point masses. If we can specify the initial velocities and positions of the point particles, then Newton's equations for the point particles (obtained from the second law) should determine all past and future motion. However, we now know that the assumption that Newton's equations can predict the future is a fallacy. Newton's equations are, of course, the correct starting point of mechanics, but in general, they only allow us to determine the long-time behavior of integrable mechanical systems, few of which can be found in nature. Newton's laws, for most systems, describe inherently random behavior and cannot determine the future evolution of any real system (except for very short times) in more than a probabilistic sense.

The belief that Newtonian mechanics is a basis for determinism was formally laid to rest by Sir Lighthill (1986) in a lecture to the Royal Society on the three-hundredth anniversary of Newton's Principia. In his lecture, Lighthill says … *I speak … once again on behalf of the broad global fraternity of practitioners of mechanics. We are all deeply conscious today that the enthusiasm of our forebears for the marvelous achievements of Newtonian mechanics led them to make generalizations in this area of predictability which, indeed, we may have generally tended to believe before 1960, but which we now recognize were false. We collectively wish to apologize for having misled the general educated public by spreading ideas about the determinism of systems satisfying Newton's laws of motion that, after 1960, were to be proved incorrect ….*

In a sense, Newton (and Western science) were fortunate because the solar system has amazingly regular behavior considering its complexity, and one can predict its short-time behavior with fairly good accuracy. Part of the reason for this is the fact that the two-body Kepler system is governed by symmetries, both space-time and hidden, and is integrable. A three body gravitational system is not integrable. Newton's derivation of Kepler's laws was based on the properties of the two-body system. However, the dynamical interactions of the many bodies that comprise the solar system lead to deviations from the predictions of Kepler's laws, and lead one to ask why the solar system is, in fact, so regular. Is the solar system stable (Moser 1975)? Will it maintain its present configuration into the future? These questions have not yet been fully answered.

Questions concerning the stability and the future evolution of the solar system have occupied scientists and mathematicians for the past 300 years. Until computers were invented, all mathematical theories used perturbation expansions of various types. In the eighteenth century, important contributions were made by Euler, Lagrange, and Laplace on predicting the change in the geometry of orbits due to small perturbations and on determining the overall stability of orbits. In addition, Lagrange (1889) reformulated Newtonian mechanics in terms of a variational principle that vastly extended our ability to analyze the behavior of dynamical systems and allowed a straight-forward extension to continuum mechanics.

In the nineteenth century, there were two very important pieces of work that laid the groundwork for our current view of mechanics. Hamilton reformulated mechanics (Hamilton 1940) so that the dynamics of a mechanical system could be described in terms of a momentum-position phase space rather than a velocity-position phase space as is the case for the Lagrangian formulation. This step is extremely important because in the Hamiltonian formulation (which describes the evolution of mechanical systems in terms of coupled first-order differential equations) the flow of trajectories in phase space is volume-preserving. Furthermore, if symmetries exist (such as the space-time symmetries), then some of the generalized momenta of the system may be conserved, thus reducing the dimension of the phase space in which we must work.

The relation between the symmetries of a system and conservation laws was first clarified by Noether (1918). Noether's work provides one of the most important tools of twentieth-century science, because the key to much of what we are able to predict in science is symmetry. Symmetries imply conservation laws, and conservation laws give conservative classical mechanics and quantum mechanics whatever predictive power they have. Conservation laws are even responsible for the existence of thermodynamics and hydrodynamics.

Another extremely important piece of work in the nineteenth century was due to Poincaré (1899). Poincaré not only closed the door on an era but created the first crack in the facade of determinism. Before Poincaré, most work on dynamics, subsequent to Newton, involved computation of deviations from KepIer-type orbits for two massive bodies that are perturbed by a third body. The idea was to take a Kepler orbit as a first approximation and then compute successive corrections to it using perturbation theory. One must then show that the perturbation expansions thus obtained converge.

