

Appendix A

A brief history of chaos

Laws of attribution

1. **Arnol'd's Law:** everything that is discovered is named after someone else (including Arnol'd's law)
2. **Berry's Law:** sometimes, the sequence of antecedents seems endless. So, nothing is discovered for the first time.
3. **Whiteheads's Law:** Everything of importance has been said before by someone who did not discover it.

—M.V. Berry

A.1 Chaos is born

(R. Mainieri and P. Cvitanović)

TRYING TO PREDICT the motion of the Moon has preoccupied astronomers since antiquity. Accurate understanding of its motion was important for determining the longitude of ships while traversing open seas.

Kepler's Rudolphine tables had been a great improvement over previous tables, and Kepler was justly proud of his achievements. He wrote in the introduction to the announcement of Kepler's third law, *Harmonice Mundi* (Linz, 1619) in a style that would not fly with the contemporary *Physical Review Letters* editors:

What I prophesied two-and-twenty years ago, as soon as I discovered the five solids among the heavenly orbits—what I firmly believed long before I had seen Ptolemy's *Harmonics*—what I had promised my friends in the title of this book, which I named before I was sure of my discovery—what sixteen

years ago, I urged as the thing to be sought—that for which I joined Tycho Brahé, for which I settled in Prague, for which I have devoted the best part of my life to astronomical contemplations, at length I have brought to light, and recognized its truth beyond my most sanguine expectations. It is not eighteen months since I got the first glimpse of light, three months since the dawn, very few days since the unveiled sun, most admirable to gaze upon, burst upon me. Nothing holds me; I will indulge my sacred fury; I will triumph over mankind by the honest confession that I have stolen the golden vases of the Egyptians to build up a tabernacle for my God far away from the confines of Egypt. If you forgive me, I rejoice; if you are angry, I can bear it; the die is cast, the book is written, to be read either now or in posterity, I care not which; it may well wait a century for a reader, as God has waited six thousand years for an observer.

Then came Newton. Classical mechanics has not stood still since Newton. The formalism that we use today was developed by Euler and Lagrange. By the end of the 1800's the three problems that would lead to the notion of chaotic dynamics were already known: the three-body problem, the ergodic hypothesis, and nonlinear oscillators.

A.1.1 Three-body problem

Bernoulli used Newton's work on mechanics to derive the elliptic orbits of Kepler and set an example of how equations of motion could be solved by integrating. But the motion of the Moon is not well approximated by an ellipse with the Earth at a focus; at least the effects of the Sun have to be taken into account if one wants to reproduce the data the classical Greeks already possessed. To do that one has to consider the motion of three bodies: the Moon, the Earth, and the Sun. When the planets are replaced by point particles of arbitrary masses, the problem to be solved is known as the three-body problem. The three-body problem was also a model to another concern in astronomy. In the Newtonian model of the solar system it is possible for one of the planets to go from an elliptic orbit around the Sun to an orbit that escaped its dominion or that plunged right into it. Knowing if any of the planets would do so became the problem of the stability of the solar system. A planet would not meet this terrible end if solar system consisted of two celestial bodies, but whether such fate could befall in the three-body case remained unclear.

After many failed attempts to solve the three-body problem, natural philosophers started to suspect that it was impossible to integrate. The usual technique for integrating problems was to find the conserved quantities, quantities that do not change with time and allow one to relate the momenta and positions at different times. The first sign on the impossibility of integrating the three-body problem came from a result of Burns that showed that there were no conserved quantities that were polynomial in the momenta and positions. Burns' result did not preclude the possibility of more complicated conserved quantities. This problem was settled by Poincaré and Sundman in two very different ways.

In an attempt to promote the journal *Acta Mathematica*, Mittag-Leffler got the permission of the King Oscar II of Sweden and Norway to establish a mathematical competition. Several questions were posed (although the king would have preferred only one), and the prize of 2500 kroner would go to the best submission. One of the questions was formulated by Weierstrass:

Given a system of arbitrary mass points that attract each other according to Newton's laws, under the assumption that no two points ever collide, try to find a representation of the coordinates of each point as a series in a variable that is some known function of time and for all of whose values the series converges uniformly.

This problem, whose solution would considerably extend our understanding of the solar system, ...

Poincaré's submission won the prize. He showed that conserved quantities that were analytic in the momenta and positions could not exist. To show that he introduced methods that were very geometrical in spirit: the importance of state space flow, the role of periodic orbits and their cross sections, the homoclinic points.

The interesting thing about Poincaré's work was that it did not solve the problem posed. He did not find a function that would give the coordinates as a function of time for all times. He did not show that it was impossible either, but rather that it could not be done with the Bernoulli technique of finding a conserved quantity and trying to integrate. Integration would seem unlikely from Poincaré's prize-winning memoir, but it was accomplished by the Finnish-born Swedish mathematician Sundman. Sundman showed that to integrate the three-body problem one had to confront the two-body collisions. He did that by making them go away through a trick known as regularization of the collision manifold. The trick is not to expand the coordinates as a function of time t , but rather as a function of \sqrt{t} . To solve the problem for all times he used a conformal map into a strip. This allowed Sundman to obtain a series expansion for the coordinates valid for all times, solving the problem that was proposed by Weierstrass in the King Oscar II's competition.

