Appendix A1

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. Whitehead’s Law: Everything of importance has been said before by someone who did not discover it.

—Sir Michael V. Berry

Writing a history of anything is a reckless undertaking, especially a history of something that has preoccupied at one time or other any serious thinker from ancient Sumer to today’s Hong Kong. A mathematician, to take an example, might see it this way: “History of dynamical systems.” Nevertheless, here comes yet another very imperfect attempt.

A1.1 Chaos is born

I’ll maybe discuss more about its history when I learn more about it.

—Maciej Zworski

(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.
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 Bruns that showed that there were no conserved quantities that were polynomial in the momenta and positions. Bruns’ result did not preclude the possibility of more complicated conserved quantities. This problem was settled by Poincaré and Sundman in two very different ways [A1.1, A1.2].

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 \(1 - e^{-\lambda}\). 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.

### A1.1.2 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. It is 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 [A1.3]. 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 [A1.4]. 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.

### A1.1.3 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.

### A1.2 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 lead 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 [A1.5], 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 lead to the work of Levinson, which in turn provided the basis for the horseshoe construction of S. Smale.

### A1.3 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” [A1.7]. 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 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.

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 [A1.8]. 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 [A1.9].

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 [A1.10], 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.

### A1.4 Periodic orbit theory

Pure mathematics is a branch of applied mathematics.

— Joe Keller, after being asked to define applied mathematics

(P. Cvitanović)

The history of periodic orbit theory is rich and curious; recent advances are equally inspired by more than a century of developments in three separate subjects: 1. classical chaotic dynamics, initiated by Poincaré and put on its modern footing by Smale [A1.7], Ruelle [A39.14], and many others, 2. quantum theory initiated by Bohr, with the modern ‘chaotic’ formulation by Gutzwiller [A1.12, A1.13], and 3. analytic number theory initiated by Riemann and formulated as a spectral problem by Selberg [A37.2, A1.15]. Following different lines of reasoning and driven by different motivations, the three separate roads all arrive at trace formulas, zeta functions and spectral determinants.

The fact that these fields are all related is far from obvious, and even today the practitioners tend to cite papers only from their sub-speciality. In Gutzwiller’s words [A1.13], “The classical periodic orbits are a crucial stepping stone in the understanding of quantum mechanics, in particular when then 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.” A posteriori, one can say that zeta functions arise in both classical and quantum mechanics because 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, \( \log(\det(L)) = \text{tr}(\log L) \). In this way the spectrum of an evolution operator becomes related to its traces, i.e. periodic orbits. A deeper way of restating this is to observe that the trace formulas perform the same role in all of the above problems; they relate the spectrum of lengths (local dynamics) to the spectrum of eigenvalues (global eigenstates), and for nonlinear geometries they play a role analogous to the one that Fourier transform plays for the circle.

Distant history is easily sanitized and mythologized. As we approach the present, our vision is inevitably more myopic; for very different accounts covering the same recent history, see V. Baladi [A1.14] (a mathematician’s perspective), and M. V. Berry [A1.17] (a quantum chaologist’s perspective). We are grateful for any comments from the reader that would help make what follows fair and balanced.

M. Gutzwiller was the first to demonstrate that chaotic dynamics is built upon unstable periodic orbits in his 1960’s work on the quantization of classical chaotic quantum systems, where the ‘Gutzwiller trace formula’ gives the semiclassical quantum spectrum as a sum over classical periodic orbits [A1.18, A1.19, A1.20, A1.12]. Equally important was D. Ruelle’s 1970’s work on hyperbolic systems, where ergodic averages associated with natural invariant measures are expressed as weighted sums on the infinite set of unstable periodic orbits embedded in the underlying chaotic set [A1.21, A1.22]. This idea can be traced back to the following sources: 1. the foundational 1967 review [A1.7], where S. Smale proposed “as a wild idea in this direction” a (technically incorrect, but prescient) zeta function over periodic orbits, 2. the 1965 Artin-Mazur zeta function for counting periodic orbits [A1.10], and 3. the 1956 Selberg number-theoretic zeta functions for Riemann surfaces of constant curvature [A37.2]. That one could compute using these infinite sets was not clear at all. Ruelle [A39.14] never attempted explicit computations, and Gutzwiller only attempted to implement summations over anisotropic Kepler periodic orbits by treating them as Ising model configurations [A39.17] (In retrospect, Gutzwiller was lucky; it turns out that the more periodic orbits one includes, the worse convergence one gets [A1.24]).