The problem of whether or not perturbation series converge was so important that it was the subject of a prize question posed by King Oscar II of Sweden in 1885. The question read as follows: *For an arbitrary system of mass points which attract each* *other according to Newton's laws, assuming that no two points ever collide, give the coordinates of the individual points for all time as the sum of a uniformly convergent series whose terms are made up of known functions (Moser 1975)*. Poincaré entered the contest and won the prize by showing that such series could be expected to diverge because of small denominators caused by internal resonances.

We now know that resonances, that give rise to these small divisors, are associated with the onset of chaos. Because of these divergences, it appears to be impossible to make long-time predictions concerning the evolution of mechanical systems (with a few exceptions such as the two-body Kepler system) using perturbation expansions.

No further progress was made on the problem of long-time prediction in mechanics until l954 when Kolmogorov (1954) outlined a proof, for systems of the type proposed in King Oscar's question, that a majority of the trajectories are quasi-periodic and can be described in terms of a special type of perturbation expansion. In 1962, Arnol'd (1963) constructed a formal proof of Kolmogorov's results for a three-body system with an analytic Hamiltonian, and Moser (1968) obtained a similar result for twist maps. The result of the work of Kolmogorov, Arnol'd, and Moser (KAM) is that series expansions describing the motion of some orbits in many-body systems are convergent, provided the natural frequencies associated with these orbits are not close to resonance. The work of Arnol'd, also showed that nonintegrable systems, with three or more degrees of freedom, are intrinsically unstable. They contain a dense web of resonance lines, the Arnol'd web, that allows diffusion to occur throughout the available phase space. The question of how rapid the diffusion will be depends on the parameters of the system.

Shenker and Kadanoff (1982) and MacKay (1983) were able to show that at the parameter value at which a given KAM torus (with quadratic irrational winding number) is destroyed, the rational approximates have self-similar structure and the areas in phase space that they occupy are related by scaling laws. They also showed that the rational approximates play a dominant role in the destruction of KAM tori. Escande and Doveil (1981) developed a renormalization theory for the destruction of KAM tori directly from the Hamiltonian for systems with two degrees of freedom. Thus, Hamiltonian systems, much like equilibrium systems near a phase transition, can exhibit self-similar structure.

Much of the behavior that occurs in classical systems also occurs in their quantum counterpart. However, because of the Heisenberg uncertainty relations, we are forced to describe classical and quantum systems from quite different perspectives. In classical systems, we can examine the evolution of individual orbits in phase space, and we can see directly the chaotic flow of trajectories in phase space. If we were to describe the evolution of the classical system in terms of the probability distribution in phase space, using the Liouville equation, we would have to search for the signatures of chaos in the behavior of the probability distributions and eigenvalues of the Liouville operator. This has been done for very simple chaotic maps (Driebe 1999), but it is a formidable task when dealing with Newtonian mechanical systems with two or more degrees of freedom.

When we study quantum systems, we have no phase space in which to describe the evolution of individual orbits because of the Heisenberg uncertainty relations. A single quantum state occupies volume of order $\hbar^d$ in the classical phase space, where $\hbar$ is Planck's constant and d is the number of degrees of freedom. We are forced from the outset to study quantum systems at the level of a linear probability (probability amplitude to be more precise) equation, namely the Schrödinger equation.

Most of the mechanisms at work in nonlinear classical systems are also at work in their quantum counterparts. For example, nonlinear resonances exist in quantum systems and can destroy constants of the motion (good quantum numbers) in local regions of the Hilbert space. They form self-similar structures, but only down to scales of order $\hbar^d$ and not to infinitely small scales as they do in classical systems. However, because the Schrödinger equation is an equation for probability amplitudes rather than probabilities, we will find some new phenomena that can occur in quantum systems but not in classical systems.

One of the most important discoveries of quantum chaos theory is that the statistical properties of energy spectra and scattering delay times indicate that the information content of a quantum system is extremized (minimized) as its classical counterpart undergoes a transition to chaos. The idea of studying the spectral statistics of quantum systems is largely due to Wigner (1951, 1957), who in the 1950s analyzed the statistical properties of nuclear scattering resonances. It was found that the nearest neighbor spacing of scattering resonances, for some nuclear scattering processes, has a distribution that agrees with the distribution of spacings of eigenvalues of ensembles of random Hermitian matrices (the Gaussian ensemble) whose matrix elements extremize information. The work of Wigner led Dyson (1962) to study the statistical properties of ensembles of random unitary matrices (the circular ensembles) that extremize information.

