Periodic orbit theory in classical and quantum mechanics

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The periodic orbit theory of classical and quantum mechanics of classically chaotic dynamical systems has recently advanced on three fronts: The cycle expansion techniques have made possible new numerical spectra evaluations; Riemann conjecture inspired functional equations have been formulated; and new methods for reducing the numbers of cycles required in cycle expansions have been proposed. However, control of the convergence of classical periodic orbit formulas remains a difficult problem.

This issue of CHAOS focuses on the periodic orbit theory of the classical and quantum mechanics of classically chaotic dynamical systems. The papers collected here were presented in the NORDITA "Physics of Quantum Chaos and Measurement" program, Copenhagen, April–June 1991, and the NATO Advanced Research Workshop "Quantum Chaos—Theory and Experiment," Niels Bohr Institute, 28 May–1 June, 1991. They represent very recent advances on at least three fronts: new, cycle-expansion-based numerical spectra evaluations; Riemann conjecture inspired functional equations; and new proposals for reduction of the numbers of cycles required in cycle expansions. Perhaps the prettiest new application presented here is D. Wintgen, K. Richter, and G. Tanner's cycle expansion evaluation of the helium spectrum; this solves a long-standing problem of quantum mechanics, the very problem which daunted the 1920s old quantum theory and led to the birth of modern quantum mechanics.

The articles in this issue of CHAOS are interrelated to an unusual degree, with some authors advocating bold new conjectures, some providing supporting evidence, and still others already attempting to shoot them down. This fairly reflects the spirit of the workshop; the participants met just as the periodic orbit theory became a straightforward computational tool, with many new provocative numerical results challenging the theory, and, conversely, with new theoretical speculations providing impetus for experimentation, both genuine and numerical. The sense was one of rapid progress, such as when surprisingly simple ideas turn out to work much better than they should—but probably, in a larger perspective, the main contribution of the work presented here will be that it helped clarify the real obstacles that stand in the way of developing a serious theory of chaotic systems.

The history of the periodic orbit theory is rich and curious, and the present advances are, to an 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] and Ruelle[2] (among many others); (2) *quantum theory,* initiated by Bohr, with the "chaotic" formulation by Gutzwiller;[3,4] and (3) analytic *number theory,* initiated by Riemann and formulated as a modern spectral problem by Selberg.[5,6] Following superficially totally different lines of reasoning and driven by very different motivations, they all arrive at formally nearly identical *zeta functions* or *functional determinants.*

That these topics should be related is far from obvious, and this is reflected in the discomfort with which the experts in each of the fields digest the results of their distant colleagues. Connection between dynamics and number theory arises from the 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 = 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 zeta functions 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.

I. VALIDITY OF THE SADDLE-POINT OR SEMICLASSICAL APPROXIMATIONS

In classical mechanics and number theory, the zeta functions are exact. The quantum-mechanical ones, derived by the Gutzwiller approach, are, at best, only the saddle-point approximations to the exact quantum functional determinants, and for quantum mechanics an important conceptual problem arises already at the level of derivation of zeta functions: How accurate are they, and can the periodic orbit theory be systematically improved? Until recently, the eigenvalues calculated from the periodic orbit theory were so inaccurate that there was not much point in investigating corrections to them. The first detailed numerical investigation of the correction terms is undertaken here by A. Wirzba. He finds that for the open two- and three-disk systems patching up the cycle expansions by including creeping (or tunneling) periodic orbits fails to bring cycle expansions significantly closer to the exact quantum mechanics, and whether the theory can be improved without abandoning periodic orbits remains to be

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seen. M. Saraceno and A. Voros investigate differences between the exact and the semiclassical quantum determinants in a clean hyperbolic system and also encounter a variety of puzzles.

II. CYCLE EXPANSIONS

In practice, all the papers presented here take the saddlepoint approximation to quantum mechanics (the Gutzwiller trace formula, possibly improved by including tunneling periodic trajectories, or with a Weyl staircase prefactor) as the starting point. Once that is assumed, what follows is *classical* in the sense that all quantities used in periodic orbit calculations—actions, stabilities, geometrical phases—are classical quantities. The problem is then to understand and control the convergence of classical periodic orbit formulas.

While various periodic orbit formulas might be formally equivalent, practice shows that some are vastly preferable to others. Today, three classes of periodic-orbit formulas are in use:

(1) *Trace formulas:* In classical dynamics, trace formulas hide under a variety of ungracious appellations such as the f-alpha or multifractal formalism; in quantum mechanics, they are known as the Gutzwiller trace formulas. In actual calculations they are hard to use for anything other than the leading eigenvalue estimates.

