Preface

The main purpose of this book is to present and discuss, in an introductory and pedagogical way, a number of important recent developments in the dynamics of Hamiltonian systems of N degrees of freedom. This is a subject with a long and glorious history, which continues to be actively studied due to its many applications in a wide variety of scientific fields, the most important of them being classical mechanics, astronomy, optics, electromagnetism, solid state physics, quantum mechanics, and statistical mechanics.

One could, of course, immediately point out the absence of biology, chemistry, or engineering from this list. And yet, even in such diverse areas, when the oscillations of mutually interacting elements arise, a Hamiltonian formulation can prove especially useful, as long as dissipation phenomena can be considered negligible. This situation occurs, for example, in weakly oscillating mechanical structures, low-resistance electrical circuits, energy transport processes in macromolecular models of motor proteins, or vibrating DNA double helical structures.

Let us briefly review some basic facts about Hamiltonian dynamics, before proceeding to describe the contents of this book.

The fundamental property of Hamiltonian systems is that they are derived from Hamilton's Principle of Least Action and are intimately related to the conservation of book, under time evolution in the phase space of their position and momentum variables $q_k, p_k, k = 1, 2, \ldots, N$, defined in the Euclidean phase space $\mathbb{R}^{2N}$. Their associated system of (first-order) differential equations of motion is obtained from a Hamiltonian function H, which depends on the phase space variables and perhaps also time. If H is explicitly time-independent, it represents a first integral of the motion expressing the conservation of total energy of the Hamiltonian system. The dynamics of this system is completely described by the solutions (trajectories or orbits) of Hamilton's equations, which lie on a $(2N - 1)$-dimensional manifold, the so-called energy surface, $H(q_1, \ldots, q_N, p_1, \ldots, p_N) = E$.

This constant energy manifold can be compact or not. If it is not, some orbits may escape to infinity, thus providing a suitable framework for studying many problems of interest to the dynamics of scattering phenomena. In the present book, however, we shall be exclusively concerned with the case where the constant energy manifold is compact. In this situation, the well-known theorems of Liouville-Arnol'd (LA) and Kolmogorov-Arnol'd-Moser (KAM) rigorously establish the following two important facts [19].

The LA theorem: If $N - 1$ global, analytic, single-valued integrals exist (besides the Hamiltonian) that are functionally independent and in involution (the Poisson bracket of any two of them vanishes), the system is called *completely integrable*, as its equations can in principle be integrated by quadratures to a single integral equation expressing the solution curves. Moreover, these curves generally lie on *N-dimensional tori* and are either periodic or quasiperiodic functions of N incommensurate frequencies.

The KAM theorem: If H can be written in the form $H = H_0 + \varepsilon H_1$ of an ε perturbation of a completely integrable Hamiltonian system H_0, *most* (in the sense of positive measure) quasiperiodic tori persist for sufficiently small ε. This establishes the fact that many near-integrable Hamiltonian systems (like the solar system for example!) are "globally stable" in the sense that most of their solutions around an isolated stable-elliptic equilibrium point or periodic orbit are "regular" or "predictable."

And what about Hamiltonian systems which are far from integrable? As has been rigorously established and numerically amply documented, they possess near their *unstable* equilibria and periodic orbits dense sets of solutions which are called *chaotic*, as they are characterized by an extremely sensitive dependence on initial conditions known as *chaos*. These chaotic solutions also exist in generic near-integrable Hamiltonian systems down to arbitrarily small values of $\varepsilon \to 0$ and form a network of regions on the energy surface, whose size generally grows with increasing $|\varepsilon|$.

In the last four decades, since KAM theory and its implications became widely known, Hamiltonian systems have been studied exhaustively, especially in the cases of $N = 2$ and $N = 3$ degrees of freedom. A wide variety of powerful analytical and numerical tools have been developed to (1) verify whether a given Hamiltonian system is integrable; (2) examine whether a specific initial state leads to a periodic, quasiperiodic, or chaotic orbit; (3) estimate the "size" of regular domains of predominantly quasiperiodic motion; and (4) analyze mathematically the "boundary" of these regular domains, beyond which large-scale chaotic regions dominate the dynamics and most solutions exhibit in the course of time statistical properties that prevail over their deterministic character.

