A Fredholm Determinant for Semi-classical Quantization

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We investigate a new type of approximation to quantum determinants, the "quantum Fredholm determinant", and test numerically the conjecture that for Axiom A hyperbolic flows such determinants have a larger domain of analyticity and better convergence than the Gutzwiller-Voros zeta functions derived from the Gutzwiller trace formula. The conjecture is supported by numerical investigations of the 3-disk repeller, a normal-form model of a flow, and a model 2-d map.

I. INTRODUCTION

[*] While various periodic orbit formulas may be formally equivalent, in practice some are vastly preferable to others. Trace formulas, such as the thermodynamic averages in classical dynamics, and the semi-classical Gutzwiller trace formula in quantum mechanics are difficult to use for anything other than the leading eigenvalue estimates. However, dynamical zeta functions [1], Fredholm determinants [2] and the Gutzwiller-Voros zeta function [3,4] have recently been established as powerful tools for evaluation of classical and quantum averages in low dimensional chaotic dynamical systems [5] - [9]. Recent advances include new, cycle expansion [10] based numerical spectra evaluations and Riemann conjecture inspired functional equations. The convergence of cycle expansions of zeta functions and Fredholm determinants depends on their analytic properties; particularly strong results exist for Axiom A hyperbolic systems, for which the dynamical zeta functions are meromorphic [11], and the classical Fredholm determinants are entire functions [12,13]. No such results exist for the determinants used in quantum theory, but formal analogies to the classical case have led to introduction of the *quantum Fredholm determinant* [14]

$$F_{qm}(E) = \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{e^{-\frac{i}{\hbar} S_p(E) + i\pi m_p/2}}{|\Lambda_p|^{1/2} \Lambda_p^k} \right)^{k+1} \qquad (1)$$

as an alternative to the Gutzwiller-Voros zeta function

$$Z_{qm}(E) = \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{e^{-\frac{i}{\hbar} S_p(E) + i\pi m_p/2}}{|\Lambda_p|^{1/2} \Lambda_p^k} \right) . \qquad (2)$$

We present here the numerical evidence in support of the conjecture of ref. [14]:

For Axiom A systems the quantum Fredholm determinant has a larger domain of analyticity than the Gutzwiller-Voros zeta function.

We shall consider here only purely hyperbolic flows with the topology of a Smale horseshoe. The important conceptual insight of Smale [15] is the realization that for such flows the associated zeta functions have nice analytic structure. In a more formal setting, such flows are called "Axiom A", and Ruelle [1] proves that for expanding analytic maps the zeta functions are meromorphic, and the spectrum is discrete. This differs very much from the intuition acquired in studies of quantum chaos; there is no "abscissa of absolute convergence" and no "entropy wall", the exponential proliferation of orbits can be controlled, and the Selberg-type zeta functions are entire and converge everywhere.

In classical mechanics and number theory, the zeta functions and the Fredholm determinants are exact. All quantum mechanical studies take a saddle-point approximation - the Gutzwiller trace formula - as the starting point, and for quantum mechanics an important conceptual problem arises already at the level of derivation of the Gutzwiller-Voros zeta functions; how accurate are they, and can the periodic orbit theory of such semi-classical approximations be systematically improved? We shall not address this problem here; in this paper we are interested in the convergence of cycle expansion truncations of the Gutzwiller-Voros zeta function.

[*] PC: version 16 sept 1993, file chaos.nbi.dk: /users/predrag/tex/articles/q_fredholm/qfred6.tex

The problem is *classical* in the sense that all quantities used in periodic orbit calculations - actions, stabilities, Maslov phases - are classical quantities.

The main limitation of the study presented here is that the Fredholm determinants are proven to be entire only for hyperbolic flows with symbolic dynamics with finite grammar (Axiom A flows). Hence our numerics is restricted to three systems with complete binary grammar and bounded nonlinearity:

(a) the 3-disk repeller
(b) a Hamiltonian Hénon map as a normal form approximation to a flow
(c) a model 2-d hyperbolic mapping

The paper is organized as follows: in sect. II we review the evolution operator formalism for smooth flows. In sect. III we explain the theorems that guarantee that Fredholm determinants for Axiom A systems are entire. In sect. IV we define and motivate the determinants used in this paper. In sect. V we review the cycle expansions, and give convergence estimates for various expansions. In sect. VI we discuss the numerical evidence in support of the quantum Fredholm determinant conjecture.

II. FLOWS, EVOLUTION OPERATORS AND THEIR SPECTRA

Functional determinants and zeta functions arise in classical and quantum mechanics because in both the dynamical evolution can be described by the action of linear evolution operators on infinite-dimensional vector spaces. The classical *evolution operator* for a d-dimensional map or a $(d+1)$-dimensional flow is given by:

$$\mathcal{L}^t(y,x) = \delta(y - f^t(x)) g^t(x) \ . \tag{3}$$

For discrete time, $f^n(x)$ is n-th iterate of the map f; for continuous flows, $f^t(x)$ is the trajectory of the initial point x. $g^t(x)$ is a weight multiplicative along the trajectory; its precise functional form depends on the dynamical average under study. For purposes of this section it suffices to take $g^t(x) = 1$, essentially the Perron-Frobenius operator case.

The global averages (escape rates, energy eigenvalues, resonances, fractal dimensions, etc.) can be extracted from the eigenvalues of the evolution operators. The eigenvalues 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, *ie.* periodic orbits. Formally, the traces $\mathrm{tr}\mathcal{L}^t$ are easily evaluated as integrals of Dirac delta functions as follows:

A. Trace formula for maps

If the evolution is given by a discrete time mapping, and all periodic points are known to have stability eigenvalues $\Lambda_k \neq 1$ strictly bounded away from unity, the trace $\mathcal{L}^n$ is given by the sum over all periodic points x of period n:

$$\begin{aligned} \mathrm{tr}\, \mathcal{L}^n &= \int dx dy \delta(x-y) \mathcal{L}^n(y,x) \\ &= \sum_p n_p \sum_{r=1}^{\infty} \frac{\delta_{n,n_p r}}{|\det \left(\mathbf{1} - \mathbf{J}_p^r\right)|} \ , \end{aligned} \tag{4}$$

where

$$\mathbf{J}_p(x) = \prod_{j=0}^{n_p-1} \mathbf{J}(f^j(x)), \quad J_{kl}(x) = \frac{\partial}{\partial x_l} f_k(x) \tag{5}$$

is the $[d \times d]$ Jacobian matrix evaluated at the periodic point x, and the product goes over all periodic points x_i belonging to a given prime cycle p. The *trace formula* is the Laplace transform of $\mathrm{tr}\, \mathcal{L}^t$ which, for discrete flows, is simply the generating function

$$\mathrm{tr}\, \mathcal{L}(z) = \sum_{n=1}^{\infty} z^n \mathrm{tr}\, \mathcal{L}^n = \sum_{\alpha=0}^{\infty} \frac{z e^{-\nu_\alpha}}{1 - z e^{-\nu_\alpha}}$$

where $e^{-\nu_0}, e^{-\nu_1}, e^{-\nu_2}, \ldots$ are the eigenvalues of $\mathcal{L}$. For large times $\det \left(\mathbf{1} - \mathbf{J}^{(n)}(x_i)\right) \to \Lambda_i$, where Λ_i is the product of the expanding eigenvalues of $\mathbf{J}^{(n)}(x_i)$, so the trace is dominated by

$$\mathrm{tr}\, \mathcal{L}(z) \approx \sum_{n=1}^{\infty} z^n \sum_{x_i \in \mathrm{Fix}(f^n)} \frac{1}{|\Lambda_i|} = \frac{z e^{-\nu_0}}{1 - z e^{-\nu_0}} + \ \ldots \ , \tag{6}$$

and diverges at the leading eigenvalue $1/z = e^{-\nu_0}$. This approximation, which in current physics literature is called the "thermodynamic" or the "f of α" formalism [16], is adequate (but far from optimal) for extraction of the leading eigenvalue of $\mathcal{L}$, and difficult to apply to extraction of the non-leading eigenvalues.

B. Trace formula for flows

For flows the eigenvalue corresponding to the eigenvector along the flow (the velocity vector) necessarily equals unity for all periodic orbits, and therefore the integral (4) requires a more careful treatment [17].

To evaluate the contribution of a prime periodic orbit p of period T_p, one choses a local coordinate system with a longitudinal coordinate $dx_\parallel$ along the direction of the flow, and d transverse coordinates $x_\perp$

$$\mathrm{tr}\,{}_p \mathcal{L}^t = \int_{V_p} dx_\perp dx_\parallel \delta(x_\perp - f_\perp^t(x)) \delta(x_\parallel - f_\parallel^t(x)) \ . \tag{7}$$

Integration is restricted to an infinitesimally thin tube V_p enveloping the cycle p.

Let $v = |\mathbf{F}(x)|$ be the velocity along the orbit, and change the longitudinal variable to $dx_\parallel = v d\tau$. Whenever the time t is a multiple of the cycle period T_p, the integral along the trajectory yields

$$\int_{V_p} dx_\parallel \delta(x_\parallel - f_\parallel^t(x)) = \sum_{r=1}^{\infty} \delta(t - rT_p) \int_p d\tau$$
$$= T_p \sum_{r=1}^{\infty} \delta(t - rT_p) \ . \qquad (8)$$

Linearization of the periodic flow in a plane perpendicular to the orbit yields the same weight as for the maps:

$$\int_{V_p} dx_\perp \delta(x_\perp - f_\perp^{-rT_p}(x)) = \frac{1}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} \ , \qquad (9)$$

where $\mathbf{J}_p$ is the p-cycle $[d\times d]$ transverse Jacobian, and we have assumed hyperbolicity, *ie.* that all transverse eigenvalues are bounded away from unity. A geometrical interpretation of weights such as (9) is that after the r-th return to a surface of section, the initial tube V_p has been stretched out along the expanding eigendirections, with the overlap with the initial volume given by $1/|\det(\mathbf{1} - \mathbf{J}_p^r)|$.

Substituting (8-9) into (7), we obtain an expression for $\mathrm{tr}\, \mathcal{L}^t$ as a sum over all prime cycles p and their repetitions

$$\mathrm{tr}\, \mathcal{L}^t = \sum_p T_p \sum_{r=1}^{\infty} \frac{\delta(t - rT_p)}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} \ .$$

A Laplace transform replaces the above sum of Dirac delta functions by the *trace formula for classical flows* [17]:

$$\mathrm{tr}\, \mathcal{L}(s) = \int_0^\infty dt\, e^{st} \mathrm{tr}\, \mathcal{L}^t = \sum_p T_p \sum_r \frac{e^{sT_p r}}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} \ . \qquad (10)$$

We should caution the reader that in taking the Laplace transform we have ignored a possible $t \to 0_+$ volume term, as we do not know how to regularize the delta function kernel in this limit. In the quantum (or heat kernel) case this limit gives rise to the Weyl or Thomas-Fermi mean eigenvalue spacing. A more careful treatment might assign to such volume term some interesting role in the theory of classical resonance spectra.