(2) *Ruelle or dynamical zeta functions*[2] are typically of the form:

$$\frac{1}{\zeta(s)} = \prod_p (1-t_p), \quad t_p = e^{sT_p}|\Lambda_p^{-1}|, \tag{1}$$

where the product is over all prime cycles p, Λ_p is the expanding p-cycle stability eigenvalue, and T_p is the p-cycle period. (1) also yields semiclassical *quantum* resonances, if t_p is the quantum amplitude associated with a given cycle,

$$t_p = (1/\sqrt{\Lambda_p})e^{(i/h)S_p(s) + i\pi m_p},$$

where S_p is the action and m_p is the Maslov index of the p cycle. Combined with cycle expansions, dynamical zeta functions are a powerful tool for determination of classical and quantum mechanical averages.

(3) *Selberg-type zeta functions, Fredholm determinants, or functional determinants* are the natural objects for spectrum calculations, with convergence better than for dynamical zeta functions, but with extra products over (1) type factors, and messier cycle expansions. A typical Selberg-type zeta function is of the form

$$Z(s) = \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{e^{iS_p/\hbar + i\pi m_p}}{\sqrt{|\Lambda_p|\Lambda_p^{-k}}}\right). \tag{2}$$

Most periodic orbit calculations presented employ cycle expansions of such determinants.

Loosely speaking, a *cycle expansion*[7] is a series representation of a zeta function, with products in (1) and (2) expanded as sums over pseudocycles, products of t_p's. The product, as it stands, is really only a shorthand notation for a zeta function—for example, the zeros of the individual factors are *not* the zeros of the zeta function, and convergence of such objects is far from obvious. In the crudest application of a cycle expansion, the practitioner simply throws in all cycles available, and extracts eigenvalues. Surprisingly, it seems that any method, no matter how cockeyed, produces a spectrum of not unreasonable accuracy. This is illustrated here by the numerical results of M. Sieber, G. Tanner and D. Wintgen, F. Christiansen and P. Cvitanović and P. Dahlqvist; popular models are the anisotropic Kepler problem, the x^2y^2 potential, and the hyperbola billiard (billiard whose walls are given by xy = const). We note with pleasure that even patently wrong formulas work up to a point: M. Sieber simply truncates the Selberg product (2) (thus all zeros of the zeta function are in wrong places)—still, by taking the real part, he obtains decent estimates for the low eigenvalues. While M. Sieber's and G. Tanner's calculations seem to support this claim, F. Christiansen finds that such truncations lead to uncontrollable numbers of spurious eigenvalues.

A more serious theory of cycle expansions requires a deeper understanding of their analyticity and convergence. While the classical, the quantum, and the number-theoretical zeta functions are formally very similar, the intuition that they give us about their convergence is very different. The real life challenges are generic dynamical flows, which fit neither schematization. At this time, the two inspiring idealizations and main sources of intuition are the Riemann zeta function, and the classical "axiom A" hyperbolic systems.

III. CONVERGENCE OF CYCLE EXPANSIONS: "AXIOM A" HYPERBOLIC FLOWS

The main conceptual insight of Smale[1] is that, if a flow has a topology of a (Smale) horseshoe, the associated zeta functions have nice analytic structure. In a more formal setting, such flows are called "axiom A," and Ruelle[2] proves that the associated zeta functions are holomorphic and the spectrum is discrete. This situation is very different from what practitioners of quantum chaos are used to: There is no "abscissa of abysmal convergence" and no "entropy wall," the exponential proliferation of cycles causes no problem, the Selberg-type zeta functions are entire and converge everywhere, and the topology dictates the choice of cycles to be used in cycle expansion truncations. The basic observation[7,8] is that the motion in dynamical systems of few degrees of freedom is in this case organized around a few *fundamental* cycles. More precisely, the cycle expansion of the product (1)

$$\frac{1}{\zeta} = 1 - \sum_f t_f - \sum_n c_n \tag{3}$$

allows a regrouping of terms into dominant *fundamental* contributions t_f and decreasing *curvature* corrections c_n. The fundamental cycles t_f have no shorter approximants; they are the "building blocks" of the dynamics in the sense that all longer orbits can be approximately pieced together from them. A typical curvature term in (3) is a *difference* of a long cycle $\{ab\}$ minus its shadowing approximation by shorter cycles $\{a\}$ and $\{b\}$:

$$t_{ab} - t_a t_b = t_{ab}(1 - t_a t_b / t_{ab}).$$

The orbits that follow the same symbolic dynamics, such as $\{ab\}$ and a "pseudoorbit" $\{a\}\{b\}$, lie close to each other, have similar weights, and for longer and longer orbits the curvature corrections are expected to fall off rapidly. Indeed, for systems that satisfy the "axiom A" requirements, such as the open disk billiards, curvature expansions converge very well.[9] D. Wintgen, K. Richter, and G. Tanner very successfully apply the curvature expansions to helium. An original application of the same technique in a classical context is given by R. Mainieri.

