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Interdisciplinary Applied Mathematics

Martin C. Gutzwiller

Chaos in Classical and Quantum Mechanics

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With 78 Illustrations

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Preface

Elementary mechanics, both classical and quantum, has become a growth industry in the last decade. A newcomer to this flourishing field must get acquainted with some unfamiliar concepts and get rid of some cherished assumptions. The change in orientation is necessary because physicists have finally realized that most dynamical systems do not follow simple, regular, and predictable patterns, but run along a seemingly random, yet well-defined, trajectory. The generally accepted name for this phenomenon is *chaos,* a term that accurately suggests that we have failed to come to grips with the problem.

This book offers a collection of ideas and examples rather than general concepts and mathematical theorems. However, an indifferent compilation of the most telling results can only discourage the novice. In order to focus on a central theme, I have singled out the questions that have a bearing on the connection between classical and quantum mechanics. In this manner we are led to ask whether there are chaotic features in quantum mechanics; the issue is still open, and all the preliminary answers suggest that quantum mechanics is more subtle than most of us had realized.

Reading this book requires a knowledge of both classical and quantum mechanics beyond a first introductory physics course. Advanced mastery of these subjects is not necessary, however, and probably not even desirable, since I am trying to appeal to the intuition rather than the analytical ability of the reader. Some of the more sophisticated concepts, such as the action function in classical mechanics and its analog in quantum mechanics, Green's function, are basic to the whole development as it is presented here. Their meaning and their use will be explained in the context in which they appear, and without the mathematical qualifications that would be necessary if I tried to offer general propositions rather than special cases.

In keeping with this informal style I have emphasized certain aspects of the whole story which are not usually found in scientific books. Whenever possible I base my arguments on elementary geometry rather than algebraic manipulations. In order to gain a better perspective on the more important results, references to the historical development are often helpful. In the same vein, related problems from different disciplines are mentioned in the same section, with particular attention to mathematics, astronomy, physics, and chemistry. Finally, I have taken the liberty to comment on the motivation behind certain efforts, to evaluate the validity and relevance of some results, and to consider future tasks, if not to speculate outright about possible developments in the field of chaos.

This book comes out of a course of the same title that I taught in the winter and spring of 1986 at the Laboratoire de Physique du Solide in Orsay, outside of Paris. I owe a debt of gratitude to my faithful audience, who helped me with a moderate amount of criticism; in particular, Francoise Axel, Oriol Bohigas, Alain Comtet, Marie Joya Giannoni, Bernard Jancovici, Maurice Kléman, Jean Marc Luck, Claude Itzykson, and André Voros provided many useful suggestions.

Most scientists have not participated in the recent development of ideas related to chaos in Hamiltonian systems; they are usually not aware of the many different viewpoints and interpretations, the new problems and methods for their solution, and the novel applications to important experiments. As far as this book is concerned, all of these ideas deal with relatively elementary questions in both classical and quantum mechanics; as soon as they are understood, some readers may be tempted to call them obvious because of their deceptive simplicity!

Since I have worked in this area for twenty years, I have benefitted from discussions with many colleagues who are interested in questions related to chaos. I want to thank them all, and apologize for not mentioning them by name. It is remarkable how many different personalities and individual tastes in scientific matters can be attracted to one central theme. I hope indeed that this book will appeal to all those who look for diversity in their pursuit of physics and its closest relatives, mathematics, astronomy, and chemistry. Thus we might eventually find harmony in chaos.

Interdisciplinary Applied Mathematics
Volume 1

To Frances and Patricia

Faithful Companions on a Long Journey

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Introduction

Elementary mechanics is the model for the physical sciences. Its principles and methods are the ideal for most other disciplines that deal with nature. Substantial parts even of mathematics have been developed to deal with the problems of mechanics. Every scientist has a fairly well-defined picture of the way mechanics works and the kind of results it yields.