The semi-classical evaluation of the quantum trace is considerably more laborious, but the final result, given in sect. IV A, is very similar in form to the above classical trace.

C. Fredholm determinants

The problem with the classical (6), (10) and the Gutzwiller trace formulas (20) is that they diverge precisely where one would like to use them (we return to this in sect. IV F). While in the physics literature on dynamically generated strange sets this does not prevent numerical extraction of reasonable "thermodynamic" averages, in the case of the Gutzwiller trace formula this leads to the perplexing observation that crude estimates of the radius of convergence seem to put the entire physical spectrum out of reach. This problem is cured by going from trace formulas to determinants, which turn out to have larger analyticity domains. For maps, the two are related by

$$F(z) = \det(1 - z\mathcal{L}) = \exp\left(-\sum_n^\infty \frac{z^n}{n} \mathrm{tr}\, \mathcal{L}^n\right)$$

For flows the classical Fredholm determinant is given by

$$F(s) = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{sT_p r}}{|\det(\mathbf{1} - \mathbf{J}_p^r)|}\right) \ , \qquad (11)$$

and the classical trace formula (10) is the logarithmic derivative of the classical Fredholm determinant

$$\mathrm{tr}\, \mathcal{L}(s) = -\frac{d}{ds} \log F(s) \ . \qquad (12)$$

With z set to $z = e^s$, the Fredholm determinant (11) applies both to maps and flows. A Fredholm determinant can be rewritten as an infinite product over periodic orbits, by noting that the r sum in (11) is close in form to expansion of a logarithm. We cast it into such a form by expanding the Jacobian weights in terms of stability eigenvalues. For a 3-dimensional Hamiltonian flow with one expanding eigenvalue Λ, and one contracting eigenvalue $1/\Lambda$, the weight in (11) may be expanded as follows:

$$\frac{1}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} = \frac{1}{|\Lambda|^r (1 - 1/\Lambda_p^r)^2}$$
$$= \frac{1}{|\Lambda|^r} \sum_{k=0}^{\infty} (k+1) \Lambda_p^{-kr} \ . \qquad (13)$$

With this we can rewrite the Fredholm determinant exponent as

$$\sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{sT_p r}}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} = \sum_{k=0}^{\infty} (k+1) \log\left(1 - \frac{e^{sT_p}}{|\Lambda_p| \Lambda_p^k}\right) \ .$$

and represent the Fredholm determinant as a Selberg-type product [17]

$$F(s) = \prod_p \prod_{k=0}^{\infty} \left(1 - t_p/\Lambda_p^k\right)^{k+1} \ ,$$
$$t_p = \frac{e^{sT_p}}{|\Lambda_p|} z^{n_p} \ . \qquad (14)$$

z is a book-keeping variable that we will use to expand zeta functions and determinants, set to $z = 1$ in calculations. In general, t_p depends on the dynamical average one wishes to evaluate; this particular weight is used in evaluation of escape rates and correlation spectra [6,18].

The above heuristic manipulations are potentially dangerous, as we are dealing with infinite-dimensional vector spaces and singular integral kernels; we outline now the ingredients of the proofs that put the above formulas on solid mathematical footing.

III. FREDHOLM DETERMINANTS CAN BE ENTIRE

As the introduction of the quantum Fredholm determinant (1) is motivated by its close analogy with the classical Fredholm determinants, we shall sketch here the basic ideas behind the proofs that the classical Fredholm determinants are entire, without burdening the reader with too many technical details (rigorous treatment is given in refs. [11–13]). The reason why one cares whether a Fredholm determinant is entire or not is that in practice one can extract many more eigenvalues, and to a higher accuracy, from entire Fredholm determinants than from functions which are not entire. The main point of the theorems explained below is that the Fredholm determinants are entire functions in any dimension, provided that

1. the evolution operator is *multiplicative* along the flow,
2. the symbolic dynamics is a *finite subshift*,
3. all cycle eigenvalues are *hyperbolic* (sufficiently bounded away from 1),
4. the map (or the flow) is *real analytic*, *ie.* it has a piecewise analytic continuation to a complex extension of the phase space.

The notion of Axiom A systems is a mathematical abstraction of 2 and 3. It would take us too far to give and explain the definition of the Axiom A systems (see refs. [15,23]). Axiom A implies, however, the existence of a Markov partition of the phase space (see below) from which 2 and 3 follow. Properties 1 and 2 enable us to represent the evolution operator as a matrix in an appropriate basis space; properties 3 and 4 enable us to bound the size of the matrix elements and control the eigenvalues. To see what can go wrong consider the following examples:

Property 1 is violated for flows in 3 or more dimensions by the following weighted evolution operator

$$\mathcal{L}^t(y,x) = |\Lambda^t(x)|^\beta \delta(y - f^t(x)) \, , \tag{15}$$

where $\Lambda^t(x)$ is an eigenvalue of the Jacobian transverse to the flow. While for the Jacobians $J_{ab} = J_a J_b$ for two successive segments a and b along the trajectory, the corresponding eigenvalues are in general *not* multiplicative, $\Lambda_{ab} \neq \Lambda_a \Lambda_b$ (unless a, b are repeats of the same cycle, so $J_a J_b = J^{n_a+n_b}$), so the above evolution operator is not multiplicative along the trajectory. The theorems require that the evolution be represented as a matrix in an appropriate polynomial basis, and thus cannot be applied to non-multiplicative kernels, *ie.* kernels that do not satisfy the semi-group property $\mathcal{L}^{t'}\mathcal{L}^t = \mathcal{L}^{t'+t}$.

Property 2 is violated by the 1-d map

$$f(x) = \alpha(1 \,-\, |1-2x|) \, , \quad 1/2 < \alpha < 1 \, .$$

All cycle eigenvalues are hyperbolic, but the critical point $x_c = \frac{1}{2}$ is in general not a pre-periodic point, there is no finite Markov partition, the symbolic dynamics does not have a finite grammar, and the theorems discussed below do not apply. In practice this means that while the leading eigenvalue of $\mathcal{L}$ might be computable, the reminder of the spectrum is very hard to control; as the parameter a is varied, nonleading zeros of the Fredholm determinant move wildly about.

Property 3 is violated by the map

$$f(x) = \begin{cases} x + 2x^2 & , \quad x \in I_0 = [0, \frac{1}{2}] \\ 2 - 2x & , \quad x \in I_1 = [\frac{1}{2}, 1] \end{cases} \, .$$

Here the interval $[0,1]$ has a Markov partition into the two subintervals I_0 and I_1 on which f is monotone. However, the fixed point at $x = 0$ has stability $\Lambda = 1$, and violates the condition 3. This type of map is called intermittent and necessitates much extra work [19]. The problem is that the dynamics in the neighborhood of a marginal fixed point is very slow, with correlations decaying as power laws rather than exponentially.

The property 4 is required as from a mathematical point of view, the heuristic approach of sect. II faces two major hurdles:

1. The trace (4) is not well defined since the integral kernel is singular.

2. The existence and properties of eigenvalues are by no means clear.

Both problems are related to how one defines the function space on which the evolution operator acts. As in physical applications one studies smooth dynamical observables, we restrict the space to smooth functions, more precisely, the space of functions analytic in a given complex domain and having a continuous extension to the boundary of the domain. In practice “real analytic” means that all expansions are polynomial expansions. In order to illustrate how this works in practice, we first work out a few simple examples.

A. Expanding maps

We start with the trivial example of a repeller with only one expanding linear branch

$$f(x) = \Lambda x \qquad |\Lambda| > 1 \, .$$

The action of the associated evolution operator is

$$\mathcal{L}\phi(y) = \int dx\delta(y-\Lambda x)\phi(x) = \frac{1}{|\Lambda|}\phi(y/\Lambda)\,.$$

From this one immediately identifies eigenfunctions and eigenvalues:

$$\mathcal{L}\, y^n = \frac{1}{|\Lambda|\Lambda^n} y^n\,, \qquad n = 0,1,2,\ldots \tag{16}$$

The ergodic theory, as presented by Sinai [20] and others, tempts one to use a space of either integrable or square integrable functions. For our purposes, this space is too big; had we not insisted on analyticity, non-integer and even complex powers could be used in the construction. In particular, in the space L^1 all $|\Lambda|^{\alpha-1}$ with α complex but $\mathrm{Re}(\alpha) < 1$ would be eigenvalues, *ie.* the eigenvalues would fill out the unit disk. We note that the eigenvalues Λ^{-n-1} fall off exponentially with n, and that the trace of $\mathcal{L}$ is given by

$$\mathrm{tr}\,\mathcal{L} = \frac{1}{|\Lambda|}\sum_{n=0}^{\infty}\Lambda^{-n} = \frac{1}{|\Lambda|(1-\Lambda^{-1})} = \frac{1}{|f'-1|}$$

in agreement with (4). A similar result is easily obtained for powers of $\mathcal{L}$, and for the Fredholm determinant one obtains:

$$\det(1-z\mathcal{L}) = \prod_{k=0}^{\infty}(1-\frac{z}{|\Lambda|\Lambda^k}) = \sum_{k=0}^{\infty} c_k t^k\,,$$

$t = -z/|\Lambda|$, where the coefficients c_k are given explicitly by the Euler formula [21]

$$c_k = \frac{1}{1-\Lambda^{-1}}\,\frac{\Lambda^{-1}}{1-\Lambda^{-2}}\cdots\frac{\Lambda^{-k+1}}{1-\Lambda^{-k}}\quad . \tag{17}$$

The coefficients decay asymptotically *faster* than exponentially, as $\Lambda^{-k(k-1)/2}$. This property ensures that for a repeller consisting of a single repelling point the classical Fredholm determinant is entire in the complex z plane.

