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Complex Hamiltonian Dynamics

With a Foreword by Sergej Flach

Springer

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To our wives Angela and Irini, our children Athena and Dimitris and our parents Athena and Christos, Niki and Dimitris.
Their love, dedication and support are a constant source of inspiration and encouragement in our lives.

Foreword

What makes a science book interesting, valuable, useful, and perhaps also worth spending the money to own it? Well, in the case of this book I guess it starts with its title which immediately attracts one's attention. Next, the intrigued reader is invited to inspect a Contents List which combines many familiar-sounding topics and chapters along with completely new and unknown ones, raising our curiosity to find out how these different topics are interrelated. Ultimately, of course, we realize that it is the reading itself which will tell us whether we have found enough new and interesting insights into this domain of the endless world of wonders in science, which the authors call *complex Hamiltonian dynamics*. This brief foreword is thus devoted to tell the reader that all the above conditions are satisfied for the book you hold in your hands (or have downloaded to your electronic device).

To begin with, the short title tells those of you who do not know it already that Hamiltonian dynamics is endlessly complex. Indeed, Hamiltonian models can be formally used for almost any problem in nature, which includes hopelessly complex systems as well. But complexity in Hamiltonian dynamics starts on much lower and seemingly simpler levels. Just get into Chap. 2, where the authors demonstrate in a pedagogical and very readable way some basic and well-known facts of chaos theory for systems with a few degrees of freedom, illustrated by a number of illuminating examples.

While reading the chapters that follow, the concept of the monograph, its title, and the intentions of the authors quickly become clear. In a nutshell, what is addressed here is the border between strongly chaotic and fully regular dynamical systems. The authors use recent progress in the study of relaxation of nonequilibrium states as a playground for applying novel tools. The models are carefully chosen from a set of well-known half-century-old paradigms, which were invented to address basic questions of statistical physics. The fact that a number of these questions still remain unanswered hints at a kind of complexity that is present at seemingly simple levels. It is indeed worth noting that the experienced authors take special care to formulate a number of exercises, which makes this monograph a combination of an introduction into the nonlinear dynamics of many degrees of freedom, a report on recent progress at the forefront of nonlinear science, and an ideal textbook for students and teachers of advanced physics courses.

An interesting attempt to describe and distinguish order from chaos in Hamiltonian systems with many degrees of freedom is given in Chap. 3. The authors discuss various types of fixed and dynamical equilibria and their local stability properties, and smoothly connect them to the issue of global stability of dynamical states. Besides discussing standard ways of characterizing chaos via Lyapunov spectra, the authors also introduce novel methods (called SALI and GALI) which connect tangent dynamics with stability of motion and the nature of the dynamical state under investigation. Both aspects of characterizing equilibria and exploring techniques to distinguish order from chaos are discussed in detail in the two subsequent chapters.

Then comes Chap. 6, where we encounter many applications of the methods introduced earlier to the classical problem of the FPU paradox, first posed by Enrico Fermi, John Pasta, and Stanislav Ulam in their pioneering studies of the early 1950s. The next chapter addresses the fascinating phenomenon of localization and reports on another recent puzzle of great interest at the border between order and chaos, namely, the spreading of nonlinear waves in ordered and disordered media.

The monograph continues in Chap. 8 with a critical discussion and comparison of many systems exhibiting "weak chaos" from the viewpoint of nonextensive statistical mechanics. Finally, the book ends in Chap. 9 with a number of open problems, which should prove quite inspiring to graduate student readers, and concludes with a brief review of additional fascinating topics of Hamiltonian dynamics, which are of great current interest and outstanding potential for practical applications.

In summary, this book constitutes in my opinion a very solid piece of work, which serves several purposes: It is very useful as an introductory textbook that familiarizes the reader with modern methods of analysis applied to Hamiltonian systems of many degrees of freedom and reviews a set of modern research areas at the forefront of nonlinear science. Last but not least, thanks to its pedagogical structure, it should prove easily exploitable as an exercise source for advanced university courses.

Dresden, Germany *Sergej Flach*

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 $d = 2, 3, \dots$ 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*

Acknowledgments

Throughout our career and, in particular, in the course of our work described in the present book, we have been privileged to collaborate with many scientists, junior and senior to us in age and scientific experience. It is impossible to do justice to all of them in the limited space available here. Among the senior scientists, Tassos Bountis (T. B.) first wishes to mention Professors Elliott Montroll and Robert Helleman of the University of Rochester, New York, and Professor Joseph Ford of Georgia Institute of Technology, who first introduced him to the wonderful world of Hamiltonian Systems and Nonlinear Dynamics in the USA. Most influential to his particular scientific viewpoint have also been Professors Grégoire Nicolis, Université Libre de Bruxelles, Giulio Casati, University of Insubria, and Hans Capel, University of Amsterdam, and, in Greece, Professors George Contopoulos, University of Athens, and John Nicolis, University of Patras. More recently, T. B. has worked on lattice dynamics based on a number of ideas and results put forth by Dr. Sergej Flach and his group at the Max Planck Institute of the Physics of Complex Systems in Dresden, Professor George Chechin of the Southern Federal University of Russia at Rostov-on-Don, and Professor Constantino Tsallis and his coworkers at the Centro Brasileiro de Pesquisas Fisicas in Rio de Janeiro.