The Sundman's series are not used today to compute the trajectories of any three-body system. That is more simply accomplished by numerical methods or through series that, although divergent, produce better numerical results. The conformal map and the collision regularization mean that the series are effectively in the variable $1 - e^{-\sqrt{t}}$. Quite rapidly this gets exponentially close to one, the radius of convergence of the series. Many terms, more terms than any one has ever wanted to compute, are needed to achieve numerical convergence. Though Sundman's work deserves better credit than it gets, it did not live up to Weierstrass's expectations, and the series solution did not "considerably extend our understanding of the solar system." The work that followed from Poincaré did.

A.1.2 Ergodic hypothesis

The second problem that played a key role in development of chaotic dynamics was the ergodic hypothesis of Boltzmann. Maxwell and Boltzmann had combined the mechanics of Newton with notions of probability in order to create statistical mechanics, deriving thermodynamics from the equations of mechanics. To evaluate the heat capacity of even a simple system, Boltzmann had to make a great simplifying assumption of ergodicity: that the dynamical system would visit every part of the phase space allowed by conservation laws equally often. This hypothesis was extended to other averages used in statistical mechanics and was called the ergodic hypothesis. It was reformulated by Poincaré to say that a trajectory comes as close as desired to any phase space point.

Proving the ergodic hypothesis turned out to be very difficult. By the end of twentieth century it has only been shown true for a few systems and wrong for quite a few others. Early on, as a mathematical necessity, the proof of the hypothesis was broken down into two parts. First one would show that the mechanical system was ergodic (it would go near any point) and then one would show that it would go near each point equally often and regularly so that the computed averages made mathematical sense. Koopman took the first step in proving the ergodic hypothesis when he realized that it was possible to reformulate it using the recently developed methods of Hilbert spaces. This was an important step that showed that it was possible to take a finite-dimensional nonlinear problem and reformulate it as an infinite-dimensional linear problem. This does not make the problem easier, but it does allow one to use a different set of mathematical tools on the problem. Shortly after Koopman started lecturing on his method, von Neumann proved a version of the ergodic hypothesis, giving it the status of a theorem. He proved that if the mechanical system was ergodic, then the computed averages would make sense. Soon afterwards Birkhoff published a much stronger version of the theorem.

A.1.3 Nonlinear oscillators

The third problem that was very influential in the development of the theory of chaotic dynamical systems was the work on the nonlinear oscillators. The problem is to construct mechanical models that would aid our understanding of physical systems. Lord Rayleigh came to the problem through his interest in understanding how musical instruments generate sound. In the first approximation one can construct a model of a musical instrument as a linear oscillator. But real instruments do not produce a simple tone forever as the linear oscillator does, so Lord Rayleigh modified this simple model by adding friction and more realistic models for the spring. By a clever use of negative friction he created two basic models for the musical instruments. These models have more than a pure tone and decay with time when not stroked. In his book *The Theory of Sound* Lord Rayleigh introduced a series of methods that would prove quite general, such as the notion of a limit cycle, a periodic motion a system goes to regardless of the initial conditions.

A.1.4 Chaos grows up

(R. Mainieri)

The theorems of von Neumann and Birkhoff on the ergodic hypothesis were published in 1912 and 1913. This line of enquiry developed in two directions. One direction took an abstract approach and considered dynamical systems as transformations of measurable spaces into themselves. Could we classify these transformations in a meaningful way? This led Kolmogorov to the introduction of the concept of entropy for dynamical systems. With entropy as a dynamical invariant it became possible to classify a set of abstract dynamical systems known as the Bernoulli systems. The other line that developed from the ergodic hypothesis was in trying to find mechanical systems that are ergodic. An ergodic system could not have stable orbits, as these would break ergodicity. So in 1898 Hadamard published a paper with a playful title of ‘... billiards ...,’ where he showed that the motion of balls on surfaces of constant negative curvature is everywhere unstable. This dynamical system was to prove very useful and it was taken up by Birkhoff. Morse in 1923 showed that it was possible to enumerate the orbits of a ball on a surface of constant negative curvature. He did this by introducing a symbolic code to each orbit and showed that the number of possible codes grew exponentially with the length of the code. With contributions by Artin, Hedlund, and H. Hopf it was eventually proven that the motion of a ball on a surface of constant negative curvature was ergodic. The importance of this result escaped most physicists, one exception being Krylov, who understood that a physical billiard was a dynamical system on a surface of negative curvature, but with the curvature concentrated along the lines of collision. Sinai, who was the first to show that a physical billiard can be ergodic, knew Krylov’s work well.