While it is not at all obvious that what is true for a single fixed point should also apply to a Cantor set of periodic points, the same asymptotic decay of expansion coefficients is obtained when several expanding branches are involved. Consider a monotone and expanding 1-d map $f(x)$, with $|f'_\epsilon(x)| > 1$ on two non-overlapping intervals

$$f(x) = \begin{cases} f_0(x), & x\in I_0 \\ f_1(x), & x\in I_1 \end{cases}\;. \tag{18}$$

The simplest non–trivial example is a piecewise-linear 2–branch repeller with slopes Λ_0 and Λ_1. By the chain rule $\Lambda_p = \Lambda_0^{n_0}\Lambda_1^{n_1}$, where the cycle p contains n_0 symbols 0 and n_1 symbols 1, so the trace (4) reduces to

$$\begin{aligned}\mathrm{tr}\,\mathcal{L}^n &= \sum_{m=0}^{n}\binom{n}{m}\frac{1}{|1-\Lambda_0^m\Lambda_1^{n-m}|}\\ &= \sum_{k=0}^{\infty}\left(\frac{1}{|\Lambda_0|\Lambda_0^k}+\frac{1}{|\Lambda_1|\Lambda_1^k}\right)^n .\end{aligned}$$

The Fredholm determinant (11) is given by

$$\det(1-z\mathcal{L}) = \prod_{k=0}^{\infty}\left(1-\frac{t_0}{\Lambda_0^k}-\frac{t_1}{\Lambda_1^k}\right)\;,$$

where $t_\epsilon = z/|\Lambda_\epsilon|$. The eigenvalues (compare with (16)) are simply

$$e^{-\nu_k} = \frac{1}{|\Lambda_0|\Lambda_0^k}+\frac{1}{|\Lambda_1|\Lambda_1^k}\;.$$

Asymptotically the spectrum is dominated by the lesser of the two fixed point slopes $\Lambda = \Lambda_0$ (if $|\Lambda_0| < |\Lambda_1|$, otherwise $\Lambda = \Lambda_1$), and the eigenvalues $e^{-\nu_k}$ fall off exponentially as $1/\Lambda^k$, just as in the single fixed-point example above.

The proof that the Fredholm determinant for a general nonlinear 1-d map (18) is entire uses the expansion

$$\det(1-z\mathcal{L}) = \sum_{k\geq 0}(-z)^k\mathrm{tr}\,\left(\wedge^k\mathcal{L}\right)$$

where $\wedge^k\mathcal{L}$ is the k'th exterior power of the operator $\mathcal{L}$. For example,

$$\wedge^2\mathcal{L}(x_1x_2,y_1y_2) = \frac{1}{2!}\left[\begin{array}{cc}\mathcal{L}(x_1,y_1) & \mathcal{L}(x_2,y_1)\\ \mathcal{L}(x_1,y_2) & \mathcal{L}(x_2,y_2)\end{array}\right]$$

so $\mathrm{Tr}\,(\wedge^2\mathcal{L}) = \frac{1}{2!}\left((\mathrm{Tr}\;\mathcal{L})^2 - \mathrm{Tr}\,(\mathcal{L}^2)\right)$. In a suitable polynomial basis $\phi_n(z)$ the operator has an explicit matrix representation

$$(\mathcal{L}\phi)_n(z) = \sum_{m=0}^{\infty}\mathcal{L}_{mn}\phi_m(z)\,.$$

In the single fixed-point example (16), $\phi_n = y^n$, and $\mathcal{L}$ is diagonal, $\mathcal{L}_{nn} = \Lambda^{-n}/|\Lambda|$.

The proof proceeds by employing Cauchy complex contour integrals in order to verify that the traces are indeed given by the heuristic formula (4). Furthermore, from bounds on the elements $\mathcal{L}_{mn}$ one calculates bounds on $\mathrm{tr}\,\left(\wedge^k\mathcal{L}\right)$ and verifies [11–13] that they again fall off as $\Lambda^{-k^2/2}$, concluding that the $\mathcal{L}$ eigenvalues fall off exponentially for a general Axiom A 1-d map. The simplest example of how the Cauchy formula is employed is provided by a nonlinear inverse map $\psi = f^{-1}$, $s = \mathrm{sgn}(\psi')$

$$\mathcal{L}\phi(w) = \int dx\;\delta(w-f(x))\phi(x) = s\;\psi'(w)\;\phi(\psi(w))\,.$$

Assume that ψ is a contraction of the unit disk, i.e.

$$|\psi(w)| < \theta < 1 \quad\text{and}\quad |\psi'(w)| < C < \infty \quad\text{for}\quad |w| < 1\,,$$

and expand ϕ in a polynomial basis by means of the Cauchy formula

$$\phi(z) = \sum_{n\geq 0} z^n \phi_n = \oint \frac{dw}{2\pi i}\,\frac{\phi(w)}{w-z}\,, \quad \phi_n = \oint \frac{dw}{2\pi i}\,\frac{\phi(w)}{w^{n+1}}\,.$$

In this basis, $\mathcal{L}$ is a represented by the matrix

$$\mathcal{L}\phi(w) = \sum_{m,n} w^m L_{mn}\phi_n\,, \quad L_{mn} = \oint \frac{dw}{2\pi i}\,\frac{s\,\psi'(w)(\psi(w))^n}{w^{m+1}}$$

Taking the trace and summing we get:

$$\mathrm{Tr}\ \mathcal{L} = \sum_{n\geq 0} L_{nn} = \oint \frac{dw}{2\pi i}\,\frac{s\,\psi'(w)}{w-\psi(w)}$$

This integral has but one simple pole at the unique fix point $w^* = \psi(w^*) = f(w^*)$. Hence

$$\mathrm{Tr}\ \mathcal{L} = \frac{s\,\psi'(w^*)}{1-\psi'(w^*)} = \frac{1}{|f'(w^*)-1|}$$

The requirement that map be analytic is needed to guarantee the inequality

$$|L_{mn}| \leq \sup_{|w|\leq 1} |\psi'(w)|\ |\psi(w)|^n \leq C\theta^n$$

which shows that finite $[N\times N]$ matrix truncations approximate the operator within an error exponentially small in N.

We note in passing that for 1-d repellers a diagonalization of an explicit truncated $\mathcal{L}_{mn}$ matrix yields many more eigenvalues than the cycle expansions [8,13]. The reasons why one persists anyway in using the periodic orbit theory are partially aestethic, and partially pragmatic. Explicit $\mathcal{L}_{mn}$ demands explicit choice of a basis and is thus non-invariant, in contrast to cycle expansions which utilize only the invariant information about the flow. In addition, we do not know how to construct $\mathcal{L}_{mn}$ for a realistic flow, such as the 3-disk problem, while the periodic orbit formulas are general and straightforward to apply.

It is a relatively simple task to generalize the above arguments to an expanding d-dimensional dynamical system $f : M \to M$ with the Markov property (for a more precise definition see ref. [11]):

Markov property: One demands that M can be divided into S subsets $\{I_0, I_1, \ldots, I_{S-1}\}$ such that either $fI_i \cap I_j = \emptyset$ or $I_j \subset fI_i$. The transition matrix takes values $t_{ij} = 0$ or 1, accordingly.

Expansion property: Each inverse $\psi_{ij} : I_j \to I_i$ (defined when $t_{ij} = 1$) is unique and a contraction.

Depending on the smoothness of the functions ψ_{ij} and the function space considered, as well as how one defines the contraction, one obtains stronger or weaker results on the spectrum of eigenvalues. We shall restrict ourselves to the space of analytic functions, and assume that there exists a set of complex neighborhoods $D_i \supset I_i$ such that $\psi_{ij} : \mathrm{Cl}(D_j) \to \mathrm{Int}(D_i)$. Mapping *closures* of domains into *interiors* is a useful way of stating the contraction property. The result is [11,12,22,13] that the expansion coefficients C_k fall off as $1/\Lambda^{k^{1+1/d}}$, and the eigenvalues as $1/\Lambda^{k^{1/d}}$. Again, the results can be proved using a multinomial basis on each domain and deducing from this an explicit matrix representation for the operator.

B. Hyperbolic maps

Theorem [Rugh 1992]: *The Fredholm determinant for hyperbolic analytic maps is entire.*

The proof, apart from the Markov property which is the same as for the purely expanding case, relies heavily on analyticity of the map in the explicit construction of the function space and its basis. The basic idea of the proof is to view the hyperbolicity as a cross product of a contracting map in the forward time and another contracting map in the backward time. In this case the Markov property introduced above has to be elaborated a bit. Instead of dividing the phase space into intervals, one divides it into rectangles. The rectangles should be viewed as a direct product of intervals (say horizontal and vertical), such that the forward map is contracting in, for example, the horizontal direction, while the inverse map is contracting in the vertical direction. For Axiom A systems the natural coordinate axes are given by the stable/unstable manifolds of the map. With the phase space divided into S rectangles $\{R_0, R_1, \ldots, R_{S-1}\}$, $R_i = I_i^h \times I_i^v$ with complex extension $D_i^h \times D_i^v$, the hyperbolicity condition (which at the same time guarantees the Markov property) can be formulated as follows:

Analytic hyperbolic property: Either $fR_i \cap \mathrm{Int}(R_j) = \emptyset$, or for each pair $w_h \in \mathrm{Cl}(D_i^h)$, $z_v \in \mathrm{Cl}(D_j^v)$ there exist unique analytic functions of w_h, z_v: $w_v = w_v(w_h, z_v) \in \mathrm{Int}(D_i^v)$, $z_h = z_h(w_h, z_v) \in \mathrm{Int}(D_j^h)$, such that $f(w_h, w_v) = (z_h, z_v)$. Furthermore, if $w_h \in I_i^h$ and $z_v \in I_j^v$, then $w_v \in I_i^v$ and $z_h \in I_j^h$. (See fig. 1).

What this means is that it is possible to replace coordinates z_h, z_v at time n by the contracting pair z_h, w_v, where w_v is the contracting coordinate at time $n+1$ for the inverse map. Specifying the closure/interior of the sets is a convenient way of defining hyperbolicity.

A map f satisfying the above condition is called analytic hyperbolic and the theorem states that the associated Fredholm determinant is entire, and that the trace formula (4) (derived heuristically in ref. [5]) is correct. We refer the reader to ref. [13] for the details of the proof. The theorem applies also to hyperbolic analytic maps in d dimensions and smooth hyperbolic analytic flows in

$(d+1)$ dimensions, provided that the flow can be reduced to a map by suspension on a Poincaré section complemented by an analytic "ceiling" function [23] which accounts for a variation in the section return times. For example, if we take as the ceiling function $g(x) = e^{sT(x)}$, where $T(x)$ is the time of the next Poincaré section for a trajectory staring at x, we reproduce the flow Fredholm determinant (14).

Examples of analytic hyperbolic maps are provided by small analytic perturbations of the cat map (where the Markov partitioning is non-trivial [24]), the 3-disk repeller, and the 2-d baker's map, the last two examples to be discussed further below.

The proofs of discreteness of the classical spectra have so far not been extended to the semi-classical Gutzwiller-Voros zeta functions, with exception of the spaces of constant negative curvature [28]. The technical problem is that the proofs require an evolution operator that is multiplicative along the trajectory; composition of the semi-classical Green's functions is not of that type, as every composition of successive semi-classical paths requires a further saddle-point approximation (see sect. IV A).