For a long time the convergence of such sums bedeviled the practitioners, until the mathematically rigorous spectral determinants for hyperbolic deterministic flows, and the closely related semiclassically exact Gutzwiller Zeta functions were recast in terms of highly convergent cycle expansions. Under these circumstances, a relatively few short periodic orbits lead to highly accurate long time averages of quantities measured in chaotic dynamics and of spectra for quantum systems. The idea, in a 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 and the exact \( n \)-cycles sum. For unstable, hyperbolic flows, this difference falls off exponentially or super-exponentially [A1.60]. Contrary to what some literature says, cycle expansions are no more clever resummations than the Plemelj-Smithies cumulant evaluation of a determinant is a ‘resummation’, and their theory is considerably more reassuring than what practitioners of quantum chaos fear: there is no ‘abscessa of absolute convergence’, there is no ‘entropy barrier’, and the exponential proliferation of cycles is not the problem.

Cvitanović derived ‘cycle expansions’ in 1986-87, in an effort to prove that the mode-locking dimension for critical circle maps discovered by Jensen, Bak and Bohr [A1.25] is universal; the same kind of periodic orbits are involved in the Hénon map, but now in renormalization ‘time’. The symbolic dynamics of the Hénon attractor (the pruning front conjecture [A1.26]) is coded by transition graphs, topological entropy is given by roots of their determinants. This observation led to the study of convergence of spectral determinants for both discrete-time (iterated maps) and continuous-time deterministic flows (both ODEs and PDEs).

Cycle expansions thus arose not from temporal dynamics, but from studies of scalings in period-doubling and cycle-map renormalizations [A1.27, A1.28, A1.29]. This work was done in collaboration with R. Artuso (PhD 1987-1989), G. Guimarães, and E. Aurell (PhD 1984-1989), and it was written under the watchful eye of parrot Gaspar in Fundaçåo de Facao, Porto Seguro, as two long Recycling of strange sets papers [A1.30, A1.27]: I. Cycle expansions and II. Applications. The main lesson was that one should never split theory and applications into papers numbered I and II, part II, which covers many interesting results, has barely been glanced at by anyone.

The first published paper on these developments was Auerbach et al. [A1.31] Exploring chaotic motion through periodic orbits (submitted March 1987). Here only a ‘level sum’ approximation (23.40),

\[
1 = \sum_{S \in \text{Prim}} t_j e^{\beta E_j}, \quad t_j = e^{-\beta E_j \Lambda_j} , \quad (A1.1)
\]

to the trace formula is presented as an nth order estimate of the leading Perron-Frobenius eigenvalue \( \lambda_0 \), and applied to the Hénon attractor (Eq. (4) of the above paper). (The exact weight of an unstable prime periodic orbit \( p \) for level sum (21.6)) had been conjectured by Kadanoff and Tang [A1.32] in 1984.) Even as it was written, the heuristics of this paper was rendered obsolete by the exact cycle expansions, and yet, mysteriously, this might be one of the most cited periodic orbits papers.

The first attempt to make cycle expansions accessible to every person was condensed into Phys. Rev. Lett. Invariant measurement of strange sets in terms of cycles (submitted March 1988) [A1.33]. However, the two long papers by Artuso et al. [A1.30, A1.27] are a better read.

Several applications of the new methodology are worth mentioning. One was the accurate calculation of the leading dozen eigenvalues of the period-doubling operator [A1.27, A1.28, A1.34]. Another breakthrough was the cycle expansion of deterministic transport coefficients [A1.35, A1.36, A1.37], such as diffusion constants without any probabilistic assumptions. The classical Boltzmann equation for the evolution of 1-particle density is based on Stosszahlansatz, the assumption that velocities of colliding particles are not correlated. In correlated orbit theory all correlations are included in cycle averaging formulas, such as the cycle expansion for a particle diffusing chaotically across a spatially-periodic array.
\[
\gamma = 0.4103348077693464893834613078192 \ldots .
\]
Try to extract this from a direct numerical simulation, or a log-log plot of level sums (A1.1)! Prior to cycle expansions, the best accuracy that Gaspard and Rice achieved by applying Markov approximations to the spectral determinant [A1.40] was 1 significant digit, \( \gamma = 0.45 \).