The work of Lord Rayleigh also received vigorous development. It prompted many experiments and some theoretical development by van der Pol, Duffing, and Hayashi. They found other systems in which the nonlinear oscillator played a role and classified the possible motions of these systems. This concreteness of experiments, and the possibility of analysis was too much of temptation for Mary Lucy Cartwright and J.E. Littlewood [A.18], who set out to prove that many of the structures conjectured by the experimentalists and theoretical physicists did indeed follow from the equations of motion. Birkhoff had found a ‘remarkable curve’ in a two dimensional map; it appeared to be non-differentiable and it would be nice to see if a smooth flow could generate such a curve. The work of Cartwright and Littlewood led to the work of Levinson, which in turn provided the basis for the horseshoe construction of S. Smale.

chapter 12

In Russia, Lyapunov paralleled the methods of Poincaré and initiated the strong Russian dynamical systems school. Andronov carried on with the study of nonlinear oscillators and in 1937 introduced together with Pontryagin the notion of coarse systems. They were formalizing the understanding garnered from the study of nonlinear oscillators, the understanding that many of the details on how these oscillators work do not affect the overall picture of the state space: there will still be limit cycles if one changes the dissipation or spring force function by a little bit. And changing the system a little bit has the great advantage of

eliminating exceptional cases in the mathematical analysis. Coarse systems were the concept that caught Smale’s attention and enticed him to study dynamical systems.

A.2 Chaos with us

(R. Mainieri)

In the fall of 1961 Steven Smale was invited to Kiev where he met Arnol’d, Anosov, Sinai, and Novikov. He lectured there, and spent a lot of time with Anosov. He suggested a series of conjectures, most of which Anosov proved within a year. It was Anosov who showed that there are dynamical systems for which all points (as opposed to a non-wandering set) admit the hyperbolic structure, and it was in honor of this result that Smale named these systems Axiom-A. In Kiev Smale found a receptive audience that had been thinking about these problems. Smale’s result catalyzed their thoughts and initiated a chain of developments that persisted into the 1970’s.

Smale collected his results and their development in the 1967 review article on dynamical systems, entitled “Differentiable dynamical systems.” There are many great ideas in this paper: the global foliation of invariant sets of the map into disjoint stable and unstable parts; the existence of a horseshoe and enumeration and ordering of all its orbits; the use of zeta functions to study dynamical systems. The emphasis of the paper is on the global properties of the dynamical system, on how to understand the topology of the orbits. Smale’s account takes you from a local differential equation (in the form of vector fields) to the global topological description in terms of horseshoes. chapter 12

The path traversed from ergodicity to entropy is a little more confusing. The general character of entropy was understood by Weiner, who seemed to have spoken to Shannon. In 1948 Shannon published his results on information theory, where he discusses the entropy of the shift transformation. Kolmogorov went far beyond and suggested a definition of the metric entropy of an area preserving transformation in order to classify Bernoulli shifts. The suggestion was taken by his student Sinai and the results published in 1959. In 1960 Rohlin connected these results to measure-theoretical notions of entropy. The next step was published in 1965 by Adler and Palis, and also Adler, Konheim, McAndrew; these papers showed that one could define the notion of topological entropy and use it as an invariant to classify continuous maps. In 1967 Anosov and Sinai applied the notion of entropy to the study of dynamical systems. It was in the context of studying the entropy associated to a dynamical system that Sinai introduced Markov partitions in 1968.

Markov partitions allow one to relate dynamical systems and statistical mechanics; this has been a very fruitful relationship. It adds measure notions to the topological framework laid down in Smale’s paper. Markov partitions divide the state space of the dynamical system into nice little boxes that map into each other. Each

box is labeled by a code and the dynamics on the state space maps the codes around, inducing a symbolic dynamics. From the number of boxes needed to cover all the space, Sinai was able to define the notion of entropy of a dynamical system. In 1970 Bowen came up independently with the same ideas, although there was presumably some flow of information back and forth before these papers got published. Bowen also introduced the important concept of shadowing of chaotic orbits. We do not know whether at this point the relations with statistical mechanics were clear to everyone. They became explicit in the work of Ruelle. Ruelle understood that the topology of the orbits could be specified by a symbolic code, and that one could associate an ‘energy’ to each orbit. The energies could be formally combined in a ‘partition function’ to generate the invariant measure of the system.

After Smale, Sinai, Bowen, and Ruelle had laid the foundations of the statistical mechanics approach to chaotic systems, research turned to studying particular cases. The simplest case to consider is 1-dimensional maps. The topology of the orbits for parabola-like maps was worked out in 1973 by Metropolis, Stein, and Stein. The more general 1-dimensional case was worked out in 1976 by Milnor and Thurston in a widely circulated preprint, whose extended version eventually got published in 1988.

A lecture of Smale and the results of Metropolis, Stein, and Stein inspired Feigenbaum to study simple maps. This led him to the discovery of the universality in quadratic maps and the application of ideas from field-theory to dynamical systems. Feigenbaum’s work was the culmination in the study of 1-dimensional systems; a complete analysis of a nontrivial transition to chaos. Feigenbaum introduced many new ideas into the field: the use of the renormalization group which led him to introduce functional equations in the study of dynamical systems, the scaling function which completed the link between dynamical systems and statistical mechanics, and the presentation functions which describe the dynamics of scaling functions.