Most systems of interest are *not* of the "axiom A" category; they are neither purely hyperbolic nor do they have a simple symbolic dynamics grammar. The importance of symbolic dynamics is grossly unappreciated by people who come from exclusively quantum chaos backgrounds; the crucial ingredient for nice analyticity properties of zeta functions is the existence of a finite grammar (coupled with uniform hyperbolicity). From the hyperbolic dynamics point of view, the Riemann zeta function is perhaps the worst possible example; understanding the symbolic dynamics would amount to being able to give a finite grammar definition of all primes. Hyperbolic dynamics suggests that a generic "chaotic" dynamical system should be approached by a sequence of finite grammar approximations,[8] pretty much as a "generic" number is approached by a sequence of continued fractions. This systematic *pruning* of forbidden orbits requires care and is carried out in only one of the papers; K. T. Hansen explores it in detail for the case of hyperbola billiards. The unhealthy effects of uncontrolled grammar are illustrated by the results of P. Cvitanović, P. Gaspard, and T. Schreiber in the context of classical deterministic diffusion.

Strictly speaking, the proofs of discreteness of the classical spectra have, so far, not been extended to the semiclassical zeta functions. The technical problem is that the proofs require a transfer operator that is multiplicative along the trajectory; composition of quantum evolution operators is not of that type, as the composition requires a further saddle point expansion. However, on the basis of heuristic arguments that work for the classical case and the numerical experience with quantum resonances for repellers, we expect the spectra to be discrete also for the "axiom A" semiclassical zeta functions.

IV. CURE FOR EXPONENTIAL PROLIFERATION?

While the exponential proliferation of cycles does not necessarily worsen the convergence of zeta functions (at least it does not for the cases discussed above), it does present a practical problem—so far, exponential increase in number of cycles is required for a linear increase in number of eigenvalues evaluated. This is unsatisfactory, and E. Bogomolny argues that a small subset of cycles should suffice for good estimates of eigenvalues up to a given cutoff energy. While G. Tanner's calculations seem to support the claim, F. Christiansen's investigation of how nonuniformly the phase space is covered casts serious doubts on it. Even so, the idea is so appealing that it is worth much more trashing.

V. CONVERGENCE OF CYCLE EXPANSIONS: FUNCTIONAL EQUATIONS

While the Riemann and the Selberg zetas might seem remote from physics problems, there is one fact that cannot be ignored: Mathematicians have developed methods for evaluating spectra in these problems that are tens of orders of magnitude more effective than what physicists use in calculating quantum spectra, and there is a great temptation to extend this mathematics to the dynamics that we study. Generally, the problem with such Riemann-zeta inspired approaches is that almost any magic property that underlies this mathematics fails for realistic dynamical zeta functions; all derivations seem to depend very explicitly on underlying integer lattices, their self-duality under Fourier transforms, etc.

A very appealing proposal[11] along these lines is discussed in this issue by J. Keating, E. Bogomolny, and M. Sieber. The idea is to improve the periodic orbit expansions by imposing unitarity as a functional equation ansatz. The cycle expansions used are the same as the original ones,[8,12] 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 at the appropriate cycle length (Berry and Keating[11]). 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, the 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 curvature corrections. While the functional equation conjecture is not yet in its final form, it is very intriguing and worth pursuing.

The dynamical systems that we are *really* interested in—for example, smooth, bounded, Hamiltonian potentials—are presumably never really chaotic,[13,14] and it is still unclear what intuition is more rewarding: Are quantum spectra of chaotic dynamics in smooth, bounded, Hamiltonian potentials more like zeros of Riemann zetas or zeros of dynamical zetas? We do not know at present, and the central question remains: how to attack the problem in a systematic and controllable fashion?

While the work collected in this issue of CHAOS is provocative, a serious improvement of the convergence of periodic orbit formulas still eludes us and seems to require a new idea. We are left with a series of open challenges, such as the following.

(1) **Symbolic dynamics:** Develop optimal sequences ("continued fraction approximants") of finite subshift ap-

proximations to generic dynamical systems. Apply to a periodic orbit evaluation of a spectrum for (a) a billiard and (b) a physically motivated Hamiltonian flow.

(2) **Exponential proliferation:** Resolve n spectral eigenvalues using as input a number of cycles that grow more slowly than exponentially with n.

(3) **Nonhyperbolicity:** Incorporate power-law corrections (marginal stability orbits, "intermittency") into cycle expansions. Apply to long-time tails in a Hamiltonian problem such as the x^2y^2 potential, deterministic diffusion in the Lorentz gas, etc.

(4)**Tunneling:** Add complex time orbits to quantum mechanical cycle expansions (the WKB theory for chaotic systems).

(5) **Unitarity:** Evaluate corrections to the Gutzwiller semiclassical periodic orbit sums, or reformulate the periodic orbit theory in such a way that unitarity is built in, and the zeros (energy eigenvalues)of the appropriate Selberg products are real.

(6) **Symmetries:** Include spin, fermions, gauge fields into the periodic orbit theory.

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