As it often happens, however, physicists are more daring than mathematicians. Impatient with the slow progress of rigorous analysis and inspired by the pioneering numerical experiments of Fermi, Pasta, and Ulam (FPU) in the 1950s, a number of statistical mechanics experts embarked on a wonderful journey in the field of $N \gg 1$ coupled nonlinear oscillator chains and lattices and discovered a goldmine. Much to the surprise of their more traditional colleagues, they discovered a wealth of extremely interesting results and opened up a path that is most vigorously pursued to this very day. They concentrated especially on one-dimensional FPU lattices (or chains) of N classical particles and sought to uncover their transport properties, especially in the $N \to \infty$ and $t \to \infty$ limits.

They were joined in their efforts by a new generation of mathematical physicists aiming ultimately to establish the validity of Fourier's law of heat conduction, unravel the mysteries of localized oscillations, understand energy transport, and explore the statistical properties of these Hamiltonian systems at far from equilibrium situations. They often set all parameters equal, but also seriously pondered the effect of disorder and its connections with nonlinearity. Although most results obtained to date concern ($d = 1$)-dimensional chains, a number of findings have been extended to the case of higher ($d > 1$)-dimensional lattices.

Throughout these studies, regular motion has been associated with quasiperiodic orbits on N-dimensional tori and chaos has been connected to Lyapunov exponents, the maximal of which is expected to converge to a finite positive value in the long time limit $t \to \infty$. Recently, however, this "duality" has been challenged by a number of results regarding longtime Hamiltonian dynamics, which reveal (a) the role of tori with a dimension as low as $d = 2, 3, \ldots$ on the $2N - 1$ energy surface and (b) the significance of regimes of "weak chaos," near the boundaries of regular regions. These phenomena lead to the emergence of a hierarchy of structures, which form what we call *quasi-stationary states*, and give rise to particularly long-lived regular or chaotic phenomena that manifest a deeper level of complexity with far-reaching physical consequences.

It is the purpose of this book to discuss these phenomena within the context of what we call *complex Hamiltonian dynamics*. In the chapters that follow, we intend to summarize many years of research and discuss a number of recent results within the framework of what is already known about N degrees of freedom Hamiltonian systems. We intend to make the presentation self-contained and introductory enough to be accessible to a wide range of scientists, young and old, who possess some basic knowledge of mathematical physics.

We do not intend to focus on traditional topics of Hamiltonian dynamics, such as their symplectic formalism, bifurcation properties, renormalization theory, or chaotic transport in homoclinic tangles, which have already been expertly reviewed in many other textbooks. Rather, we plan to focus on the progress of the last decade on one-dimensional Hamiltonian lattices, which has yielded, in our opinion, a multitude of inspiring discoveries and new insights, begging to be investigated further in the years to come.

More specifically, we propose to present in Chap. 1 some fundamental background material on Hamiltonian systems that would help the uninitiated reader build some basic knowledge on what the rest of the book is all about. As part of this introductory material, we mention the pioneering results of A. Lyapunov and H. Poincaré regarding local and global stability of the solutions of Hamiltonian systems. We then consider in Chap. 2 some illustrative examples of Hamiltonian systems of $N = 1$ and 2 degrees of freedom and discuss the concept of integrability and the departure from it using singularity analysis in *complex time* and perturbation theory. In particular, the occurrence of chaos in such systems as a result of intersections of invariant manifolds of saddle points will be examined in some detail.

In Chap. 3, we present in an elementary way the mathematical concepts and basic ingredients of equilibrium points, periodic orbits, and their local stability analysis for arbitrary N. We describe the method of Lyapunov exponents and examine their usefulness in estimating the Kolmogorov entropy of certain physically important Hamiltonian systems in the thermodynamic limit, that is, taking the total energy E and the number of particles N very large with $E/N =$ constant. Moreover, we introduce some alternative methods for distinguishing order from chaos based on the more recently developed approach of Generalized Alignment Indices (GALIs) described in detail in Chap. 5.