IV. CLASSICAL AND QUANTUM DETERMINANTS

Though the only objective of this paper is to compare the convergence of the semi-classical determinants (1) and (2), theoretical motivation demands a plethora of related zeta functions and determinants. In this section we introduce and define the additional determinants and zeta functions that will be required in what follows.

A. The Gutzwiller-Voros zeta function

The semi-classical periodic orbit theory for hyperbolic flows was developed by Gutzwiller in terms of traces of Van Vleck semi-classical Green's functions [3], and subsequently re-expressed in terms of determinants by Voros [4]. In contrast to the sharp delta-function kernel for the classical evolution, the *quantum evolution operator* is the smeared-out Green's function kernel

$$G(q'', q'; t) \tag{19}$$

defined only on half of the phase space (typically either the spatial coordinates q, or the momentum coordinates p). The Gutzwiller trace formula follows by replacing the quantum Green's function by the semi-classical Van Vleck propagator $K_c(q'', q'; t)$, and evaluating the trace $\mathrm{tr}\, K_c(q'', q'; t)$ by saddle-point methods. The result is a periodic orbit formula of topologically the same structure as the classical trace (10), but with different weights: the semi-classical *Gutzwiller trace formula* [3]:

$$\mathrm{tr}\, G(E) = \overline{g}(E) + \frac{1}{i\hbar} \sum_p T_p \sum_r^{\infty} \frac{e^{-\frac{i}{\hbar} S_p(E) r + i\pi \frac{m_p}{2} r}}{|\det\left(\mathbf{1} - \mathbf{J}_p^r\right)|^{\frac{1}{2}}} \ . \tag{20}$$

Here T_p is the p-cycle period, S_p its action, m_p the Maslov index, and $\mathbf{J}_p$ is the transverse Jacobian of the flow. As in many applications the wave number k is a more natural choice of variable than the energy E, we shall henceforth replace $E \to k$ in all semi-classical formulas.

For 2-d flows the Gutzwiller trace formula is of the form (see (13))

$$\mathrm{tr}\, G(k) = \overline{g}(k) + \frac{1}{i\hbar} \sum_p T_p \sum_r^{\infty} \frac{e^{-\frac{i}{\hbar} S_p(k) r + i\pi m_p r/2}}{|\Lambda_p^r|^{1/2}\left(1 - 1/\Lambda_p^r\right)} \ . \tag{21}$$

and the corresponding determinant (12) is the 2-d *Gutzwiller-Voros zeta function*

$$Z_{qm}(k) = \exp\left(-\sum_p \sum_r^{\infty} \frac{1}{r} \frac{t_p^r}{\left(1 - 1/\Lambda_p^r\right)}\right) \ ,$$
$$t_p = z^{n_p} \frac{e^{-\frac{i}{\hbar} S_p + i\pi m_p/2}}{\sqrt{|\Lambda_p|}} \ . \tag{22}$$

z is a book-keeping variable that keeps track of the topological cycle length n_p, used to expand zeta functions and determinants (see sect. V). Unlike the classical Fredholm determinant, which is exact, the Gutzwiller-Voros zeta function is the leading term of a semi-classical approximation, and the size of corrections to it remain unknown [25].

The Gutzwiller trace formula, apart from the quantum and Maslov phases, differs from the classical trace formula in two aspects. One is the volume term $\overline{g}(E)$ in (20) which is a missing from our version of the classical trace formula. While an overall pre-factor does not affect the location of zeros of the determinants, it might play a role in relations such as functional equations for zeta functions. The other difference is that the quantum kernel leads to a square root of the cycle Jacobian determinant, a reflection of the relation probability = (amplitude)^2. The $1/\sqrt{\det(1 - \mathbf{J}_p)}$ weight leads in turn to the product representation (2)

$$Z_{qm}(k) = \prod_p \prod_{k=0}^{\infty} \left(1 - t_p/\Lambda_p^k\right) \ , \tag{23}$$

which differs from the classical Fredholm determinant (14) by missing exponent $k+1$.

B. The quantum Fredholm determinant

The conjecture tested in this paper asserts that one may replace the Gutzwiller-Voros zeta function (23) by the *quantum Fredholm determinant* (1), *ie.* the Fredholm determinant (14) with the *quantum* weights t_p, without disturbing the leading semi-classical eigenvalues, but improving the convergence of cycle expansions used in evaluating the spectrum, and revealing a part of the spectra inaccessible to the Gutzwiller-Voros zeta function (see sect. VI A for an example).

The form of the quantum weight (22) suggests that the quantum evolution operator should be approximated by a classical evolution operator with a quantum weight:

$$\mathcal{L}^t(y,x) = \delta(y - f^t(x))\sqrt{|\Lambda^t(x)|}e^{-\frac{i}{\hbar}S^t(x)+i\pi m_p(x)/2} \,.$$

As explained in sect. III, this operator is not multiplicative along the trajectory, and consequently does not satisfy the assumptions required by the theorems that guarantee that a Fredholm determinant is entire. Nevertheless, our numerical results support the conjecture that the $|\Lambda|^{1/2}$ weighted determinant has a larger domain of analyticity than the commonly used Gutzwiller-Voros zeta function and that some related determinant might even be entire.

C. The dynamical zeta function

The Ruelle or the dynamical zeta function [1] are defined by

$$1/\zeta = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} t_p^r\right) \,, \tag{24}$$

and have the Euler product representation

$$1/\zeta = \prod_p (1 - t_p) \,, \tag{25}$$

where the product is over all prime cycles p, and the cycle weight t_p depends on the average computed; the simplest example is the weight (14) used in computation of escape rates and correlation spectra. (25) also yields the leading semi–classical *quantum* resonances, if t_p is the quantum weight (22) associated with the cycle p.

Historical antecedents of the dynamical zeta function are the fixed-point counting functions introduced by Artin-Mazur and Smale [15], and the determinants of transfer operators of statistical mechanics [20]. While $1/\zeta$ is the natural object in these applications, in dynamical systems theory dynamical zeta functions arise naturally only for piecewise linear mappings; for smooth flows the natural object for study of classical and quantal spectra are the determinants introduced above. However, dynamical zeta functions will here be useful objects in relating various determinants and explaining the geometrical meaning of curvature expansions.

D. Weighted Fredholm determinants

The theorems of sect. III apply not only to the evolution operator (3), but also to more general evolution operators multiplicative along the flow. In particular, transport of k-forms transverse to the flow is given by the exterior products of the Jacobian (5) of the flow

$$\mathcal{L}^t_{(k)}(y,x) = \delta(y - f^t(x)) \cdot \wedge^k \mathbf{J} \,. \tag{26}$$

In d dimensions (transverse to the flow), the non-vanishing exterior powers are $\mathbf{J}$, $\wedge^1\mathbf{J}$, $\wedge^2\mathbf{J}$, …, $\wedge^d\mathbf{J}$. The $k = 0$ case describes the scalar density transport (3); $k = 1$ describes vector transport (utilized in evaluation of strange set stabilities [5,26,8] and fast dynamo rates [27]); $k = 2$ describes $dx \wedge dy$ area transport, and so on. $\mathcal{L}^t_{(k)}$ is a $[d^k \times d^k]$ matrix; for example, in the explicit index notation $\wedge^2\mathbf{J}$ is given by the antisymmetric exterior product

$$(\wedge^2\mathbf{J})_{ac,bd} = \frac{1}{2}\left(\delta^e_a\delta^f_c - \delta^f_a\delta^e_c\right) J_{eb}J_{fd} \,.$$

As $\left(\wedge^k\mathbf{A}\right)\left(\wedge^k\mathbf{B}\right) = \wedge^k\mathbf{AB}$, $\mathcal{L}^t_{(k)}$ are multiplicative operators along the flow, so if $\det(1-\mathcal{L})$ is entire, $\det(1-\mathcal{L}_{(k)})$ are also entire. The trace formula for $\mathcal{L}_{(k)}$ is

$$\mathrm{tr}\,\mathcal{L}_{(k)}(s) = \sum_p T_p \sum_r^{\infty} \frac{\mathrm{tr}\,\left(\wedge^k\mathbf{J}^r_p\right) e^{sT_p r}}{|\det\left(\mathbf{1} - \mathbf{J}^r_p\right)|} \,, \tag{27}$$

where $\mathrm{tr}\,\mathbf{J} = \Lambda_1 + \Lambda_2 + \ldots + \Lambda_d$, $\mathrm{tr}\,\wedge^2\mathbf{J} = \Lambda_1\Lambda_2 + \Lambda_1\Lambda_3 + \ldots + \Lambda_{d-1}\Lambda_d$, and so on. The corresponding Fredholm determinants are:

1-d case:

$$\det(1 - \mathcal{L}_{(1)}) = \prod_p \prod_{k=0}^{\infty} \left(1 - t_p/\Lambda_p^{k-1}\right) \,,$$

2-d Hamiltonian case:

$$\det(1 - \mathcal{L}_{(1)}) = \prod_p \prod_{k=0}^{\infty} \left(1 - \frac{t_p}{\Lambda_p^{k-1}}\right)^{k+1} \left(1 - \frac{t_p}{\Lambda_p^{k+1}}\right)^{k+1}$$

$$\det(1 - \mathcal{L}_{(2)}) = \prod_p \prod_{k=0}^{\infty} \left(1 - t_p/\Lambda_p^k\right)^{k+1} = \det(1 - \mathcal{L}) \,,$$

where we have used the Hamiltonian volume conservation in $\mathrm{tr}\ \wedge^2\mathbf{J}_p = \Lambda_p \cdot 1/\Lambda_p = 1$.

In order to discuss relations between various determinants and zeta functions, it is convenient to also define following weighted dynamical zeta functions:

$$1/\zeta_k = \prod_p (1 - t_p/\Lambda_p^k) = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{t_p^r}{\Lambda_p^{kr}}\right) \,, \tag{28}$$

and weighted Fredholm determinants

$$F_k = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(t_p/\Lambda_p^k)^r}{(1 - 1/\Lambda_p^r)^2}\right) \,. \tag{29}$$

($F_0 = F$). For 2-dimensional Hamiltonian flows the classical Fredholm determinant (14) can be written as

$$F = \prod_{k=0}^{\infty} 1/\zeta_k^{k+1} \ . \tag{30}$$

F_k can be interpreted as the Fredholm determinant $\det(1-\mathcal{L}_k)$ of the weighted evolution operator

$$\mathcal{L}_k^t(y,x) = \frac{g^t(x)}{\Lambda^t(x)^k}\delta(y - f^t(x)) \ ,$$

where $\Lambda^t(x)$ is the expanding eigenvalue of the Jacobian transverse to the flow, and $g^t(x)$ is any analytic weight function multiplicative along the trajectory. As discussed in sect. III, there is no guarantee that $\det(1-\mathcal{L}_k)$, the Fredholm determinant for this operator, should be entire for $k \neq 0$.