The work in more than one dimension progressed very slowly and is still far from completed. The first result in trying to understand the topology of the orbits in two dimensions (the equivalent of Metropolis, Stein, and Stein, or Milnor and Thurston’s work) was obtained by Thurston. Around 1975 Thurston was giving lectures “On the geometry and dynamics of diffeomorphisms of surfaces.” Thurston’s techniques exposed in that lecture have not been applied in physics, but much of the classification that Thurston developed can be obtained from the notion of a ‘pruning front’ formulated independently by Cvitanović.

Once one develops an understanding of the topology of the orbits of a dynamical system, one needs to be able to compute its properties. Ruelle had already generalized the zeta function introduced by Artin and Mazur so that it could be used to compute the average value of observables. The difficulty with Ruelle’s zeta function is that it does not converge very well. Starting out from Smale’s observation that a chaotic dynamical system is dense with a set of periodic orbits, Cvitanović used these orbits as a skeleton on which to evaluate the averages of observables, and organized such calculations in terms of rapidly converging cycle expansions. This

convergence is attained by using the shorter orbits used as a basis for shadowing the longer orbits.

This account is far from complete, but we hope that it will help get a sense of perspective on the field. It is not a fad and it will not die anytime soon.

A.2.1 Periodic orbit theory

Pure mathematics is a branch of applied mathematics.
— Joe Keller, after being asked to define applied mathematics

The history of the periodic orbit theory is rich and curious, and the recent advances are to equal degree inspired by a century of separate development of three disparate subjects; 1. *classical chaotic dynamics*, initiated by Poincaré and put on its modern footing by Smale [1.27], Ruelle [1.32], and many others; 2. *quantum theory* initiated by Bohr, with the modern ‘chaotic’ formulation by Gutzwiller [21.13, A.28]; and 3. *analytic number theory* initiated by Riemann and formulated as a spectral problem by Selberg [A.31, A.32]. Following totally different lines of reasoning and driven by very different motivations, the three separate roads all arrive at formally nearly identical *trace formulas*, *zeta functions* and *spectral determinants*.

That these topics should be related is far from obvious. Connection between dynamics and number theory arises from Selberg’s observation that description of geodesic motion and wave mechanics on spaces of constant negative curvature is essentially a number-theoretic problem. *A posteriori*, one can say that zeta functions arise in both classical and quantum mechanics because in both the dynamical evolution can be described by the action of linear evolution (or transfer) operators on infinite-dimensional vector spaces. The spectra of these operators are given by the zeros of appropriate determinants. One way to evaluate determinants is to expand them in terms of traces, $\log \det = \text{tr} \log$, and in this way the spectrum of an evolution operator becomes related to its traces, i.e., periodic orbits. A perhaps deeper way of restating this is to observe that the trace formulas perform the same service in all of the above problems; they relate the spectrum of lengths (local dynamics) to the spectrum of eigenvalues (global averages), and for nonlinear geometries they play a role analogous to that the Fourier transform plays for the circle.

In Gutzwiller’s words:

“The classical periodic orbits are a crucial stepping stone in the understanding of quantum mechanics, in particular when the classical system is chaotic. This situation is very satisfying when one thinks of Poincaré who emphasized the importance of periodic orbits in classical mechanics, but could not have had any idea of what they could mean for quantum mechanics. The set of energy levels and the set of periodic orbits are complementary to each other since they are essentially related through a Fourier transform. Such

a relation had been found earlier by the mathematicians in the study of the Laplacian operator on Riemannian surfaces with constant negative curvature. This led to Selberg's trace formula in 1956 which has exactly the same form, but happens to be exact. The mathematical proof, however, is based on the high degree of symmetry of these surfaces which can be compared to the sphere, although the negative curvature allows for many more different shapes."

A.2.2 Dynamicist's vision of turbulence

The key theoretical concepts that form the basis of dynamical theories of turbulence are rooted in the work of Poincaré, Hopf, Smale, Ruelle and Gutzwiller. In his 1889 analysis of the three-body problem [1.22] Poincaré introduced the geometric approach to dynamical systems and methods that lie at the core of the theory developed here: qualitative topology of state space flows, Poincaré sections, the key roles played by equilibria, periodic orbits, heteroclinic connections, and their stable/unstable manifolds. Poincaré's work and parallel work by Lyapunov's school in Russia was followed up by steady development of dynamical systems theory through the 20th century.

In a seminal 1948 paper [A.11], Hopf visualized the function space of allowable Navier-Stokes velocity fields as an infinite-dimensional phase space, parameterized by viscosity, boundary conditions and external forces, with instantaneous state of a flow represented by a point in this state space. Laminar flows correspond to equilibrium points, globally stable for sufficiently large viscosity. As the viscosity decreases (as the Reynolds number increases), 'turbulent' states set in, represented by chaotic state space trajectories.

Hopf's observation that viscosity causes a contraction of state space volumes under the action of dynamics led to his key conjecture: that long-term, typically observed solutions of the Navier-Stokes equations lie on finite-dimensional manifolds embedded in the infinite-dimensional state space of allowed states. Hopf's manifold, known today as the 'inertial manifold,' is well-studied in the mathematics of spatio-temporal PDEs. Its finite dimensionality for non-vanishing 'viscosity' parameter has been rigorously established in certain settings by Foias and collaborators [A.39].