The connection between chaos theory and random matrix theory was made in 1979 by McDonald and Kaufman (1979), who found that classically chaotic quantum billiards have spectral spacing distributions given by the Gaussian ensembles. Comparison between statistical properties of deterministic quantum systems with underlying classical chaos and predictions of random matrix theories that extremize information is now a standard tool of quantum mechanics.

In the early days of quantum mechanics, before the work of Heisenberg and Schrödinger, the quantum version of a classical system was obtained by quantizing the action variables. This is straightforward if the classical system is integrable and one can find the action variables. However, Einstein, who knew of the work of Poincaré, as early as 1917 (Einstein 1917) pointed out that there may be difficulties with this method of quantization if invariant tori do not exist in the classical phase space, as is the case with chaotic systems.

Indeed, until the work of Gutzwiller in the early 1980s (Gutzwiller 1982), there was no way to link classically chaotic systems to their quantum counterparts. However, Gutzwiller showed that Feynman path integrals, in the semiclassical limit, provide such a link, and the spectral properties of a quantum system, whose classical counterpart is chaotic are determined largely in terms of an infinite sum over the unstable periodic orbits of the classical system.

Probably the most widely studied systems, as regards to the transition to chaos, are systems driven by time-periodic external fields. With a time-periodic force, one can cause a nonlinear system, with only one degree of freedom, to undergo a transition to chaos. In such systems, energy is not conserved but due to a discrete time translation invariance, the Floquet energy (quasi-energy) is conserved. Thus all the techniques used in energy-conserving systems can be applied to these driven systems.

1.3 Plan of the Book

The goal of this book is to provide a thorough grounding in classical and quantum chaos theory, with the focus on topics that impact current and future research topics.

Chapters 2–5 provide a description of processes underlying chaotic classical dynamics in conservative systems. Chapter 2 lays the foundations of the relevant classical mechanics for understanding chaos, and focuses on those aspects of chaotic behavior that will be used throughout the remainder of the book.

Chapter 3 deals primarily with systems that have two degrees of freedom. For these systems it is possible to visualize the processes that lead to the onset of chaos, because one can construct area preserving maps to follow the process. In Chap. 3, we also focus on the fractal nature of structures in the phase space that lead to global chaos, as parameters of the system are changed.

Chapter 4 deals with classical scattering processes and the fractal nature of scattering dynamics, when the scatterer is chaotic or partially chaotic. Finally, Chap. 5 focuses on the Arnold web that exists in nonlinear, non-integrable systems with three of more degrees of freedom. The Arnol'd web provides the mechanism for the global transition to chaos in systems with three or more degrees of freedom.

The remaining chapters of the book, Chaps. 6–10, examine the quantum manifestations of chaos. We start in Chap. 6 with a discussion of random matrix theory, as applied to conservative Hamiltonian systems. Random matrix theory is based on the assumption that the matrix elements of a hermitian or unitary matrix are independent random variables. This implies certain behaviors of the eigenvalues and eigenvectors of such systems that have been observed in quantum systems whose classical counterpart is chaotic. As we also show in Chap. 6, a conservative quantum system that shows random matrix-like behavior has become thermalized.

In Chap. 7, we discuss the behavior of some bounded quantum systems whose classical counterparts undergo a transition to chaos. The Schrödinger equation for these systems is linear. Nonlinearities appear in the Hamiltonian. We consider chaotic billiards, spin systems, and small molecules which are anharmonic oscillators. A number of the results we describe have been realized in microwave cavity experiments.