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The next stop of H. S.'s journey in the tangled world of Chaotic Dynamics was Paris, France, where he had the privilege to work together with Professor Jacques Laskar at the Observatory of Paris. H. S. is grateful to Jacques for broadening his knowledge on chaos detection methods (which is one of his most loved subjects) and symplectic integration techniques as well as for giving him the opportunity to work on the dynamics of real accelerators.

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Contents

Acronyms

BEC	Bose Einstein Condensation: Important physical phenomenon related to the behavior of bosons at very low temperatures.
BG	Boltzmann Gibbs: Ensembles of classical equilibrium statistical mechanics proposed by Boltzmann and Gibbs in the late nineteenth and early twentieth centuries.
CLT	Central Limit Theorem: The classical theorem, according to which sums of N identically and independently distributed random variables tend, in the limit $N \rightarrow \infty$, to a Gaussian distribution with the same mean and variance as the original variables.
CPU	Central Processing Unit: The part of a computer system that performs the basic arithmetical, logical, and input/output operations required by a computer program. The time required by the CPU for the completion of the tasks of a particular computer program (CPU time) is used to characterize the efficiency of the program.
DNLS	Discrete Nonlinear Schrödinger Equation: The Hamiltonian system of equations emanating from the NLS by the discretization of its second derivative with respect to the space variable.
DDNLS	Disordered Discrete Nonlinear Schrödinger Equation: The DNLS when some of its parameters are chosen randomly and uniformly from within a specified interval.
dof	Degree(s) of freedom: The number of canonical conjugate pairs of position and momentum variables characterizing a Hamiltonian system.
FPU	Fermi, Pasta and Ulam: Names of the researchers who first integrated numerically a chain (one-dimensional lattice) of identical oscillators coupled by quadratic as well as cubic and/or quartic nearest neighbor interaction terms in their Hamiltonian.
FPU$-\alpha$	FPU lattice whose interaction terms in the Hamiltonian, beyond the harmonic ones, are only of the cubic type.
FPU$-\beta$	FPU lattice whose interaction terms in the Hamiltonian, beyond the harmonic ones, are only of the quartic type.

GALI_k	Generalized Alignment Index of order $k \geq 2$: Chaos indicator related to the book of the parallelepiped formed by k deviation vectors in the tangent space of an orbit of a dynamical system.
IPM	In Phase Mode: A particular NNM of one-dimensional lattices, where all particles oscillate identically and in phase.
KAM	Kolmogorov Arnol'd Moser: Name of a theorem that establishes an important rigorous result regarding the behavior of weakly perturbed integrable Hamiltonian systems.
KdV	Korteweg de Vries: Name of an equation exhibiting solitary wave solutions first obtained by Korteweg and de Vries in the 1890s. In the 1960s these waves were named solitons and formed an integral part of the theory of completely integrable evolution equations.
KG	Klein Gordon: It refers to the so-called Klein Gordon potential of classical and quantum physics, which consists of a quadratic and a quartic part.
LA	Liouville Arnol'd: Name of a theorem that establishes an important rigorous result regarding the solvability of integrable Hamiltonian systems of N dof and the existence of N-dimensional tori on which their bounded solutions lie.
LCE(s)	Lyapunov Characteristic Exponent(s): Exponents characterizing the rates of divergence of nearby trajectories of dynamical systems in phase space.
MLE	Maximum Lyapunov Exponent: The LCE with the maximal value.
NLS	Nonlinear Schrödinger Equation: A completely integrable PDE which consists of the linear Schrödinger equation plus a cubic nonlinearity and is of particular importance in the field of nonlinear optics.
NNM(s)	Nonlinear Normal Mode(s): Extension of the normal modes of a linear system of coupled harmonic oscillators in the nonlinear regime.
NME(s)	Normal Mode Eigenvector(s): Eigenvector(s) of a linear problem, used as a basis for the expansion of the solutions of the associated perturbed nonlinear problem.
ODE(s)	Ordinary Differential Equation(s): Differential equations involving derivatives with respect to only one independent variable.
OPM	Out of Phase Mode: A particular NNM of one-dimensional lattices, where all particles oscillate identically out of phase with respect to each other in all neighboring pairs.
PDE(s)	Partial Differential Equation(s): Differential equations involving derivatives with respect to more than one independent variable.
pdf(s)	Probability distribution function(s): Function(s) representing the probability density of observables related to the long time evolution of variables of a dynamical system in chaotic regimes.
PSS	Poincaré Surface of Section: Cross-section of orbits of a Hamiltonian system with certain lower dimensional subspace of its phase space. For example, in the case of a two dof Hamiltonian system the PSS is a two-dimensional plane defined by one pair of position and momentum

coordinates, say (x, p_x), at times when the second position coordinate has a prescribed value, say $y = 0$, and the second momentum a prescribed sign, say $p_y > 0$.

QSS — Quasi-stationary states: Weakly chaotic dynamical states of Hamiltonian systems that persist for very long times and are generally characterized by pdfs that are different from Gaussian.

SALI — Smaller Alignment Index: Chaos indicator related to the area of a parallelogram formed by two deviation vectors in the tangent space of an orbit of a dynamical system. It is analogous to $GALI_2$.

SPO(s) — Simple Periodic Orbit(s): Periodic orbit(s) of a dynamical system returning to their initial state after a single oscillation of its variables.