Hopf noted "[t]he great mathematical difficulties of these important problems are well known and at present the way to a successful attack on them seems hopelessly barred. There is no doubt, however, that many characteristic features of the hydrodynamical phase flow occur in a much larger class of similar problems governed by non-linear space-time systems. In order to gain insight into the nature of hydrodynamical phase flows we are, at present, forced to find and to treat simplified examples within that class."

Hopf's call for geometric state space analysis of simplified models first came to fulfillment with the influential Lorenz's truncation [2.8] of the Rayleigh-Bénard convection state space (see example 2.2), and was brought a bit closer to true hydrodynamics with the Cornell group's POD models of boundary-layer turbulence [A.19,

A.12]. Further significant progress has proved possible for systems such as the 1-spatial dimension Kuramoto-Sivashinsky flow [A.13, A.14], a paradigmatic model of turbulent dynamics, and one of the most extensively studied spatially extended dynamical systems.

Today, as we hope to have convinced the reader, with modern computation and experimental insights, the way to a successful attack on the full Navier-Stokes problem is no longer "hopelessly barred." We address the challenge in a way Hopf could not divine, employing methodology developed only within the past two decades, explained in depth in this book. Hopf presciently noted that "the geometrical picture of the phase flow is, however, not the most important problem of the theory of turbulence. Of greater importance is the determination of the probability distributions associated with the phase flow". Hopf's call for understanding of probability distributions under phase flow has indeed proven to be a key challenge, the one in which dynamical systems theory has made the greatest progress in the last half century, namely, the Sinai-Ruelle-Bowen ergodic theory of 'natural' or SRB measures for far-from-equilibrium systems [1.27, 1.28, 1.29, 1.32].

The story so far goes like this: in 1960 Edward A. Spiegel was Robert Kraichnan's research associate. Kraichnan told him: "Flow follows a regular solution for a while, then another one, then switches to another one; that's turbulence." It was not too clear, but Kraichnan's vision of turbulence moved Ed. In 1962 Spiegel and Derek Moore investigated a set of 3rd order convection equations which seemed to follow one periodic solution, then another, and continued going from periodic solution to periodic solution. Ed told Derek: "This is turbulence!" and Derek said "This is wonderful!" and was moved. He went to give a lecture at Caltech sometime in 1964 and came back angry as hell. They pilloried him there: "Why is this turbulence?" they kept asking and he could not answer, so he expunged the word 'turbulence' from their 1966 article [A.15] on periodic solutions. In 1970 Spiegel met Kraichnan and told him: "This vision of turbulence of yours has been very useful to me." Kraichnan said: "That wasn't my vision, that was Hopf's vision." What Hopf *actually* said and where he said it remains deeply obscure to this very day. There are papers that lump him together with Landau, as the 'Landau-Hopf's incorrect theory of turbulence,' but he did not seem to propose incommensurate frequencies as building blocks of turbulence, which is what Landau's guess was.

Starting with the introduction of 'cycle expansions' [20.1] in 1988, the classical, mathematically rigorous SRB, and the closely related semiclassical Gutzwiller theory, were refashioned into effective tools for computing long time averages of quantities measured in chaotic dynamics. The idea that chaotic dynamics is built upon unstable periodic orbits first arose in Ruelle's work on hyperbolic systems, with ergodic averages associated with natural invariant measures expressed as weighted summations of the corresponding averages about the infinite set of unstable periodic orbits embedded in the underlying chaotic set. For a long time the convergence of such sums bedeviled the practitioners, until the periodic orbit theory was recast in terms of highly convergent *cycle expansions* [20.2] for which relatively few short periodic orbits led to highly accurate transport rates for classical

systems, and quantal spectra for quantum systems. The idea, in nutshell, is that long orbits are shadowed by shorter orbits, and the n th term in a cycle expansion is the difference between the shorter cycles estimate of the period n -cycles' contribution from the exact n -cycles sum. For hyperbolic, everywhere unstable flows, this difference falls off exponentially or super-exponentially. Implementing the cycle expansions theory, the group of Wintgen soon obtained a surprisingly accurate helium spectrum [A.20] from a small set of shortest cycles, 50 years after failure of the old quantum theory to do so, and 20 years after Gutzwiller first introduced his quantization of chaotic systems.

In 1996 Christiansen *et al.* [A.40] proposed (in what is now the gold standard for an exemplary ChaosBook.org project) that the periodic orbit theory be applied to infinite-dimensional flows, such as the Navier-Stokes, using the Kuramoto-Sivashinsky model as a laboratory for exploring the dynamics close to the onset of spatiotemporal chaos. The main conceptual advance in this initial foray was the demonstration that the high-dimensional (16-64 mode Galérkin truncations) dynamics of this dissipative flow can be reduced to an approximately 1-dimensional Poincaré return map $s \rightarrow f(s)$, by choosing the unstable manifold of the shortest periodic orbit as the intrinsic curvilinear coordinate from which to measure near recurrences. For the first time for any nonlinear PDE, some 1,000 unstable periodic orbits were determined numerically.