The connection between the quantum manifestations of chaos and random matrix theory was first observed in nuclear scattering experiments. In Chap. 8, we describe the theory originally developed by Wigner and Eisenbud (W-E) 1947 that allowed analysis of nuclear scattering processes in terms of random matrix theory. We then use these tools to define scattering phenomena such as resonance, quasibound states, and delay times for scattering processes. Finally, in Chap. 8, we show a variety of experimental and numerical data on nuclear and molecular energy-Ievel sequences and show that these systems are exhibiting the manifestations of chaos.

Another connection between classically chaotic systems and their quantum counterpart involves the use of semiclassical path integrals. In Chap. 9, we use the semiclassical limit of Feynman path integrals to derive the Gutzwiller trace formula, which expresses the trace of the Green's function of a quantum system in terms of periodic orbits of the classical system. We show that the trace formula gives very good results for the energy levels of the anisotropic Kepler system, a classically chaotic system. Finally, we conclude Chap. 9 with a numerical and experimental study of the influence of periodic orbits on the absorption spectrum of diamagnetic hydrogen.

Chapter 10 is devoted to periodically driven quantum systems, which can be described using Floquet theory. We show that nonlinear resonances exist in the Hilbert space of quantum systems, and we use Floquet theory to interpret the results of dynamic tunneling experiments using cold atoms confined to optical lattices. We decribe the behavior of the quantum delta-kicked rotor, which was the first system in which dynamic Anderson localization was observed numericaly. We also describe extensive experiments on microwave-driven hydrogen that give experimental confirmation of the existence of higher-order nonlinear resonances in quantum systems. Finally, we show that the Arnol'd web exists in quantum systems and plays an important role in destablizing their dynamics, and we show the influence of chaos on quantum control.

This book contains several appendices that give background on subjects of importance to this book. For example, there is a review of the effect of symmetries on the structure of Hamiltonian matrices. There is a derivation of the measures for Hermitian and unitary matrices used in random matrix theory. There is a derivation of the normalization constants and expressions for probability distributions of the Gaussian and circular ensembles in terms of quaternion matrices. There are other appendices as weIl that will aid the reader with some of the theory concepts in this book.

We do not have room in this book to discuss in detail all of the interesting applications of classical and quantum chaos theory, so in the concluding section of each chapter we have given references to additional topics of interest.

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Chapter 2
Fundamental Concepts

Abstract The dynamical behavior of nonlinear conservative systems is determined by global and hidden symmetries that constrain dynamical flow to lower-dimensional surfaces in the phase space. When the number of global symmetries equals the number of degrees of freedom, the dynamical system is integrable. This rarely happens,

Symmetry-breaking terms added to a Hamiltonian cause nonlinear resonances to occur on all scales in the phase space and give rise to a fractal structuring of the phase space. Chaos appears in the neighborhood of the nonlinear resonances. The Poincaré surfaces of section provide a numerical tool for testing integrability of conservative dynamical systems. Non-linear resonances may appear or disappear as mparameters of the system are varied and the overlap of nonlinear resonances leads to the onset of chaos.

Kolmogorov, Arnol'd, and Moser (collectively called KAM) developed a rapidly converging perturbation theory that describes non-resonant regions of the phase space. In chaotic regions of the phase space, neighboring orbits move apart exponentially in any direction. The rate of exponential divergence of pairs of orbits is given by Lyapounov exponents. Systems with positive Lyapounov exponents also have positive KS metric entropy.

Keywords Noether's theorem · Integrability · Global symmetries · Hidden symmetries · KAM tori · Poincaré surface of section · Nonlinear resonance · Definition of chaos · Lyapounov exponents · Baker's transformation

2.1 Introduction

The dynamical behavior of nonlinear conservative systems is determined by the nature of the symmetries that govern their behavior. These dynamical symmetries can be categorized as *global symmetries* or *hidden symmetries*. Both types of symmetry constrain the dynamical flow of the system to lower-dimensional surfaces in the phase space. Global symmetries are related to the space-time symmetries of the system. The other symmetries do not have an obvious source and were

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first called *hidden symmetries* by Moser (1979). When there are as many *global* symmetries as numbers of degrees of freedom, the dynamical system is said to be *integrable*.