E. Relations between determinants and zeta functions

Ruelle [11] has observed that the elementary identity for d-dimensional matrices

$$1 = \frac{1}{\det(1-\mathbf{J})}\sum_{k=0}^{d}(-1)^k \mathrm{tr}\left(\wedge^k \mathbf{J}\right) \ ,$$

inserted into the exponential representation (24) of the dynamical zeta function, relates the dynamical zeta function to weighted Fredholm determinants. In one dimension this identity

$$1 = \frac{1}{(1-1/\Lambda)} - \frac{1}{\Lambda}\frac{1}{(1-1/\Lambda)}$$

expresses the dynamical zeta function as a ratio of two Fredholm determinants

$$1/\zeta = \frac{\det(1-\mathcal{L})}{\det(1-\mathcal{L}_{(1)})} \tag{31}$$

and shows that $1/\zeta$ is meromorphic, with poles given by the zeros of $\det(1-\mathcal{L}_{(1)})$. In refs. [6,26] heuristic arguments were developed for 1-dimensional mappings to explain how the poles of individual $1/\zeta_k$ cancel against the zeros of $1/\zeta_{k+1}$, and thus conspire to make the corresponding Fredholm determinants entire. Numerical checks verify both the heuristic arguments, and the formula (31).

For 2-dimensional Hamiltonian flows this yields

$$1/\zeta = \frac{\det(1-\mathcal{L})\det(1-\mathcal{L}_{(2)})}{\det(1-\mathcal{L}_{(1)})} = \frac{F^2}{F_1 F_{-1}}$$

This establishes that $1/\zeta$ is meromorphic in 2-d as well, but the relation is not particularly useful for our purposes. Instead we insert the identity

$$1 = \frac{1}{(1-1/\Lambda)^2} - \frac{2}{\Lambda}\frac{1}{(1-1/\Lambda)^2} + \frac{1}{\Lambda^2}\frac{1}{(1-1/\Lambda)^2}$$

into the exponential representation (28) of $1/\zeta_k$, and obtain

$$1/\zeta_k = \frac{F_k F_{k+2}}{F_{k+1}^2} \ . \tag{32}$$

Even though we have no guarantee that F_k are entire, we do know (by arguments explained in the next section) that the upper bound on the leading zeros of F_{k+1} lies strictly below the leading zeros of F_k, and therefore we expect that for 2-dimensional Hamiltonian flows the dynamical zeta function $1/\zeta_k$ has generically a *double* leading pole coinciding with the leading zero of the F_{k+1} Fredholm determinant. This might fail if the poles and leading eigenvalues come in wrong order, but we have not encountered such situation in our numerical investigations. This result can also be stated as follows: the theorem that establishes that the classical Fredholm determinant (30) is entire, implies that the poles in $1/\zeta_k$ must have right multiplicities in order that they be cancelled in the $F = \prod 1/\zeta_k^{k+1}$ product.

Both the quantum Fredholm determinant and the quantum zeta function yield the same leading zeros, given by $1/\zeta_0$. They differ in non-leading zeros (zeros with larger imaginary part of the complex energy), but as the Gutzwiller-Voros zeta function (23) is only the leading term of a semi-classical approximation, with the size of corrections unknown, the physical significance of these non-leading zeros remains unclear.

F. Abscissa of absolute convergence

Consider the "thermodynamic" approximation (6) in the case of the Gutzwiller trace formula (21):

$$\mathrm{tr}\, G(k) \approx \sum_p T_p \sum_r^{\infty} \frac{e^{-\frac{i}{\hbar}S_p(k)r + i\pi m_p r/2}}{|\Lambda_p^r|^{1/2}} \ .$$

This approximation omits the non-leading $\approx 1/\Lambda_p$ terms that vanish in the $t \to \infty$ limit and do not affect the leading eigenvalues. If the phases conspire to partially cancel contributing terms, the sum diverges for a larger value of $\mathrm{Im}(k)$. The abscissa of absolute convergence in the complex k plane is obtained by maximizing the sum, *ie.* replacing all terms by their absolute values:

$$\mathrm{tr}\, G(k) \approx \sum_p T_p \sum_r^{\infty} \frac{e^{T_p \mathrm{Im}(k) r}}{|\Lambda_p^r|^{1/2}} \ .$$

(we have for simplicity taken S_p to be the action for billiards, $S_p/\hbar = T_p k$). Value of $\mathrm{Im}(k)$ for which this sum diverges determines the abscissa of absolute convergence. In the case of the Gutzwiller trace formula (21) this leads to the disappointing result that all eigenvalues of interest are outside the domain of convergence. However, for determinants and zeta functions the eigenvalues are given by locations of the zeros, and the analyticity domain is larger. We can also use determinants to accurately estimate this abscissa of absolute convergence, by replacing all cycle weights t_p in (14) by their absolute values.

To evaluate the abscissa of absolute convergence of the Gutzwiller-Voros zeta function we first note that inserting the identity $1 = (1-1/\Lambda_p^r)/(1-1/\Lambda_p^r)$ into the exponent of Gutzwiller-Voros zeta function (22), one obtains the following relation between the Gutzwiller-Voros zeta function and the quantum Fredholm determinant:

$$Z_{qm}(k) = \frac{F_{qm}(k)}{F_{\frac{1}{2}}(k)} ,$$

where

$$F_{\frac{1}{2}}(k) = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{t_p^r}{\Lambda_p^r (1-1/\Lambda_p^r)^2} \right) . \qquad (33)$$

The radius of convergence of $Z_{qm}(k)$ is therefore determined by the leading zeros of $F_{\frac{1}{2}}(k)$. To estimate the upper bound on $\mathrm{Im}(k)$ for the zeros of $F_{\frac{1}{2}}$, we omit all signs and phases in the weights in $F_{\frac{1}{2}}$:

$$\hat{F}_{\frac{1}{2}}(k) = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{|t_p^r|}{|\Lambda_p^r|(1-1/\Lambda_p^r)^2} \right) , \qquad (34)$$

and compute its leading zero at $\mathrm{Re}(k) = 0$. An example is given in sect. VI A.

G. The Gutzwiller-Voros zeta function puzzle: a classical determinant?

On the basis of close analogy between the classical and the quantum zeta functions, it has been hoped [9] that for Axiom A systems the Gutzwiller-Voros zeta functions (23) should also be entire. This hope was dashed by Eckhardt and Russberg [31] who have established by numerical studies that the Gutzwiller-Voros zeta functions for the 3-disk repeller have poles. They find numerically that in the Gutzwiller-Voros zeta function (23) product representation $1/\zeta_0$ has a double pole coinciding with the leading zero of $1/\zeta_1$. Consequently $1/\zeta_0$, $1/\zeta_0\zeta_1$ and Z_{qm} all have the same leading pole, and coefficients in their cycle expansions fall off exponentially with the same slope. Our numerical tests on the 3-disk system (see sect. VI A) support this conclusion.

Why should $1/\zeta_0$ have a *double* leading pole? The double pole is not as surprising as it might seem at the first glance; indeed, for the classical Fredholm determinant (14) $1/\zeta_0$ must have a double pole in order to cancel the leading double zero of the $(1/\zeta_1)^2$ factor. In other words, the numerics indicates that the semi-classical determinants and zeta functions have analyticity properties characteristic of *classical* determinants. As *a priori* any determinant or zeta function which yields the same *leading* semi-classical resonances is equally good, one is lead to pose the conjecture tested in this paper: quantum Fredholm determinants are preferable to Gutzwiller-Voros zeta functions, as they yield the same leading spectrum, but with better analyticity properties.

As we have no proof, we resort to numerical tests of the conjecture; but first we need to briefly explain how such determinants are investigated numerically.

V. CYCLE EXPANSIONS

A *cycle expansion* [10] is a series representation of a zeta function or a Fredholm determinant, expanded as a sum over *pseudo-cycles*, products of prime cycle weights t_p, ordered by increasing cycle length and instability. The products (23), (25) are really only a shorthand notation for zeta functions and determinants - for example, the zeros of the individual factors in infinite products (23), (25) are *not* the zeros of the corresponding zeta functions and determinants, and convergence of such objects is far from obvious.

A. Curvature expansions

Curvature expansions are based on the observation [10,5] that the motion in dynamical systems with finite grammar is organized around a few *fundamental* cycles; more precisely, that the cycle expansion of the dynamical zeta function (25) allows a regrouping of terms into dominant *fundamental* contributions t_f and decreasing *curvature* corrections c_n:

$$1/\zeta = 1 - \sum_f t_f - \sum_n c_n . \qquad (35)$$

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. In piecewise linear approximations to the flow, $1/\zeta$ is given by the determinant for a finite Markov transition matrix, and all c_n vanish identically. Hence the designation "curvatures"; size of c_n is an indication how far the flow is from a piecewise linearization.

A typical curvature term in (35) is a difference of a long cycle $\{ab\}$ and 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 the "pseudo orbit" $\{a\}\{b\}$, lie close to each other, have similar weights, and for longer and longer orbits the differences are expected to fall off rapidly. For systems that satisfy Axiom A requirements, such as the 3-disk repeller, curvature expansions converge very well [18]. It is crucial that the curvature expansion is grouped (and truncated) by topologically related cycles and pseudo-cycles; truncations that ignore topology, such as inclusion of all cycles with $T_p < T_{max}$, will contain un-shadowed orbits, and exhibit a mediocre convergence compared with the curvature expansions.

B. Fredholm determinant cycle expansions

While for the dynamical zeta function cycle expansions the shadowing is easy to explain, the resulting convergence is not the best achievable; as explained above, Fredholm determinants are expected to be entire, and their cycle expansions should converge faster than exponentially. The Fredholm determinant cycle expansions are somewhat more complicated than those for the dynamical zeta functions. We expand the exponential representation (11) of $F(s)$ as a multinomial in prime cycle weights t_p

$$F_p = 1 - \sum_{r=1}^{\infty} \frac{1}{r} \frac{t_p^r}{|\det\left[\mathbf{1} - \mathbf{J}_p^r\right]|} + \frac{1}{2}(\dots)^2 - \dots.$$
$$= \sum_{r=1}^{\infty} C_{p^k} t_p^k \,.$$

This yields the cycle expansion for $F(s)$:

$$F(s) = \sum_{k_1 k_2 k_3 \dots = 0}^{\infty} \tau_{p_1^{k_1} p_2^{k_2} p_3^{k_3} \dots}$$
$$\tau_{p_1^{k_1} p_2^{k_2} p_3^{k_3} \dots} = \prod_{i=1}^{\infty} C_{{p_i}^{k_i}} t_{p_i}^{k_i} \,,$$

where the sum goes over all pseudo-cycles. The coefficients have a simple form only in 1-d, given by the Euler formula (17). Expansions for the 2-d case are discussed in refs. [22,31].