What was novel about this work? First, dynamics on a strange attractor embedded in a high-dimensional space was reduced to an *intrinsic* nearly 1-dimensional dynamics, an approximate 1 – *dimensional* map from the segment of the unstable manifold bracketed by the primary turning points onto itself. Second, the solutions found provided both a *qualitative description*, and highly accurate *quantitative predictions* for the given PDE with the given boundary conditions and the given system parameter values.

The 1996 project went as far as one could with methods and computation resources available, until 2002, when new variational methods were introduced [29.15, A.41, 26.12]. Considerably more unstable, higher-dimensional regimes have become accessible [26.14], and the full Navier-Stokes analysis of wall-bounded flows has become feasible [A.42].

A.2.3 Gruppenpest

How many Tylenols should I take with this?... (never took group theory, still need to be convinced that there is any use to this beyond mind-numbing formalizations.)

— Fabian Waleffe, forced to read a version of chapter 9.

If you are not fan of chapter 9 “World in a mirror,” and its elaborations, you are not alone. Or, at least, you were not alone in 1930s. That is when the articles by two young mathematical physicists, Eugene Wigner and Johann von

Neumann [A.23], and Wigner’s 1931 Gruppentheorie [A.24] started *Die Gruppenpest* that plagues us to this very day.

According to John Baez [A.25], the American physicist John Slater, inventor of the ‘Slater determinant,’ is famous for having dismissed groups as unnecessary to physics. He wrote:

“It was at this point that Wigner, Hund, Heitler, and Weyl entered the picture with their ‘Gruppenpest:’ the pest of the group theory [actually, the correct translation is ‘the group plague’] ... The authors of the ‘Gruppenpest’ wrote papers which were incomprehensible to those like me who had not studied group theory... The practical consequences appeared to be negligible, but everyone felt that to be in the mainstream one had to learn about it. I had what I can only describe as a feeling of outrage at the turn which the subject had taken ... it was obvious that a great many other physicists we are disgusted as I had been with the group-theoretical approach to the problem. As I heard later, there were remarks made such as ‘Slater has slain the ‘Gruppenpest’’. I believe that no other piece of work I have done was so universally popular.”

A. John Coleman writes in *Groups and Physics - Dogmatic Opinions of a Senior Citizen* [A.26]: “The mathematical elegance and profundity of Weyl’s book [Theory of Groups and QM] was somewhat traumatic for the English-speaking physics community. In the preface of the second edition in 1930, after a visit to the USA, Weyl wrote, “It has been rumored that the ‘group pest’ is gradually being cut out of quantum physics. This is certainly not true in so far as the rotation and Lorentz groups are concerned; ...” In the autobiography of J. C. Slater, published in 1975, the famous MIT physicist described the “feeling of outrage” he and other physicists felt at the incursion of group theory into physics at the hands of Wigner, Weyl et al. In 1935, when Condon and Shortley published their highly influential treatise on the “Theory of Atomic Spectra”, Slater was widely heralded as having “slain the Gruppenpest”. Pages 10 and 11 of Condon and Shortley’s treatise are fascinating reading in this context. They devote three paragraphs to the role of group theory in their book. First they say, “We manage to get along without it.” This is followed by a lovely anecdote. In 1928 Dirac gave a seminar, at the end of which Weyl protested that Dirac had said he would make no use of group theory but that in fact most of his arguments were applications of group theory. Dirac replied, “I said that I would obtain the results without previous knowledge of group theory!” Mackey, in the article referred to previously, argues that what Slater and Condon and Shortley did was to rename the generators of the Lie algebra of SO(3) as “angular momenta” and create the feeling that what they were doing was physics and not esoteric mathematics.”

From AIP Wigner interview: AIP: “In that circle of people you were working with in Berlin, was there much interest in group theory at this time?” WIGNER: “No. On the opposite. Schrödinger coined the expression, ‘Gruppenpest’ must be abolished.” “It is interesting, and representative of the relations between mathematics and physics, that Wigner’s paper was originally submitted to a Springer physics journal. It was rejected, and Wigner was seeking a physics journal that might take it when von Neumann told him not to worry, he would get it into the Annals of

Mathematics. Wigner was happy to accept his offer [A.27].”

A.3 Death of the Old Quantum Theory

In 1913 Otto Stern and Max Theodor Felix von Laue went up for a walk up the Uetliberg. On the top they sat down and talked about physics. In particular they talked about the new atom model of Bohr. There and then they made the ‘Uetli Schwur.’ If that crazy model of Bohr turned out to be right, then they would leave physics. It did and they didn’t.

— A. Pais, *Inward Bound: of Matter and Forces in the Physical World*

In an afternoon of May 1991 Dieter Wintgen is sitting in his office at the Niels Bohr Institute beaming with the unparalleled glee of a boy who has just committed a major mischief. The starting words of the manuscript he has just penned are

The failure of the Copenhagen School to obtain a reasonable ...

34 years old at the time, Dieter was a scruffy kind of guy, always in sandals and holed out jeans, the German flavor of a 90’s left winger and a mountain climber, working around the clock with his students Gregor and Klaus to complete the work that Bohr himself would have loved to see done back in 1916: a ‘planetary’ calculation of the helium spectrum.