A second concept that is important for understanding the dynamics of nonlinear systems is *nonlinear resonance*. As Kolmogorov (1954), Arnol'd (1963), and Moser (1962) have shown, when a small symmetry-breaking term is added to the Hamiltonian of system, most of the phase space continues to behave as if the symmetries still exist. However, in regions where the symmetry-breaking term allows resonance to occur between otherwise uncoupled degrees of freedom, the dynamics begins to change its character. When resonances do occur, they generally occur on all scales in the phase space and give rise to a fractal structuring of the phase space.

The third concept that is essential for understanding conservative nonlinear dynamics is *chaos* or *sensitive dependence on initial conditions*. For the class of systems in which symmetries can be broken by adding small symmetry-breaking terms, chaos first appears in the neighborhood of the nonlinear resonances. As the strength of the symmetry-breaking term increases and the size of the resonance regions increases, ever larger regions of the phase space become chaotic.

The dynamical evolution of systems with broken symmetry cannot be determined using conventional perturbation theory, because of the existence of nonlinear resonances. In Sect. 2.2, we show that nonlinear resonances cause a topological change locally in the structure of the phase space, and that conventional perturbation theory is not adequate to deal with such topological changes.

In Sect. 2.3, we introduce the concept of integrability. A system is integrable if it has as many *global* constants of the motion as degrees of freedom. The connection between global symmetries and global constants of motion was first proven for dynamical systems by Noether (1918). We will give a simple derivation of Noether's theorem in Sect. 2.3.

It is usually impossible to tell if a system is integrable just by looking at the equations of motion. As we show in Sect. 2.4, the Poincaré surface of section provides a very useful numerical tool for testing integrability and will be used throughout the remainder of this book. We will illustrate the use of the Poincaré surface of section for the classic model of Henon and Heiles (1964) and for a model of the HOCl molecule.

In Sect. 2.5, we introduce the concept of nonlinear resonances and illustrate their behavior for some simple models originally introduced by Walker and Ford (1969). These models are interesting because they show that resonances may appear or disappear as parameters of the system are varied and the overlap of nonlinear resonances leads to the onset of chaos.

Conventional perturbation theory does not work when nonlinear resonances are present. But Kolmogorov, Arnol'd, and Moser (collectively called KAM) have developed a rapidly converging perturbation theory that can be used to describe non-resonant regions of the phase space, precisely because it is constructed to avoid the resonance regions. KAM perturbation theory will be described in Sect. 2.6.

In practice, chaos is defined in terms of the dynamical behavior of pairs of orbits that initially are close together in the phase space. If the orbits move apart exponentially in any direction in the phase space, the flow is said to be chaotic. The rate of exponential divergence of pairs of orbits is measured by the so-called *Lyapounov exponents*. There will be one such exponent for each dimension in the phase space. If all the Lyapounov exponents are zero, the dynamical flow is regular. If even one exponent is positive, the flow will be chaotic. A detailed discussion of the behavior of Lyapounov exponents for conservative systems is given in Sect. 2.7 and is illustrated in terms of the Henon-Heiles system. Systems with positive Lyapounov exponents also have positive KS metric entropy. The KS metric entropy is defined in Sect. 2.7 and computed for the baker's transformation, one of the simplest known chaotic dynamical systems.

Finally, in Sect. 2.8, we make some concluding remarks.

2.2 Conventional Perturbation Theory

Historically the first cracks in a deterministic view of the world, and an appreciation of the difficulties in obtaining long-time predictions regarding the evolution of dynamical systems, were brought into focus with Poincaré's proof that conventional perturbation expansions generally diverge. When they diverge they cannot be used as a tool to provide long-time predictions.