In practice we do not do anything as complicated. We evaluate numerically the exponent in (11) as a power series in the book-keeping variable z, truncated to maximal cycle length N. The we expand the exponential, keeping terms up to N and obtain

$$F_N(s, z) = \sum_{k=0}^{N} C_k(s) z^k \,, \tag{36}$$

and similarly for the Gutzwiller-Voros zeta function and the dynamical zeta functions. In the final evaluation z is set to $z = 1$, but the organization by powers of z^k is crucial to the convergence of cycle expansions. For example, for 1-d Axiom A mappings $C_k(s) \approx C^{-k^2}$ for any s - this super-exponential convergence is precisely the reason why the variable z was introduced in the first place. The zeros of $F_N(s, 1)$ are determined by standard methods, such as the Newton-Raphson algorithm.

Russberg and Eckhardt [31] have generalized curvature expansions to Fredholm determinants; they work to a point, but are less powerful than the general theorems on Axiom A flows. For example, they predict that the classical Fredholm determinant could have poles, in violation of the theorem explained above.

C. Convergence of cycle expansions

It is fairly easy to establish that for Axiom A systems the trace formulas converge exponentially with the number of cycles included. As explained in sect. IV F, the trace formulas are not absolutely convergent where you need them, and in addition, shadowing of longer orbits by nearby pseudo-orbits is not implemented, so we will not use trace formulas at all. However, it should be noted that for systems other than Axiom A, we do not know how to improve convergence by shadowing cancellations, or define determinants that are guaranteed to be entire, and it is still possible that for generic systems determinants do not converge any better than traces.

For dynamical zeta functions geometrical estimates [5] imply that for Axiom A systems the curvature expansion coefficients fall off exponentially, $C_k \approx \tilde{C}^k$, and the expansion sums up to a pole

$$\sum_{n=0}^{\infty} C_k z^k \simeq \sum_{n=0}^{\infty} (\tilde{C} z)^k = \frac{1}{1 - \tilde{C} z}.$$

Such poles are expected from Ruelle's relation (31) between dynamical zeta functions and Fredholm determinants, and are indeed observed numerically [26]. Convergence of dynamical zeta functions cycle expansions can be accelerated by a variety of numerical methods, but both on theoretical grounds and in practice, the preferred alternative is to use Fredholm determinants instead.

As shown in sect. III, for Axiom A maps the coefficients in the classical Fredholm determinant $F(z) = \sum_n C_n z^n$ expansions fall off faster than exponentially, as $C_n \approx \Lambda^{-n^2}$ for 1-d maps, as $C_n \approx \Lambda^{-n^{3/2}}$ for 2-dimensional maps / 3-dimensional flows, and in d dimensions as $\Lambda^{-n^{1+1/d}}$. These estimates are confirmed by the numerical tests of ref. [13], numerical results for the 3-disk repeller ref. [31], as well as the numerical results presented below.

VI. NUMERICAL RESULTS

In this section we present the evidence that the quantum Fredholm determinant is numerically as convergent as the classical Fredholm determinant, in contrast to the Gutzwiller-Voros zeta function which has a finite radius of convergence.

A. 3-disk resonances

Following refs. [18,31,29,30], we start by performing our numerical tests on the 3-disk repeller. The 3-disk repeller is the simplest physical realization of an Axiom A system, particularly convenient for numerical investigations. The methods that we use to extract periodic orbits, their periods and their stability eigenvalues are described in ref. [32]. For billiards the cycle weight t_p required for evaluation of the classical escape rates and correlation spectra is given by (14). The action S_p is proportional to the cycle period T_p, and the Maslov index changes by +2 for each disk bounce, $m_p = 2n_p$, so the quantum weight (22) is given by

$$t_p = (-1)^{n_p} \frac{e^{-ikT_p}}{\sqrt{|\Lambda_p|}} z^{n_p} , \qquad (37)$$

where $k = (\text{momentum})/2\pi$ is the wave-number, and we take velocity = 1, mass = 1.

Cycle expansion (36) coefficients $|C_n|$ for different determinants and zeta functions are plotted in figs. 2 and 3 as function of the topological cycle length n. Zeta functions exhibit exponential falloff, implying a pole in the complex plane, while both the classical and the quantum Fredholm determinants appear to exhibit a faster than exponential falloff, with no indication of a finite radius of convergence within the numerical validity of our cycle expansion truncations.

In particular, the quantum Fredholm determinant enables us to uncover a larger part of the quantum resonances than what was hitherto accessible by means of the dynamical zeta functions [30–32]. The eye is conveniently guided to the zeros by means of complex s plane contour plots, with different intervals of the absolute value of the function under investigation assigned different colors; zeros emerge as centers of elliptic neighborhoods of rapidly changing colors. Detailed scans of the whole area of the complex s plane under investigation and searches for the zeros of classical and quantum Fredholm determinants, fig. 4, reveal complicated patterns of resonances, with the classical and the semi-classical resonance patterns surprisingly similar. It is known [18] that the leading semi-classical resonances are very accurate approximations to the exact quantum resonances; the semi-classical resonances further down in the s complex plane in fig. 4 have not yet been compared with the exact quantum values. It would be of interest to check whether also all quantum Fredholm determinant resonances correspond to the true quantum resonances.

An interpretation of the resonance spectrum of the classical Fredholm determinant is given in ref. [30], where the resonances are related to the oscillations in $N(t)$, the number of particles that have not escaped by the time t, with the basic frequency $\overline{\omega} = 2\pi/\overline{T}$ given by the inverse of $\overline{T}$, the mean flight time between the disks. $\overline{\omega}$ yields the mean spacing of the resonances along the imaginary k axis. In the 3-disk system there are two fundamental frequencies, ω_0 and ω_1, determined by the inverse periods of the two fundamental cycles $\overline{0}$ and $\overline{1}$. Corresponding beat frequency [34] $f = 2\pi/(T_1 - T_0)$ is clearly visible in fig. 4. A rough measurement of the period of the beats in fig. 4 yields some 23.7 units along the real k axis, to be compared to $2\pi/(T_1 - T_0) = 23.4$.

Effect of sub-dominant resonances on the measurable spectra are exponentially small, and presumably of little physical interest. We investigate them in detail here mostly in order to demonstrate that our determinants indeed exhibit better convergence than the Gutzwiller-Voros zeta function.

Contour plots are also helpful in comparing the domain of convergence of the Fredholm determinant to that of the Gutzwiller-Voros zeta function. As can be seen from fig. 6, the quantum Fredholm determinant can be continued considerably farther down in the complex k plane, in contrast to the dynamical zeta function scans such as those given in ref. [30]. While the zeta functions clearly exhibit a finite radius of convergence, in agreement with the arguments of sect. IV, both the classical Fredholm determinant and the quantum Fredholm determinant behave as entire functions. We compute the abscissa of absolute convergence for the Gutzwiller-Voros zeta function by means of (34); for the case at hand we obtain the leading zero at $k_{ac} = 0.0 - i\,0.699110157151\ldots$. Indeed, comparison of the contour plots of fig. 6 shows that no feature of the Gutzwiller-Voros zeta function countor plot below k_c is significant. Interestingly enough, the apparent border of Gutzwiller-Voros zeta function convergence in fig. 6 seems to coincide with $\mathrm{Re}(s) = 0$, $\mathrm{Im}(s) = -1.09653395\ldots$, the zero obtained from $F_{1/2}(k)$ by removing quantum phases, $t_p \to |t_p|$, but keeping the eigenvalue Λ_p sign. in eq. (33).

As discussed above, for 1-d systems the pole of ζ_0^{-1} coincides with the leading zero of ζ_1^{-1}, and the resulting product remains finite and has a zero close [5,8] to the leading ζ_1^{-1} zero. In simple examples, such as the symmetric 1-dimensional tent map repeller, the non-leading / leading zeros of the classical F_0 / F_1 maps are identical. This suggests that some of the *non-leading* zeros of F are shadows of the ζ_1^{-1} zeros and hence likely to lie close to the *leading* zeros of F_1. For example, the non-leading resonance $k = 0.9915231008 + i\,12.5163342128$ of the classical Fredholm determinant (see fig. 4), while distinct from the leading resonance of F_1 at $k = 0.99197582677 + i\,12.5029206443798$, belongs to a family of resonances that all lie very close to the leading F_1 resonances. We are confident that such resonances are distinct, as their cycle expansions converge super-exponentially to all digits listed above, in agreement with the general theory.

The F spectrum that is not echoed by the F_1 spectrum can be isolated by "subtracting" the F_1 spectrum, *ie.* removing those resonances from the F spectrum that lie closer than some ϵ to a F_1 resonance. The resulting spectrum is depicted in fig. 5.

What is particularly interesting about this spectrum is that with the resonances associated with the F_1 spectrum removed, families that connect non-leading resonances at $\mathrm{Re}(k) = 0$ with the leading part of the resonance spectrum for larger $\mathrm{Re}(k)$ are clearly visible in fig. 5. This makes it rather clear that the evaluation of leading resonances for large $\mathrm{Re}(k)$ requires inclusion of longer cycles, the same that are required to control the spectrum for large negative $\mathrm{Im}(k)$ at $\mathrm{Re}(k) = 0$. This is the conundrum of semi-classical cycle expansions; while semi-classical intuition implies that the Gutzwiller-Voros zeta function should be applicable for large $\mathrm{Re}(k)$, in practice the semi-classical cycle expansions work best for the bottom of the spectrum.