According to the prevailing views, a dynamical system runs along a predictable and regular course, and ends up in some periodic and steady state. If very many particles are involved and we are either unable or unwilling to follow each one individually, then we are satisfied with knowing the statistical properties of a dynamical system. The phenomena of *thermodynamics*, of *friction*, and of *diffusion* have a probabilistic character because we don't really need to know everything there is. The situation is subject to random processes because we choose to be ignorant. By contrast, the mechanical behavior of simple systems is assumed to be entirely comprehensible, easily described, perhaps even dull.

This erroneous impression is created by the special examples discussed in school, from elementary to graduate: two bodies attracting each other with an inverse-square-of-the-distance force, as in planetary motion and in the hydrogen atom; several oscillators coupled by linear springs; and a rotating symmetric rigid body in a uniform gravitational field, the gyroscope. The general methods for solving more difficult problems are presented as technical refinements best left to the experts -- astronomers working in celestial mechanics and theoreticians in atomic and molecular physics.

A century ago mathematicians discovered that some apparently simple mechanical systems can have very complicated motions. Not only is their behavior exceedingly sensitive to the precise starting conditions, but they never settle to any reasonable final state with a recognizable fixed pattern. Although their movements look smooth over short times, they seem to jump unpredictably and indefinitely when their positions and momenta are checked over large time intervals.

Astronomers became increasingly aware of this problem during the last 60 years, but physicists began to recognize it only some 20 years ago. The phenomenon, which now goes under the name *chaos,* has since become a very fashionable topic of investigation. Innocent onlookers might suspect one more passing fad. I do not think it will turn out that way, though. Chaos is not only here to stay, but will challenge many of our assumptions about the typical behavior of dynamical systems. Since mechanics underlies our view of nature, we will probably have to modify some of our ideas concerning the harmony and beauty of the universe.

As a first step, we will have to study entirely different basic examples in order to re-form our intuition. We must become familiar with certain novel specimens of simple mechanical systems based on chaotic rather than regular behavior. General abstract propositions do not serve that purpose, although they are desirable once we become knowledgeable about the issues involved.

This book is, therefore, committed to the discussion of specific examples, in particular the hydrogen atom in a magnetic field, the donor impurity in a semiconductor where the effective mass of the electron is different in different directions, and the motion of a particle on a surface of negative curvature. Other equally instructive systems, which are chaotic, yet simple enough to be understood thoroughly, will be mentioned without detailed discussion. Among them is the *hydrogen atom in a strong microwave field;* an adequate treatment would almost require a monograph by itself, if the recent experiments on this system are to be presented, and everything put into proper perspective.

These unfamiliar examples must be seen in full contrast with the familiar ones. A discussion of the regular behavior and of some borderline systems will therefore precede the main part of this book. In particular the *three-body problem of celestial mechanics* will be discussed in some detail with special attention to the *Moon-Earth-Sun* system. The important ideas of classical mechanics were first conceived and tested in this area, and their practical application can be observed in the sky without elaborate instruments. Chaos made its first appearance there.

Mathematicians have put a lot of effort into proving the formal equivalence between various abstract dynamical systems. Although one hopes that these endeavors will ultimately embrace all mechanical systems, the different kinds of chaotic behavior have not been characterized to the point where an exhaustive classification can be attempted. The study of further examples will eventually get us there. Meanwhile some simple practical distinctions are sufficient. I see no reason to split the phenomenon into more than two broad categories: *soft chaos*, which allows an approach starting from regular behavior by perturbation or breaking the symmetry as it were, and *hard chaos*, where each trajectory is isolated as the intersection of a stable and an unstable manifold. Such general features as bound states versus scattering, or conservative versus time-dependent forces remain important; but there will be *no discussion of friction, nor of any other dissipation of energy*.

Only systems with a *finite number of degrees of freedom* will be considered. This selection is dictated by a fundamental problem on which I have worked for two decades and which serves as the focus in this book: How can the classical mechanics of Newton, Euler, and Lagrange be understood as a limiting case within the quantum mechanics of Heisenberg, Schroedinger, and Dirac? Einstein in 1917 was the first, and for 40 years the only, scientist to point out the true dimensions of this problem when the classical dynamical system is chaotic. While we are still a long way from a satisfactory answer, I can think of no better issue to guide our thinking.