In order to build some intuition concerning the origin of these divergences, let us consider a 2 DoF system from celestial mechanics, the relative motion of a moon of mass m_1, orbiting a planet of mass m_2 (the Kepler system). The Hamiltonian can be written

$$H_0 = \frac{{p_r}^2}{2\mu} + \frac{{p_\phi}^2}{2\mu r^2} - \frac{k}{r} = E, \tag{2.1}$$

where (p_r, p_ϕ) and (r, ϕ) are the relative momentum and positions, respectively, of the two bodies in polar coordinates, E is the total energy of the system, $\mu = \frac{m_1 m_2}{m_1+m_2}$ is the reduced mass, and $k = Gm_1m_2$ (G is the gravitational constant). The total angular momentum, $\mathbf{L}$, is conserved for this problem so the plane of motion, (r, ϕ), is taken to lie in the plane perpendicular to $\mathbf{L}$.

After a canonical transformation from coordinates (p_r, p_ϕ, r, ϕ) to action-angle coordinates $(J_1, J_2, \theta_1, \theta_2)$, the Hamiltonian takes the form (Goldstein 1980)

$$H_0(J_1, J_2) = \frac{-\mu k^2}{2(J_1 + J_2)^2} = E. \tag{2.2}$$

The motion is fairly complicated (elliptic or hyperbolic orbits) in terms of coordinates (p_r, p_ϕ, r, ϕ), but in terms of action-angle coordinates it is simple. Hamilton's equations of motion yield $\frac{dJ_i}{dt} = -\frac{\partial H_0}{\partial \theta_i} = 0$ and $\frac{d\theta_i}{dt} = \frac{\partial H_0}{\partial J_i} = \omega_i(J_1, J_2)$, where

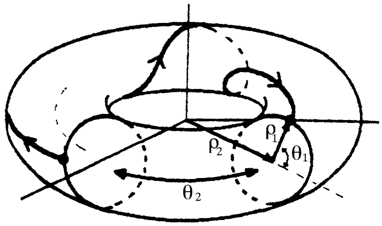

Fig. 2.1 For integrable systems with two DoF, each trajectory lies on a torus constructed from the action-angle variables $(J_1, J_2, \theta_1, \theta_2)$. The radii of the torus are $\rho_i = \sqrt{2J_i}$ for $i = (1, 2)$. If the frequencies $\omega_i = \frac{d\theta_i}{dt}$ $(i = 1, 2)$ are commensurate, the trajectory will be periodic. If the frequencies are incommensurate, the trajectory will never repeat

$i = (1, 2)$ and t is the time. Thus, we find that $J_i = c_i$ and $\theta_i = \omega_i t + d_i$, where c_i and d_i are constants determined by the initial conditions. We see immediately that the energy of this system is constant.

It is useful to picture the motion of this system as lying on a torus as shown in Fig. 2.1. The torus will have two constant radii, which we define as $\rho_i = \sqrt{2J_i}$ for $i = (1, 2)$, and two angular variables (θ_1, θ_2). A single orbit of the Kepler system will evolve on this torus according to equations $J_i = c_i$ and $\theta_i = \omega_i t + d_i$, so there are two frequencies associated with this system, ω_1 and ω_2. If these two frequencies are commensurate (that is, if $m\omega_1 = n\omega_2$, where m and n are integers), then the trajectory will be periodic and the orbit will repeat itself. If the two frequencies are incommensurate (irrational multiples of one another), then the trajectory will never repeat itself as it moves around the torus and eventually will cover the entire surface of the torus. Note also that the frequencies themselves depend on the action variables and therefore on the energy of the system. This is a characteristic feature of a nonlinear system.

Let us now assume that a perturbation acts in the plane of motion due to the presence of another planet. We shall treat this perturbation as an external field. In the presence of this perturbation, the Hamiltonian will take the form

$$H = H_0(J_1, J_2) + \epsilon V(J_1, J_2, \theta_1, \theta_2), \tag{2.3}$$

where ϵ is a small parameter, $\epsilon \ll 1$. We wish to find corrections to the unperturbed trajectories, $J_i = c_i$, due to the perturbation. Since we cannot solve the new equations of motion exactly, we can hope to obtain approximate solutions using perturbation expansions in the small parameter ϵ. Let's try it.