B. Hénon mapping as a normal form for a flow

Our next example is a model of a 3-dimensional flow $\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x})$, $\mathbf{x} = (x_1, x_2, x_3)$. We assume that the flow of interest is recurrent, and that given a convenient Poincaré section coordinatized by coordinate pair (x, y), the flow can be described by a 2-dimensional Poincaré map

$$P : \begin{cases} x' = f_1(x, y) \\ y' = f_2(x, y) \end{cases} , \tag{38}$$

together with the "ceiling" [23] function $T(x, y)$ which gives the time of flight to the next section for a trajectory starting at (x, y). A trajectory $(x_1, y_1), (x_2, y_2), (x_3, y_3), \ldots$ induces a sequence of flight times $T_1, T_2, T_3, \ldots$, $T_k = T(x_k, y_k)$. This sequence can be used to construct an embedding space, with the pair (T_k, T_{k+1}) serving as the embedding coordinates. The embedding theories [33] imply that the sequence (x_k, y_k) generated by the original map is dynamically equivalent with the sequence (T_k, T_{k+1}) (provided that the coordinate transformation is non-singular, for example $T =$const is excluded), and that the mapping

$$M : \ (T_k, T_{k+1}) \to \ (T_{k+1}, T_{k+2}) \tag{39}$$

gives us the full invariant information about the dynamical system. In particular, both the return times T_k and the stability eigenvalues of periodic orbits computed from (39) are equal to those of the original map (38). While the functional form of (39) can be complicated in actual implementation, we shall use here these ideas only as a motivation for the following rather simple model:

Assume that the Poincaré map of the flow can be modelled by a single analytic map for the whole T range of interest:

$$T_{k+1} = G(T_k, T_{k-1}). \tag{40}$$

In general G can be a complicated function, but the essential properties of a continuous flow can be modelled by the Hénon map, which we take as a local normal form (up to quadratic terms) of the time mapping. In the Hamiltonian case, the form of the Hénon map is

$$\begin{aligned} T_k &= \overline{T} + \alpha x_k \\ x_{k+1} &= 1 - a x_k^2 - x_{k-1} \, . \end{aligned} \tag{41}$$

$\overline{T}$ is essentially the mean time of flight between Poincaré sections which we shall set to $\overline{T} = 1$, and the parameter α allows us to choose a narrow or a broad return time distribution around the mean return time. For $\alpha = 0$ the flow reduces to the usual Hénon map, with constant time between the iterations. For example, the $R : a = 6 : 1$ 3-disk repeller has a rather thin repeller, and can be roughly fit with $a \approx 20$ in (41).

We relate this hypothetic flow to a semi-classical system by interpreting the flight times (41) as the lengths of segments of billiard trajectories, with the action of the periodic orbit p given by

$$\frac{1}{\hbar} S_p(k) = k \sum_{i=1}^{n_p} T_i = k(n_p + \alpha \sum_{i=1}^{n_p} x_{p,i}) \, , \tag{42}$$

where $x_{p,i}$ is the coordinate of the i-th cycle point of prime cycle p, and k is the wave number. For billiards, the Maslov index m_p is taken equal to 0 for cycles with positive stability eigenvalue Λ_p, and 1 for Λ_p negative. We take unit velocity, so $T_p = L_p$.

For the complete repeller case (all binary sequences are realized), the cycles are evaluated as follows. According to (41), the coordinates of a periodic orbit of length n_p satisfy the equation

$$x_{p,i+1} + x_{p,i-1} = 1 - a x_{p,i}^2 \, , \quad i = 1, ..., n_p \, , \tag{43}$$

with the periodic boundary condition $x_{p,0} = x_{p,n_p}$. In the complete repeller case, the Hénon map is a realization of the Smale horseshoe, and the symbolic dynamics has a very simple description in terms of the binary alphabet $\epsilon = 0, 1$, $\epsilon_{p,i} = (1 + S_{p,i})/2$, where $S_{p,i}$ are the signs of the corresponding cycle point coordinates, $S_{p,i} = \mathrm{sign}(x_{p,i})$. We start with a preassigned sign sequence $S_{p,1}, S_{p,2}, \ldots, S_{p,n_p}$, and a good initial guess for the coordinates $x'_{p,i}$. Using the inverse of the equation (43)

$$x''_{p,i} = S_{p,i} \sqrt{\frac{1 - x'_{p,i+1} - x'_{p,i-1}}{a}}, \ \ i = 1, ..., n_p \tag{44}$$

we converge iteratively, at exponential rate, to the desired cycle points $x_{p,i}$. Given the cycle points, the cycle stabilities and periods are easily computed. The times and the stabilities of the short periodic orbits for the Hénon repeller (41) at $a = 6$ are listed in table I; in actual calculations we use all prime cycles up to topological length $n = 12$ (when needed, all cycles up to length $n = 20$ have been computed). Once we have constructed a table of lengths and stabilities, extraction of the eigenvalues proceeds as in the three-disk example discussed above.

We consider first the discrete time approximation, with the parameter α set equal to zero. Then the lengths of the periodic orbits are simply $T_p = n_p$, the spectrum in the complex wave-number k plane is periodic along the real direction, and it is sufficient to consider the $0 \leq \mathrm{Re}(k) < 2\pi$ strip. Fig. 7 shows well separated eigenvalues for both the classical Fredholm determinant and the quantum Fredholm determinant, with no hint of a border of analyticity. In contrast, a corresponding contour plot of Gutzwiller-Voros zeta function (not included here) shows very clearly the finite radius of convergence, similar to what is observed in figs. 6(a) and 10.

When we switch from a map to a model of a flow by introducing a time spread, $\alpha \neq 0$ in (42), the spectrum is no longer periodic in $\mathrm{Re}(k)$. In fig. 8 we plot the classical Fredholm determinant and the quantum Fredholm determinant resonances on the same scale as in fig. 7, and in fig. 9 we plot a wider $\mathrm{Re}(k)$ range. Both classical Fredholm determinant and the quantum Fredholm determinant converge as well as in the $\alpha = 0$ discrete time case (where the theorem of sect. III guarantees that at least the classical Fredholm determinant is entire), and in the $\mathrm{Re}(k)$ direction a quasi-periodic pattern of eigenvalues can be observed, similar to the 3-disk resonance spectrum of fig. 4.

The unexpected feature of this spectrum is that the leading quantum resonance in the $0 \leq \mathrm{Re}(k) < 2\pi$ domain has larger imaginary part then the leading resonances in the sectors $2\pi n \leq \mathrm{Re}(k) < 2\pi(n+1) \quad n = 1, 2, \ldots$. This is a consequence of the partial cancellation of the contributions from the two fundamental cycles $\bar{0}$ and $\bar{1}$ in the cycle expansion (22), due to relative minus sign arising from the Maslov phases. A partial cancelation of the leading terms in the cycle expansion diminishes the leading coefficients in the $1/\zeta_0$ cycle expansion, hence the leading zero has a larger imaginary part. In the 3-disk example these contributions were positive in the A_1 subspace, but in the A_2 subspace they partially cancel in the same way as in our example. For the classical Fredholm determinant, the weight (14) depends only on the absolute magnitude of the stability, so the imaginary part of the leading zero of the classical Fredholm determinant in the domain $0 \leq \mathrm{Re}(k) < 2\pi$ is smaller then the imaginary part of the Gutzwiller-Voros zeta function's leading zero. This goes contrary to the usual expectation that the quantum escape rate should be slower than the classical one [29].

This model of a flow could also be applied to smooth potentials, with other choices for the Maslov indices, and the other forms of the action. We have computed the spectra with Maslov indices appropriate to flows in smooth potentials, and found qualitatively similar analytic properties of the quantum Fredholm determinant.

C. Baker's map

As the third and the last illustration of the improved convergence obtained by use of the quantum Fredholm determinants, we evaluate both the quantum Fredholm determinant and Gutzwiller-Voros zeta function for a model 2-d map that takes the unit square into itself by the following piecewise analytic transformations:

for $0 < x_2 < 2/5$:

$$f_1(x_1, x_2) = \frac{2}{5}x_1 + x_2(\frac{2}{5} - x_2)x_1(1 - x_1)$$
$$f_2(x_1, x_2) = \frac{5}{2}x_2 + 2x_2(\frac{2}{5} - x_2)x_1(1 - x_1)$$

for $2/5 < x_2 < 1$:

$$f_1(x_1, x_2) = \frac{3}{10}x_1 + \frac{7}{10}$$
$$f_2(x_1, x_2) = \frac{5}{3}(x_2 - \frac{2}{5}) \,. \tag{45}$$

The model has a binary symbolic dynamics and no particular physical motivation; it was introduced in ref. [13] to illustrate numerically the theorem that the classical Fredholm determinant for an Axiom A hyperbolic flow is entire. We study it here merely as another convenient model for numerical investigations of the convergence of the contracting map equivalents of the quantum Fredholm determinant and the Gutzwiller-Voros zeta function. For this discrete time example, we assume no Maslov indices, and chose the action to be equal to the (integer) time. The "Gutzwiller trace formula" for this map is defined by assigning cycles weight $1/\sqrt{|\det(1 - \mathbf{J}_p)|}$, with the corresponding "Gutzwiller-Voros zeta function".

The convergence of the cycle expansions (36) for the two determinants is illustrated by fig. 11. Starting with cycle length $n = 13$, and up to $n = 24$, the highest cycle length computed, the quantum Fredholm determinant performs better than the Gutzwiller-Voros zeta function. The convergence is also illustrated by the table II, where the zeros of the two determinants are shown. Even though the map is not area preserving and the "Gutzwiller-Voros zeta function" is quite artificial, the convergence is much the same as for the 3-disk repeller.

The numerical evidence from baker's map on whether the quantum Fredholm determinant and weighted Fredholm determinants are entire is inconclusive; zeros of F_{-1}, F_{qm}, F_0, F_1 cycle expansion truncations up to $n_{max} = 22$ have qualitatively the same distribution in the complex plane. $1/\zeta(k)$ and $Z_{qm}(k)$ exhibit somewhat worse convergence than the Fredholm determinants. In all cases, only a few leading zeros are true zeros; for example, table II lists 7 true zeros, the remaining 17 form a "wedge" in the complex plane (see fig. 12), which slowly drifts toward higher $\mathrm{Im}(k)$ with increased cycle truncation length.

We conclude our discussion of numerics with a word of caution: as we do not know how quickly the asymptotics should set in, our numerical results can easily be misleading. For example, for a larger disk-disk spacing, pre-asymptotic oscillations are visible in fig. 2, and one might mistakenly conclude [31] from such data that the classical Fredholm determinant has a pole. There is no substitute for theorems that established that appropriate determinants are entire; such oscillations make numerical convergence uncertain already in the simplest 1-dimensional repellers [36].

VII. CONCLUSIONS AND SUMMARY

In conclusion, we have tested numerically the conjecture that the new approximation to the quantum determinant, the quantum Fredholm determinant, has better analyticity properties than the commonly used Gutzwiller-Voros zeta function. The existence of such a determinant suggests a starting approximation to the quantum propagator different from the usual Van Vleck semi-classical propagator. As we do not know an operator whose determinant is the quantum Fredholm determinant, we have no proof that such determinant is entire, only numerical evidence that its convergence is superior to the Gutzwiller-Voros zeta function. The new determinant could be of practical utility, as for nice hyperbolic systems its convergence is superior to that of the Gutzwiller-Voros zeta functions.

We were guided here by the Axiom A intuition developed by Smale, Ruelle, and others: if the dynamical evolution can be cast in terms of an evolution operator multiplicative along the flow, if the corresponding mapping (for ex., return map for a Poincaré section of the flow) is analytic hyperbolic, and if the topology of the repeller is given by a finite Markov partition, then the Fredholm determinant (14) is entire. An alternative approach, inspired by the theory of the Riemann zeta function, is due to M.V. Berry and J. Keating [35]. 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 [5,6], 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 semi-classical zeta function, cut at the appropriate cycle period.