A 3-disk billiard is exceptionally nice, uniformly hyperbolic repellor. More often than not, good symbolic dynamics for a given flow is either not available, or its grammar is not finite, or the convergence of cycle expansions is affected by non-hyperbolic regions of state space. In those cases truncations such as the stability cutoff of Dahlgqvist and Russberg [A1.46, A1.47] and Dettmann and Morris [A1.48] might be helpful. The idea is to truncate the cycle expansion by only including the shadowing combinations of pseudo-cycles \( \{p_1, p_2, \ldots, p_s\} \) such that \( |\Lambda_{p_1} \cdots \Lambda_{p_s}| \leq \Lambda_{\text{max}} \), with the cutoff \( \Lambda_{\text{max}} \) equal to or smaller than the most unstable \( \Lambda_p \) in the data set.

It is pedagogically easier to motivate sums over periodic orbits by starting with discrete time dynamical systems, but most flows of physical interest are continuous in time. The weighted averages of periodic orbits for continuous time flows were introduced by Bowen, who treated them as Poincaré section suspensions weighted by the ‘time ceiling’ function, and were incorporated into dynamical zeta functions by Parry and Pollicott [A1.49] and Ruelle [A1.50]. For people steeped in quantum mechanics it all looked very unfamiliar, so in 1991 Cvitanović and Eckhardt reformulated spectral determinants for continuous time flows along the lines of Gutzwiller’s derivation of the semi-classical trace formula [A1.51]. As a consequence, quantum mechanicians [A1.17, A1.52, A1.53] tend to cite this paper as the first paper on cycle expansions.

2D billiards are only toys, but quantization of helium is surely not just a game. By implementing cycle expansions in 1991, the group of Dieter Wintgen obtained a surprisingly accurate helium spectrum [A39.11, A1.55] from a small set of its shortest cycles. This happened 50 years after old quantum theory had failed to do so and 20 years after Gutzwiller first introduced his quantization of chaotic systems [A1.12].

The Copenhagen group gave many conference and seminar talks about cycle expansions. In December 1986, Cvitanović presented results on the periodic-orbit description of the topology of Lozi and Hénon attractors and the periodic-orbit computation of associated dynamical averages, at the meeting on “Chaos and Related Nonlinear Phenomena: Where do we go from here?” This meeting was organized by Moshe Shapiro and Itamar Procaccia and held in the kibutz Kiryat Anavim. A great meeting, and Celso Grebogi was in the audience. After the “Where do we go from here?” meeting, the Maryland group wrote a series of papers on unstable periodic orbits, or ‘UPOs’. In the first paper [A1.56], Unstable periodic orbits and the dimensions of multifractal chaotic attractor (submitted September 1987), the focus was on fractal dimensions of chaotic attractors, as was the fashion in the late 1980’s. They prove that the natural measure \( \rho_0 \) of a mixing hyperbolic attractor is given by the limit of a sum over the unstable periodic points \( \mathbf{s} \) of long period \( n \), embedded in a chaotic attractor. Each periodic point is weighted by the inverse of the product of its periodic orbit’s expanding Floquet multipliers \( \Lambda_j \), Eq. (14) in their paper:

\[
\rho_0(\mathbf{M}_S) = \lim_{N \to \infty} \sum_{\mathbf{x}_j \in \mathbf{M}_S} \frac{1}{\prod \Lambda_j}, \quad \mathbf{x}_j \in \mathbf{M}_S.
\] (A1.2)

This is an approximate level sum formula for natural measure, a special case of (A1.1), with leading Perron-Frobenius eigenvalue \( s = 0 \) (no escape), and \( \beta = 0 \) (observable \( = 1 \)). The first paper does cite Auerbach et al. [A1.31], in which the same approximate level sum seems to have been published for the first time. Ever since then, various cyclist teams cite exclusively their own papers and some of the mathematicians of the 1970’s.

So you have now written a paper that uses periodic orbits. What is one to cite? Work by Sinai-Bowen-Ruelle is smarter and more profound than the vast majority of ‘chaos’ publications from the 1980s on. If you are not actually computing anything using periodic orbits and are reluctant to refer to recent contributions, you can safely credit Rueffle [A1.22, A39.14] for deriving the dynamical (or Rueffle) zeta function, and Gutzwiller for formulating semiclassical quantization as a Zeta function over unstable periodic orbits [A1.12, A1.13]. There are no cycle expansions in these papers or in Bowen’s work (see, for example, the description in Scholarpedia.org). If you have computed something using sums weighted by periodic-orbit weights, cite the first paper that introduced them, as well as a useful, continuously updated, hyperlinked and reliable reference has its virtues.