Never mind that the ‘Copenhagen School’ refers not to the old quantum theory, but to something else. The old quantum theory was no theory at all; it was a set of rules bringing some order to a set of phenomena which defied logic of classical theory. The electrons were supposed to describe planetary orbits around the nucleus; their wave aspects were yet to be discovered. The foundations seemed obscure, but Bohr’s answer for the once-ionized helium to hydrogen ratio was correct to five significant figures and hard to ignore. The old quantum theory marched on, until by 1924 it reached an impasse: the helium spectrum and the Zeeman effect were its death knell.

Since the late 1890’s it had been known that the helium spectrum consists of the orthohelium and parahelium lines. In 1915 Bohr suggested that the two kinds of helium lines might be associated with two distinct shapes of orbits (a suggestion that turned out to be wrong). In 1916 he got Kramers to work on the problem, and wrote to Rutherford: “I have used all my spare time in the last months to make a serious attempt to solve the problem of ordinary helium spectrum ... I think really that at last I have a clue to the problem.” To other colleagues he wrote that “the theory was worked out in the fall of 1916” and of having obtained a “partial agreement with the measurements.” Nevertheless, the Bohr-Sommerfeld theory, while by and large successful for hydrogen, was a disaster for neutral helium.

Heroic efforts of the young generation, including Kramers and Heisenberg, were of no avail.

For a while Heisenberg thought that he had the ionization potential for helium, which he had obtained by a simple perturbative scheme. He wrote enthusiastic letters to Sommerfeld and was drawn into a collaboration with Max Born to compute the spectrum of helium using Born’s systematic perturbative scheme. In first approximation, they reproduced the earlier calculations. The next level of corrections turned out to be larger than the computed effect. The concluding paragraph of Max Born’s classic “Vorlesungen über Atommechanik” from 1925 sums it up in a somber tone:

(...) the systematic application of the principles of the quantum theory (...) gives results in agreement with experiment only in those cases where the motion of a single electron is considered; it fails even in the treatment of the motion of the two electrons in the helium atom.

This is not surprising, for the principles used are not really consistent. (...) A complete systematic transformation of the classical mechanics into a discontinuous mechanics is the goal towards which the quantum theory strives.

That year Heisenberg suffered a bout of hay fever, and the old quantum theory was dead. In 1926 he gave the first quantitative explanation of the helium spectrum. He used wave mechanics, electron spin and the Pauli exclusion principle, none of which belonged to the old quantum theory, and planetary orbits of electrons were cast away for nearly half a century.

Why did Pauli and Heisenberg fail with the helium atom? It was not the fault of the old quantum mechanics, but rather it reflected their lack of understanding of the subtleties of classical mechanics. Today we know what they missed in 1913-24: the role of conjugate points (topological indices) along classical trajectories was not accounted for, and they had no idea of the importance of periodic orbits in nonintegrable systems.

Since then the calculation for helium using the methods of the old quantum mechanics has been fixed. Leopold and Percival [A.5] added the topological indices in 1980, and in 1991 Wintgen and collaborators [A.8, A.9] understood the role of periodic orbits. Dieter had good reasons to gloat; while the rest of us were preparing to sharpen our pencils and supercomputers in order to approach the dreaded 3-body problem, they just went ahead and did it. What it took—and much else—is described in this book.

One is also free to ponder what quantum theory would look like today if all this was worked out in 1917. In 1994 Predrag Cvitanović gave a talk in Seattle about helium and cycle expansions to—inter alia—Hans Bethe, who loved it so much that after the talk he pulled Predrag aside and they trotted over to Hans’ secret place: the best lunch on campus (Business School). Predrag asked: “Would quantum mechanics look different if in 1917 Bohr and Kramers *et al.* figured out how to use the helium classical 3-body dynamics to quantize helium?”

Bethe was very annoyed. He responded with an exasperated look - in Bethe Deutschinglish (if you have ever talked to him, you can do the voice over yourself):

“It would not matter at all!”

Commentary

Remark A.1 Notion of global foliations. For each paper cited in dynamical systems literature, there are many results that went into its development. As an example, take the notion of global foliations that we attribute to Smale. As far as we can trace the idea, it goes back to René Thom; local foliations were already used by Hadamard. Smale attended a seminar of Thom in 1958 or 1959. In that seminar Thom was explaining his notion of transversality. One of Thom's disciples introduced Smale to Brazilian mathematician Peixoto. Peixoto (who had learned the results of the Andronov-Pontryagin school from Lefschetz) was the closest Smale had ever come until then to the Andronov-Pontryagin school. It was from Peixoto that Smale learned about structural stability, a notion that got him enthusiastic about dynamical systems, as it blended well with his topological background. It was from discussions with Peixoto that Smale got the problems in dynamical systems that lead him to his 1960 paper on Morse inequalities. The next year Smale published his result on the hyperbolic structure of the non-wandering set. Smale was not the first to consider a hyperbolic point, Poincaré had already done that; but Smale was the first to introduce a global hyperbolic structure. By 1960 Smale was already lecturing on the horseshoe as a structurally stable dynamical system with an infinity of periodic points and promoting his global viewpoint. (R. Mainieri)

Remark A.2 Levels of ergodicity. In the mid 1970's A. Katok and Ya.B. Pesin tried to use geometry to establish positive Lyapunov exponents. A. Katok and J.-M. Strelcyn carried out the program and developed a theory of general dynamical systems with singularities. They studied uniformly hyperbolic systems (as strong as Anosov's), but with sets of singularities. Under iterations a dense set of points hits the singularities. Even more important are the points that never hit the singularity set. In order to establish some control over how they approach the set, one looks at trajectories that approach the set by some given ϵ^n , or faster.