Chapter 4 introduces the fundamental notions of *nonlinear normal modes* (NNMs), resonances, and their implications for global stability of motion in Hamiltonian systems with a finite number of degrees of freedom N. In particular, we examine the importance of discrete symmetries and the usefulness of group theory in analyzing periodic and quasiperiodic motion in Hamiltonian systems with periodic boundary conditions. Next, we discuss in Chap. 5 a number of analytical and numerical results concerning the GALI method (and its ancestor the Smaller Alignment Index—SALI—method), which uses properties of wedge products of deviation vectors and exploits the tangent dynamics to provide indicators of stable and chaotic motion that are more accurate and efficient than those proposed by other approaches. All this is then applied in Chap. 6 to explain the paradox of *FPU recurrences* and the associated transition from “weak” to “strong” chaos. We introduce the notion of *energy localization* in normal mode space and discuss the existence and stability of low-dimensional “q-tori,” aiming to provide a more complete interpretation of FPU recurrences and their connection to energy equipartition in FPU models of particle chains.

In Chap. 7 we proceed to discuss the phenomenon of *localized oscillations* in the configuration space of nonlinear one-dimensional lattices with $N \to \infty$, concentrating first on the so-called periodic (or translationally invariant) case where all parameters in the on-site and interaction potentials are identical. We also mention in this chapter recent results regarding the effects of *delocalization* and diffusion due to *disorder* introduced by choosing some of the parameters (masses or spring constants) randomly at the initialization of the system.

Next, in Chap. 8 we examine the statistical properties of chaotic regions in cases where the orbits exhibit “weak chaos,” for example, near the boundaries of islands of regular motion where the positive Lyapunov exponents are relatively small. We demonstrate that “stickiness” phenomena are particularly important in these regimes, while probability density functions (pdfs) of sums of orbital components (treated as random variables in the sense of the Central Limit Theorem) are well approximated by functions that are far from Gaussian! In fact, these pdfs closely resemble q-Gaussian distributions resulting from minimizing Tsallis’ q-entropy (subject to certain constraints) rather than the classical Boltzmann Gibbs (BG) entropy and are related to what has been called *nonextensive statistical mechanics* of strongly correlated dynamical processes.

In this context, we discuss chaotic orbits close to unstable NNMs of multidimensional Hamiltonian systems and show that they give rise to certain very interesting quasi-stationary states, which last for very long times and whose pdfs (of the above type) are well fitted by functions of the q-Gaussian type. Of course, in most cases, as

t continues to grow, these pdfs are expected to converge to a Gaussian distribution ($q \to 1$), as chaotic orbits exit from weakly chaotic regimes into domains of strong chaos, where the positive Lyapunov exponents are large and BG statistics prevail. Still, we suggest that the complex statistics of these states need to be explored further, particularly with regard to the onset of energy equipartition, as their occurrence is far from exceptional and their long-lived nature implies that they may be physically important in unveiling some of the mysteries of Hamiltonian systems in many dimensions.

The book ends with Chap. 9 containing our conclusions, a list of open research problems, and a discussion of future prospects in a number of areas of Hamiltonian dynamics. Moreover, at the end of every chapter we have included a number of exercises and problems aimed at training the uninitiated reader to learn how to use some of the fundamental concepts and techniques described in this book. Some of the problems are intended as projects for ambitious postgraduate students and offer suggestions that may lead to new discoveries in the field of complex Hamiltonian dynamics in the years ahead.

In the Acknowledgments that follow this Preface, we express our gratitude to a number of junior and senior scientists, who have contributed to the present book in many ways: Some have provided useful comments and suggestions on many topics treated in the book, while others have actively collaborated with us in obtaining many of the results presented here.

Whether we have done justice to all those whose work is mentioned in the text and listed in our References is not for us to judge. The fact remains that, beyond the help we have received from all acknowledged scientists and referenced sources, the responsibility for the accurate presentation and discussion of the scientific field of complex Hamiltonian dynamics lies entirely with the authors.

Patras, Greece *Tassos Bountis*
Dresden, Germany *Haris Skokos*