Depending on the context, one should also cite 1) Zoldi and Greenside [A1.57] for being the second to determine unstable periodic orbits (127 of them) for Kuwamoto-Sivasinsky, on a domain larger than what was studied in ref. [A1.79], 2) Lopéz et al. [A1.58] for being the first to determine relative periodic orbits in a spatio-temporal PDE (complex Landau-Ginzburg), and 3) Kazantsev [A1.59] for being the first to determine periodic orbits in a weather model, and for his variational method for finding periodic orbits. We love these authors, but not for their ‘escape-time weighting’.

While derivations of (A1.1) by Kadanoﬀ and Tang 1984 and Auerbach et al. 1987 were heuristic, Grebogi, Ott and Yorke 1987 prove (A1.2) by taking the
n → ∞ limit. In actual computations it would be madness to attempt to take such limit, as longer and longer periodic orbits are exponentially more and more unstable, exponentially growing in number, and non-computable: and the natural measure \( \rho_0 \) is everywhere singular, with support on a fractal set, with its \( n → ∞ \) limit even more impossible to compute. And why would one take this limit? The whole point of cycle expansions is that it is smarter to compute averages without constructing \( \rho_0 \).

Taking a limit to obtain a proof is good mathematics, but in statistical mechanics a partition function is not a limit of anything; it is the full sum of all states. Likewise, its ergodic theory cousin, the spectral determinant is not a long-time limit; it is the exact sum over all periodic orbits. Cycle expansions were introduced in a non-rigorous manner, on purpose [A1.33]: the exposition was meant not to frighten a novice, innocent of Borel measurable \( \alpha \) to \( \Omega \) sets. This was set right in the elegant PhD thesis of H. H Rugh’s in 1992, The correlation spectrum for hyperbolic analytic maps [A1.60], which proves that the zeros of spectral determinants are indeed the Ruelle-Pollicott resonances [A1.61, A1.62, A1.63]. The proof is well within mathematicians’ comfort zone, so they tend to cite Rugh’s paper as the paper on ‘Fredholm determinants’, and, as always, throw in “a sense of Grothendieck” for good measure [A1.16, A1.64], without citing earlier papers on cycle expansions.

If you intend to determine and use periodic orbits, here is the message: Heuristic ‘level sums’ are approximations to the exact trace formulas (that are derived here, in ChaosBook, and Gaspard monograph [A1.65] with no more effort than the geometric approximations), not smart for computations; faster convergence is obtained by utilizing the shadowing that is built into the exact cycle expansions of dynamical zeta functions and spectral determinants. Cycle expansions are not heuristic, in classical deterministic dynamics they are exact expansions in the unstable periodic orbits [A1.33, A1.30, A1.27]; in quantum mechanics and stochastic mechanics they are semi-classically exact. So why would one prefer a limit of a heuristic sum such as (A1.2) to the exact spectral determinant, convergent exact periodic orbits sums, and exact periodic orbits formulas for dynamical averages of observables? It is not even wrong. Perhaps if one is very fond of baker’s maps [A1.66], which, being piecewise linear, have no cycle expansion curvature terms, one does not appreciate the shadowing cancelations built into the spectral determinants and their cycle expansions. That might be the reason why linear thinkers stop at the level sum (A1.2).

A1.5 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, Gutzwiller and Spiegel. In Poincaré’s 1889 analysis of the three-body problem [A1.67], he 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, key roles played by equilibria, periodic orbits, heteroclinic connections, and their stable/unstable manifolds.

In a seminal 1948 paper [2.4], Eberhardt Hopf visualized the function space of allowable Navier-Stokes velocity fields as an infinite-dimensional state 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.

As non-vanishing ‘viscosity’ parameter has been rigorously established in certain settings by Foias and collaborators [A1.69]. 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 probability distributions associated with the phase flow has indeed proven to be a key challenge, one in which dynamical systems theory has made the greatest progress in the last half century. In particular, the Sinai-Ruelle-Bowen ergodic theory of ‘natural’ or SRB measures has played a critical role in understanding dissipative systems with chaotic behavior [A1.14, A1.70, A1.71].