Ya.G. Sinai, L. Bunimovich and N.I. Chernov studied the geometry of billiards in a very detailed way. A. Katok and Ya.B. Pesin's idea was much more robust: look at the discontinuity set, take an ϵ neighborhood around it. Given that the Lebesgue measure is ϵ^n and the stability grows not faster than $(\text{distance})^n$. A. Katok and J.-M. Strelcyn proved that the Lyapunov exponent is non-zero.

In mid 1980's Ya.B. Pesin studied the dissipative case. Now the problem has no invariant Lebesgue measure. Assuming uniform hyperbolicity, with singularities, and tying together Lebesgue measure and discontinuities, and given that the stability grows not faster than $(\text{distance})^n$, Ya.B. Pesin proved that the Lyapunov exponent is non-zero, and that SRB measure exists. He also proved that the Lorenz, Lozi and Byelikh attractors satisfy these conditions.

In the systems that are uniformly hyperbolic, all trouble is in differentials. For the Hénon attractor, already the differentials are nonhyperbolic. The points do not separate uniformly, but the analogue of the singularity set can be obtained by excising the regions that do not separate. Hence there are 3 levels of ergodic systems:

1. Anosov flow

2. Anosov flow + singularity set: For the Hamiltonian systems the general case is studied by A. Katok and J.-M. Strelcyn, and the billiards case by Ya.G. Sinai and L. Bunimovich. The dissipative case is studied by Ya.B. Pesin.
3. Hénon case: The first proof was given by M. Benedicks and L. Carleson [12.27]. A more readable proof is given in M. Benedicks and L.-S. Young [A.21].

(based on Ya.B. Pesin's comments)

Remark A.3 Einstein did it? The first hint that chaos is afoot in quantum mechanics was given in a note by A. Einstein [A.22]. The total discussion is a one sentence remark. Einstein being Einstein, this one sentence has been deemed sufficient to give him the credit for being the pioneer of quantum chaos [A.28, A.29]. We asked about the paper two people from that era, Sir Rudolf Peierls and Abraham Pais; neither had any recollection of the 1917 article. However, Theo Geisel has unearthed a reference that shows that in early 20s Born did have a study group meeting in his house that studied Poincaré's *Mécanique Céleste* [1.22]. In 1954 Fritz Reiche, who had previously followed Einstein as professor of physics in Breslau (now Wrocław, Poland), pointed out to J.B. Keller that Keller's geometrical semiclassical quantization was anticipated by the long forgotten paper by A. Einstein [A.22]. In this way an important paper written by the physicist who at the time was the president of German Physical Society, and the most famous scientist of his time, came to be referred to for the first time by Keller [A.30], 41 years later. But before Ian Percival included the topological phase, and Wintgen and students recycled the Helium atom, knowing *Mécanique Céleste* was not enough to complete Bohr's original program.

Remark A.4 Berry-Keating conjecture. A very appealing proposal in the context of semiclassical quantization is due to M. Berry and J. Keating [A.33]. The idea is to improve cycle expansions by imposing unitarity as a functional equation ansatz. The cycle expansions that they use are the same as the original ones [20.2, 22.1] described above, but the philosophy is quite different; the claim is that the optimal estimate for low eigenvalues of classically chaotic quantum systems is obtained by taking the real part of the cycle expansion of the semiclassical zeta function, cut off at the appropriate cycle length. M. Sieber, G. Tanner and D. Wintgen, and P. Dahlqvist find that their numerical results support this claim; F. Christiansen and P. Cvitanović do not find any evidence in their numerical results. The usual Riemann-Siegel formulas exploit the self-duality of the Riemann and other zeta functions, but there is no evidence of such symmetry for generic Hamiltonian flows. Also from the point of hyperbolic dynamics discussed above, proposal in its current form belongs to the category of crude cycle expansions; the cycles are cut off by a single external criterion, such as the maximal cycle time, with no regard for the topology and the curvature corrections. While the functional equation conjecture is not in its final form yet, it is very intriguing and fruitful research inspiration.

The real life challenge are generic dynamical flows, which fit neither of extreme idealized settings, Smale horseshoe on one end, and the Riemann zeta function on the other.

Remark A.5 Sources. The tale of appendix A.3, aside from a few personal recollections, is in large part lifted from Abraham Pais' accounts of the demise of the old quantum

theory [A.6, A.7], as well as Jammer's account [A.2]. In August 1994 Dieter Wintgen died in a climbing accident in the Swiss Alps.

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