First we note that since we are dealing with periodic bound state motion, we can expand the perturbation in a Fourier series, and write the Hamiltonian in Eq. (2.3) in the form

$$H = H_0(J_1, J_2) + \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} V_{n_1,n_2}(J_1, J_2) \cos(n_1\theta_1 + n_2\theta_2). \tag{2.4}$$

Next, we introduce a generating function, $G(\mathcal{J}_1, \mathcal{J}_2, \theta_1, \theta_2)$, which we define as

$$G(\mathcal{J}_1, \mathcal{J}_2, \theta_1, \theta_2) = \mathcal{J}_1\theta_1 + \mathcal{J}_2\theta_2 + \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} g_{n_1,n_2}(\mathcal{J}_1, \mathcal{J}_2) \sin(n_1\theta_1 + n_2\theta_2), \qquad (2.5)$$

where g_{n_1,n_2} will be determined below. The generating function in Eq. (2.5) generates a canonical transformation from the set of action-angle variables, $(J_1, J_2, \theta_1, \theta_2)$, to a new set of canonical action-angle variables, $(\mathcal{J}_1, \mathcal{J}_2, \Theta_1, \Theta_2)$, via the following equations:

$$J_i = \frac{\partial G}{\partial \theta_i} = \mathcal{J}_i + \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} n_i g_{n_1,n_2} \cos(n_1\theta_1 + n_2\theta_2) \qquad (2.6)$$

and

$$\Theta_i = \frac{\partial G}{\partial \mathcal{J}_i} = \theta_i + \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \frac{\partial g_{n_1,n_2}}{\partial \mathcal{J}_i} \sin(n_1\theta_1 + n_2\theta_2). \qquad (2.7)$$

The new Hamiltonian, $H'(\mathcal{J}_1, \mathcal{J}_2, \Theta_1, \Theta_2)$, is obtained from Eq. (2.4) by solving Eqs. (2.6) and (2.7) for (J_i, θ_i) as a function of $(\mathcal{J}_i, \Theta_i)$ and plugging into Eq. (2.4). If we do that and then expand $H'(\mathcal{J}_1, \mathcal{J}_2, \Theta_1, \Theta_2)$ in a Taylor series in the small parameter ϵ, we find

$$\begin{aligned} H'(\mathcal{J}_1, \mathcal{J}_2, \Theta_1, \Theta_2) &= H_0'(\mathcal{J}_1, \mathcal{J}_2) + \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} (n_1\omega_1 + n_2\omega_2) g_{n_1,n_2} \cos(n_1\Theta_1 + n_2\Theta_2) \\ &+ \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} V_{n_1,n_2}(\mathcal{J}_1, \mathcal{J}_2) \cos(n_1\Theta_1 + n_2\Theta_2) + O(\epsilon^2), \end{aligned} \qquad (2.8)$$

where the frequencies are defined as $\omega_i = \frac{\partial H_o'}{\partial \mathcal{J}_i}$.

We can now remove terms of order ϵ by choosing

$$g_{n_1,n_2} = -\frac{V_{n_1,n_2}(\mathcal{J}_1, \mathcal{J}_2)}{(n_1\omega_1 + n_2\omega_2)}. \qquad (2.9)$$

Then

$$H'(\mathcal{J}_1, \mathcal{J}_2, \Theta_1, \Theta_2) = H_o'(\mathcal{J}_1, \mathcal{J}_2) + O(\epsilon^2) \qquad (2.10)$$

and

$$J_i = \mathcal{J}_i - \epsilon \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \frac{n_i V_{n_1,n_2} \cos(n_1\Theta_1 + n_2\Theta_2)}{(n_1\omega_1 + n_2\omega_2)} + O(\epsilon^2). \tag{2.11}$$

To lowest order in ϵ, this is the solution to the problem. New actions, $\mathcal{J}_i$, have been obtained that contain corrections due to the perturbation. If, for example, $\epsilon = 0.01$, then by retaining only first-order corrections, we neglect terms of order $\epsilon^2 = 0.0001$. To first order in ϵ, $\mathcal{J}_i$ is a constant and Θ_i varies linearly in time. At least, this is the hope. However, there is a catch! For the expansion in Eq. (2.11) to have meaning, we must have

$$|n_1\omega_1 + n_2\omega_2| \gg \epsilon V_{n_1,n_2}. \tag{2.12}$$

However, the condition in Eq. (2.12) breaks down when internal nonlinear resonances occur and causes the perturbation expansion to diverge. Poincaré showed that perturbation expansions of this type can generally be expected to diverge and therefore, cannot be used for long-time predictions.