Hopf noted [[the great mathematical difficulties of these important problems are well known and at present the way to a successful attack on them seems hopelessly barred. However, there is no doubt 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 [A1.72] of the Rayleigh-Bénard convection state space. The Proper Orthogonal Decomposition (POD) models of boundary-layer turbulence brought this type of analysis closer to physical hydrodynamics [A1.73, A1.74]. Further significant progress has proved possible for systems such as the 1-spatial dimension Kuramoto-Sivashinsky flow [A1.75, A1.76], which is a paradigmatic model of turbulent dynamics, as well as 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, however, to the best of our knowledge, never suggested that turbulent flow should be analyzed in terms of ‘recurrent flows’, i.e. time-periodic solutions of the defining PDEs. The story so far goes like this: in 1960 Ed 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!” He gave a lecture at Caltech in 1964 and came back very angry. 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 paper [A1.77] 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,’ a proposal to deploy incommensurate frequencies as building blocks of turbulence. This was Landau’s guess and was the only one that could be implemented at the time.

The first paper to advocate a periodic orbit description of turbulent flows is thus the 1966 Spiegel and Moore paper [A1.77, A1.78]. Thirty years later, in 1996 Christiansen et al. [A1.79] proposed (in what is now the gold standard for exemplary ChaosBook.org/projects) 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 Galerkin 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 essentially reduced to 1-dimensional dynamics. Second, the solutions found provided both a qualitative description and highly accurate quantitative predictions for the given PDE with the given boundary conditions and system parameter values.

How is it possible that the theory originally developed for low dimensional dynamical systems can work in the $\infty$-dimensional PDE state spaces? For dissipative flows the number of unstable, expanding directions is often finite and even low-dimensional, perturbations along the $\infty$ of contracting directions heal themselves, and play only a minor role in cycle weights - hence the long-time dynamics is effectively finite dimensional. For a more precise statement, see Ginelli et al. [A1.80].

The 1996 project went as far as one could with methods and computation resources available, until 2002, when new variational methods were introduced [A1.81, A1.82, A1.83]. Considerably more unstable, higher-dimensional regimes have become accessible [A1.84]. Of course, nobody really cares about Kuramoto-Sivashinsky. It is only a model; it was not until the full Navier-Stokes calculations of Eckhardt, Kerswell and collaborators [A1.85, A1.86, A1.87] that the fluid dynamics community started to appreciate that the dynamical (as opposed to statistical) analysis of wall-bounded flows is now feasible [A1.88].

### A1.6 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 chapter 10.

If you are not fan of chapter 10 “Flips, slides and turns,” and its elaborations, you are not alone. Or, at least, you were not alone in the 1930s. That is when the articles by two young mathematical physicists, Eugene Wigner and Johann von Neumann [A1.89], and Wigner’s 1931 Gruppentheorie [A1.90] started Die Gruppenpest that plagues us to this very day.

According to John Baez [A1.91], 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 were 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 [A1.92]: “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 hav-
ing “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 [A1 93].”

A1.7 Death of the Old Quantum Theory

In 1913 Otto Stern and Max Theodor Felix von Lange 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

One afternoon in 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 …

Wintgen was 34 years old at the time, a scruffy kind of guy, always wearing sandals and holey out jeans, the German flavor of a 90’s left winger and mountain climber. He worked around the clock with his students Gregor Tanner and Klaus Richter to complete the work that Bohr himself would have loved to have seen 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 defined 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 in 1917 he 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. To a 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 [A1 94]:

(…) 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. As a result, 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 [A1.95] added the topological indices in 1980, and in 1991 Wintgen and collaborators [A39.11, A1.55] 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 Deutchinglish (if you have ever talked to him, you can do the voice over yourself):

“It would not matter at all!”

Commentary

Remark A1.1 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 A1.2 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 $\epsilon^n$, 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 $\epsilon$ neighborhood around it. Given that the Lebesgue measure is $\epsilon^n$ and the stability grows not faster than (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 (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


*(based on Ya.B. Pesin’s comments)*

**Remark A1.3** Einstein did it. The first hint that chaos is afoot in quantum mechanics was given in a note by A. Einstein [A1.100]. 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 [A1.13, A1.101]. 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 [A1.67]. 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 [A1.100]. 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 [36.3], 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 A1.4** Berry-Keating conjecture. A very appealing proposal in the context of semiclassical quantization is due to M. Berry and J. Keating [A1.102]. 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 described above [A1.30], but the philosophy is quite different; the claim is that the optimal estimate for low eigenvalues of classically chaotic Hamiltonian 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 A1.5** Sources. The tale of appendix A1.7, aside from a few personal recollections, is in large part lifted from Abraham Pais’ accounts of the demise of the old quantum theory [A1.103, A1.104], as well as Jammer’s account [A1.105]. In August 1994 Dieter Wintgen died in a climbing accident in the Swiss Alps.


References


[A1.91] J. Baez, “This Week’s Finds in Mathematical Physics Week 236.”