The real life challenge are generic dynamical flows, which fit neither schematization. Unfortunately we know of no smooth potential which is both Axiom A, and has bound states. 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 crucial ingredient for nice analyticity properties of zeta functions is existence of finite grammar (coupled with uniform hyperbolicity). From the hyperbolic dynamics point of view, the Riemann zeta 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 [5], pretty much as a "generic" number is approached by a sequence of continued fractions.

The dynamical systems that we are *really* interested in - for example, smooth bound Hamiltonian potentials - are presumably never really chaotic, and it is still unclear what intuition is more rewarding: are quantum spectra of chaotic dynamics in smooth bound Hamiltonian potentials more like zeros of Riemann zetas or zeros of dynamical zeta functions?

Note added in proof: Since completion of this work, Vattay *et al.* [37] have succeeded in constructing a multiplicative evolution operator for semi-classical quantum mechanics, whose Fredholm determinant is

$$F(\beta, E) \,=\, \exp\left(-\sum_{p,r}\frac{1}{r}\frac{|\Lambda_p|^{-r\beta}e^{i(S_p(k)/\hbar+\nu_p\pi/2)r}}{(1-1/\Lambda_p^r)^2(1-1/\Lambda_p^{2r})}\right). \tag{46}$$

This determinant is entire for the Axiom A flows. The results presented in this paper remain valid, but the new formulation makes it possible to reformulate our conjectures as theorems. In particular, the quantum Fredholm determinant can now be written as a ratio of two Vattay determinants

$$F_{qm}(k) = \frac{F(\frac{1}{2},k)}{F(\frac{5}{2},k)}.$$

As explained in sect. IV F, the abscissa of convergence for such ratio is given by the upper bound on the leading zeros of $F(\frac{5}{2},k)$. For example, for the 3-disk, $R:a=6:1$ system we find

$$\mathrm{Im}(k_{ac}) = -1.276625955\ldots$$

so the quantum Fredholm determinant can be continued almost a factor 2 down in the complex k plane beyond the region of applicability of the Gutzwiller-Voros zeta function. This explains why for all practical purposes the quantum Fredholm determinants behave as entire functions: only careful numerics reveals the difference between the quantum Fredholm determinant and the Vattay determinant in higher order terms in cycle expansions. The difference is illustrated by fig. 13; the suspicious straight section visible in the quantum Fredholm determinant ($\triangle$) in fig. 3 turns out to indeed indicate a pole, while the Vattay determinant converges super-exponentially.

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FIG. 1. For a analytic hyperbolic map, specifying the contracting coordinate w_h at the initial rectangle and the expanding coordinate z_v at the image rectangle defines a unique trajectory between the two rectangles. In particular, w_v and z_h (not shown) are uniquely specified.

FIG. 2. $\log_{10}|C_n|$, the contribution of cycles of topological length n to the cycle expansion $\sum C_n z^n$ for 3-disk repeller. Shown are: ($\circ$) $1/\zeta_0$, (∇) the Gutzwiller-Voros zeta function, ($\Box$) $1/\zeta_0\zeta_1^2$, and ($\triangle$) the quantum Fredholm determinant. Exponential falloff implies that $1/\zeta_0$ and the Gutzwiller-Voros zeta function have the same leading pole, cancelled in the $1/\zeta_0\zeta_1^2$ product. For comparison, ($\diamond$) the classical Fredholm determinant coefficients are plotted as well; cycle expansions for both Fredholm determinants appear to follow the asymptotic estimate $C_n \approx \Lambda^{-n^{3/2}}$. A_1 symmetric subspace, with center spacing - disk radius ratio $R : a = 3 : 1$, evaluated at the lowest resonance, wave number $k = 7.8727 - 0.3847\, i$, maximal cycle length $n = 8$.

FIG. 3. Same as fig. 2, but with $R : a = 6 : 1$. This illustrates possible pitfalls of numerical tests of asymptotics; the quantum Fredholm determinant appears to have the same pole as the quantum $1/\zeta_0\zeta_1^2$, but as we have no estimate on the size of pre-asymptotic oscillations in cycle expansions, it is difficult to draw reliable conclusions from such numerics. See fig. 13 for estimate of the quantum Fredholm determinant abscissa of absolute convergence.

FIG. 4. Leading resonances in the 3-disk repeller A_1 subspace, (a) for the classical Fredholm determinant, and (b) the 952 leading resonances of the quantum Fredholm determinant F_{qm}. Ratio $R : a = 6 : 0$, cycle expansions truncated at cycle length $n = 8$.

FIG. 5. "Difference" between the classical F_0 and F_1 spectrum for the 3-disk repeller. All resonances $s_{0,\alpha}$ of F_0 that fall within $|\mathrm{Re}(s_{0,\alpha}) - \mathrm{Re}(s_{1,\beta})| < 0.1$, $|\mathrm{Im}(s_{0,\alpha}) - \mathrm{Im}(s_{1,\beta})| < 0.08$, of a resonance $s_{1,\beta}$ of F_1, are deleted from fig. 4. Note that while the non-leading families of resonances $s_{0,\alpha}$ almost coincide with the leading $s_{1,\beta}$ resonances, they are not degenerate. With the resonances associated with the F_1 spectrum removed, families that connect nonleading resonances at $\mathrm{Re}(s) = 0$ with the leading part of the resonance spectrum for larger $\mathrm{Re}(s)$ are clearly visible. $R : a = 6 : 1$, A_1 subspace, maximal cycle length $n = 8$.

FIG. 6. Complex s plane countor plot comparison of (a) the Gutzwiller-Voros zeta function $\log|Z_{qm}(s)|$ with (b) the quantum Fredholm determinant $\log|F_{qm}(s)|$. The border of the convergence of the Gutzwiller-Voros zeta function agrees with the location of the abscissa of absolute convergence, given by the $\hat{F}_{1/2}$ leading eigenvalue at $\mathrm{Re}(s) = 0$, $\mathrm{Im}(s) = -0.699110157151\ldots$. The quantum Fredholm determinant can be continued at least a factor 2 further down in the complex plane. 3-disk repeller, $R : a = 6 : 1$, A_1 subspace, maximal cycle length $n = 8$.

FIG. 7. Contour plot of $\log_{10}|F(s)|$ for (a) the classical Fredholm determinant, and for (b) the quantum Fredholm determinant for the Hénon map, $\alpha = 0$ in (41), prime cycles up to topological length 12.

FIG. 8. Contour plot of $\log_{10}|F(s)|$ for (a) the classical Fredholm determinant, and for (b) the quantum Fredholm determinant for the model flow (41) with $\alpha = 1/2$, prime cycles up to topological length 12.

FIG. 9. Contour plot of $\log_{10}|F(s)|$ for the quantum Fredholm determinant; same as fig. 8, but for a wider range of $Re(k)$.

FIG. 10. Same as fig. 8 for the Gutzwiller-Voros zeta function. The single leading pole of the Gutzwiller-Voros zeta function manifests itself as the border of the convergence; only two leading eigenvalues from fig. 8(b) remain within the domain of convergence.

FIG. 11. $\log_{10}|C_n|$, the contribution of cycles of topological length n to the cycle expansion $\sum C_n z^n$, for the ($\square$) "Gutzwiller-Voros zeta function" and ($\circ$) "quantum Fredholm determinant" for the baker's map (45).

FIG. 12. The "quantum Fredholm determinant" zeros for the baker's map (45) computed from all cycles to cycle length $n_{max} = 22$. A few leading zeros are true zeros; table II lists the 7 true zeros, the remaining 17 forming a "wedge" in the complex plane which slowly drifts toward higher $\mathrm{Im}(k)$ with increased cycle truncation length.

FIG. 13. Same parameter values 3-disk system as fig. 2: ($\circ$) the quantum Fredholm determinant compared with ($\square$) the Vattay determinant. While the quantum Fredholm determinant is expected to have a pole at $\mathrm{Im}(k) = -1.276625955\ldots$, the Vattay determinant should be entire, and exhibits numerically faster than exponential convergence.

TABLE I. All periodic orbits up to 6 bounces for the Hamiltonian Hénon mapping (41) with $a = 6$. Listed are the topological length of the cycle, its expanding eigenvalue Λ_p, the variation in the period of the cycle, and its binary code.

n_p	Λ_p	$\sum x_{p,i}$	code
1	$0.71516752438\times10^{1}$	-0.6076252185107	0
1	$-0.29528463259\times10^{1}$	0.2742918851774	1
2	$-0.98989794855\times10^{1}$	0.3333333333333	10
3	$-0.13190727397\times10^{3}$	-0.2060113295833	100
3	$0.55896964996\times10^{2}$	0.5393446629166	110
4	$-0.10443010730\times10^{4}$	-0.8164965809277	1000
4	$0.57799826989\times10^{4}$	0.0000000000000	1100
4	$-0.10368832509\times10^{3}$	0.8164965809277	1110
5	$-0.76065343718\times10^{4}$	-1.4260322065792	10000
5	$0.44455240007\times10^{4}$	-0.6066540777738	11000
5	$0.77020248597\times10^{3}$	0.1513755016405	10100
5	$-0.71068835616\times10^{3}$	0.2484632276044	11100
5	$-0.58949885284\times10^{3}$	0.8706954728949	11010
5	$0.39099424812\times10^{3}$	1.0954854155465	11110
6	$-0.54574527060\times10^{5}$	-2.0341342556665	100000
6	$0.32222060985\times10^{5}$	-1.2152504370215	110000
6	$0.51376165109\times10^{4}$	-0.4506624359329	101000
6	$-0.47846146631\times10^{4}$	-0.3660254037844	111000
6	$-0.63939998436\times10^{4}$	0.3333333333333	110100
6	$-0.63939998436\times10^{4}$	0.3333333333333	101100
6	$0.39019387269\times10^{4}$	0.5485837703548	111100
6	$0.10949094597\times10^{4}$	1.1514633582661	111010
6	$-0.10433841694\times10^{4}$	1.3660254037844	111110

TABLE II. The "quantum" eigenvalues obtained from the Gutzwiller-Voros zeta function $Z_{qm}(s)$ and the quantum Fredholm determinant $F_{qm}(s)$ for the baker's map. Only the leading eigenvalues are expected to coincide. The digits listed correspond to those unchanged between the cycle length $n = 23$ and $n = 24$ truncations.

	$Z_{qm}(s)$	$F_{qm}(s)$	
k	Real part	Real part	Im. part
1	0.34051779186	+0.3405177918632516	
2	-0.39	-0.3500689652275	
3		-0.7175716624	
4-5		-1.099684	$\pm$ 0.115118
6-7		-1.59	$\pm$ 0.227