In this manner we are led straight into the main question of *quantum chaos:* Is there anything within quantum mechanics to compare with the chaotic behavior of classical dynamical systems? It seems unlikely, although there are cases of smooth chaos in quantum mechanics which border on the enigmatic, e.g., the scattering of waves on a two-dimensional box. Their discussion requires a certain degree of mathematical sophistication which is well worth the effort.

Mechanics, classical as well as quantal, with all the above restrictions in the choice of examples, seems almost simple enough to be within the grasp of purely algebraic and analytical methods. There are, however, striking examples where *numerical calculations* have given the investigator clues to the analytical solution of a problem. Furthermore, the ready availability of computers has led to many interesting numerical results, with as many intuitive interpretations, all in need of further sorting to find the relevant ideas. A somewhat arbitrary choice among these computational efforts is almost inevitable, particularly in view of the rapid accumulation of partial results. I have tried to concentrate on the work which tests the limit toward classical mechanics, and which is not the subject of some recent monograph, such as, for instance, the hydrogen atom in a microwave field, one of the few cases of quantum chaos with a wealth of experimental material.

Some readers may be disappointed because they do not find a satisfactory account of what interests them most. The number of articles in this general area has become overwhelming in the last decade. Since I think that new examples are of the essence, I regret that some particularly interesting ones are not dicussed here.

Among the most serious omissions I want to mention specifically almost everything connected with time-dependent Hamiltonian systems such as the *hydrogen-atom in a strong microwave field* (Bayfield and Koch 1974, for a review cf. Bayfield 1987) as well as the closely related *kicked rotator* (Casati, Chirikov, Izraelev, and Ford 1979; Fishman, Grempel, and Prange 1982, 1984). *Discrete maps and their quantum analog* get very little attention (Balazs and Voros 1989), and almost nothing is said about rotating bodies like gyroscopes and *coupled spins* (Magyari, Thomas, Weber, Kaufmann, and Müller 1987; Srivastava et al. 1988), nor about related work in *nuclear physics* (Meredith, Koonin, and Zirnbauer 1988; Swiatecki 1988). The above references are supposed to point to some of the seminal work in one of these areas.

Every author is entitled to use the lack of space as an excuse, although a lack of competence, interest, and/or hard work in certain subjects might occasionally provide a more adequate explanation for some shortcomings. Such obvious reasons, however, are based on the author's personal preferences and his perspective on the whole enterprise of theoretical physics. They are not easily condensed into simple declarations of intent, or statements explaining general views and methods, because they are always intimately mixed with the author's personal and professional experiences. The organization of this book and the choice of the several topics has to be seen as one possible, and to some extent coherent, approach to a novel and very active area in science.

CHAPTER 1

The Mechanics of Lagrange

The most general starting point for the discussion of any mechanical system is the *variational principle*. It was first proposed as a particularly concise formulation of Newton's laws of motion, and it turns out to be extremely useful for some simple manipulations such as the transition between different coordinate systems. Feynman (1948, 1965), with the inspiration of Dirac (1933, 1935), then found a complete analog for it in quantum mechanics. Indeed, the *path integral* provides the most direct link between the classical and the quantum regime (cf. Section 13.4).

The ideas concerning the variational principle of Lagrange are the backbone of this whole book. They will be explained in general terms assuming that the reader has met them before; they will also be illustrated explicitly using the example of space travel in the solar system.

The titles of this chapter and the next one are somewhat misleading. The historical development of mechanics is more complicated than the simple division into two kinds of mechanics, Lagrange's depending on time as the primary parameter, and Hamilton-Jacobi's depending on the energy. This distinction is important in quantum mechanics, however, and since our presentation is skewed in that direction, the relevant differences are brought out already at the classical level. The first two chapters are not meant to trace the origin of all the ideas back to their authors except where this is specifically mentioned.