2.3 Integrable Systems

Integrable systems form an important reference point when discussing the behavior of dynamical systems. We define an integrable system as follows. Consider a dynamical system with N degrees of freedom. Its phase space has $2N$ dimensions. The system is *integrable* if there exist N independent isolating integrals of motion, I_i, such that

$$I_i(p_1, \ldots, p_N, q_1, \ldots, q_N) = C_i, \tag{2.13}$$

for $i = 1, \ldots, N$, where C_i is a constant and p_i and q_i are the canonical momentum and position associated with the ith degree of freedom. The functions I_i are independent if their differentials, dI_i, are linearly independent.

It is important to distinguish between isolating and non-isolating integrals (Wintner 1947). *Non-isolating integrals* (an example is the initial coordinates of a trajectory) generally vary from trajectory to trajectory and usually do not provide useful information about a system. On the other hand, *isolating integrals of motion*, by Noether's theorem, are due to symmetries (some "hidden") of the dynamical system and define surfaces in phase space.

The condition for integrability may be put in another form. A classical system with N degrees of freedom is integrable if there exist N independent globally defined functions, $I_i(p_1, \ldots, p_N, q_i, \ldots, q_N)$, for $i = 1, \ldots, N$, whose mutual Poisson brackets vanish,

$$\{I_i, I_j\}_{Poisson} = 0, \tag{2.14}$$

for $i = 1, \ldots, N$ and $j = 1, \ldots, N$. Then the quantities I_i form a set of N phase space coordinates. In conservative systems, the Hamiltonian, $H(p_1, \ldots, p_N, q_1, \ldots, q_N)$, will be one of the constants of the motion. In general, the equation of motion of a phase function, $f = f(p_1, \ldots, p_N, q_1, \ldots, q_N, t)$, is given by

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{H, f\}_{Poisson}. \tag{2.15}$$

Thus Eqs. (2.14) and (2.15) imply that $\frac{dI_i}{dt} = 0$. If a system is integrable, there are no internal nonlinear resonances leading to chaos. All orbits lie on N-dimensional surfaces in the $2N$-dimensional phase space.

2.3.1 Noether's Theorem

As was shown by Noether (1918), isolating integrals result from symmetries. For example, the total energy is an isolating integral (is a constant of the motion) for systems that are homogeneous in time (invariant under a translation in time). Total angular momentum is an isolating integral for systems that are isotropic in space.

Noether's theorem is generally formulated in terms of the Lagrangian (see Goldstein 1980 and Appendix A). Let us consider a dynamical system with N degrees of freedom whose state is given by the set of generalized velocities and positions $(\{\dot{q}_i\}, \{q_i\})$. Let us consider a system whose Lagrangian, $L = L(\{\dot{q}_i\}, \{q_i\})$, is known. For simplicity, we consider a system with a time-independent Lagrangian. The equations of motion are given by the Lagrange equations

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0, \quad (i = 1, \ldots, N). \tag{2.16}$$

For such systems, Noether's theorem may be stated as follows.

- *Noether's Theorem* If a transformation

$$t \to t' = t + \delta t, \quad q_i(t) \to q_i'(t') = q_i(t) + \delta q_i(t), \quad \text{and}$$
$$\dot{q}_i \to \dot{q}_i'(t') = \dot{q}_i(t) + \delta \dot{q}_i(t)$$

(for $i = 1, \ldots, N$) leaves the Lagrangian form invariant,

$$L(\{\dot{q}_i(t)\}, \{q_i(t)\}) \to L'(\{\dot{q}_i'(t')\}, \{q_i'(t')\}) = L(\{\dot{q}_i'(t')\}, \{q_i'(t')\}), \tag{2.17}$$