

# A New Determinant for Quantum Chaos

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## Abstract

We propose a new type of approximation to quantum determinants, “quantum Fredholm determinant”, and conjecture that, compared to the quantum Selberg zeta functions derived from Gutzwiller semiclassical trace formulas, such determinants have a larger domain of analyticity for Axiom A hyperbolic systems. The conjecture is supported by a numerical investigation of the 3-disk repeller.

Dynamical zeta functions [1], Fredholm determinants [2] and quantum Selberg zeta functions [3, 4] have recently been established as powerful tools for evaluation of classical and quantum averages in low dimensional chaotic dynamical systems [5] - [8]. The convergence of cycle expansions [9] of zeta functions and Fredholm determinants depends on their analytic properties; particularly strong results exist for nice (Axiom A) hyperbolic systems, for which the dynamical zeta functions are holomorphic [10], and the Fredholm determinants are entire functions [11, 12]. In this note, motivated by the recent results of Eckhardt and Russberg [13], we conjecture that in contrast to the quantum Selberg zeta function, for nice hyperbolic systems the *quantum* Fredholm determinant (introduced below) is entire, *i.e.* free of poles.

For 2-dimensional Hamiltonian systems the dynamical zeta function [1] is given by

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

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the Fredholm determinant [5, 12, 14] is given by

$$F = \prod_p \prod_{k=0}^{\infty} (1 - t_p/\Lambda_p^k)^{k+1} = \prod_{k=0}^{\infty} 1/\zeta_k^{k+1} , \quad (2)$$

and the quantum Selberg zeta function [4] is given by

$$Z = \prod_p \prod_{k=0}^{\infty} (1 - t_p/\Lambda_p^k) = \prod_{k=0}^{\infty} 1/\zeta_k . \quad (3)$$

In the above,  $t_p$  is a weight associated with the cycle  $p$ , and the subscript  $p$  runs through all distinct prime cycles. A prime cycle is a single traversal of the orbit; its label is a non-repeating symbol string. The cycle weight  $t_p$  depends on the average evaluated. Following refs. [13, 15, 16] we shall perform our numerical tests on the 3-disk repeller. For such systems, the cycle weight is given by [17]

$$t_p = z^{n_p} e^{sT_p} / |\Lambda_p| , \quad (4)$$

in the evaluation of escape rates and correlation spectra, and by

$$t_p = z^{n_p} \frac{e^{-iS_p/\hbar + \nu_p}}{\sqrt{|\Lambda_p|}} , \quad (5)$$

in the evaluation of the semiclassical approximation [4, 18] to quantum resonances. Here  $T_p$  is the  $p$ -cycle period,  $S_p$  is its action,  $\nu_p$  the Maslov index and  $\Lambda_p$  the expanding eigenvalue.  $z$  is a bookkeeping variable that keeps track of the topological cycle length  $n_p$ , used to expand zeta functions and determinants:

$$F(z) = \sum_{k=0}^{\infty} C_k z^k . \quad (6)$$

In calculations  $z$  is set to  $z = 1$ .

If the dynamical evolution can be cast in terms of a transfer operator multiplicative along the flow, if the corresponding mapping (for ex., return map for a Poincaré section of the flow) is analytic, and if the topology of the repeller is given by a finite Markov

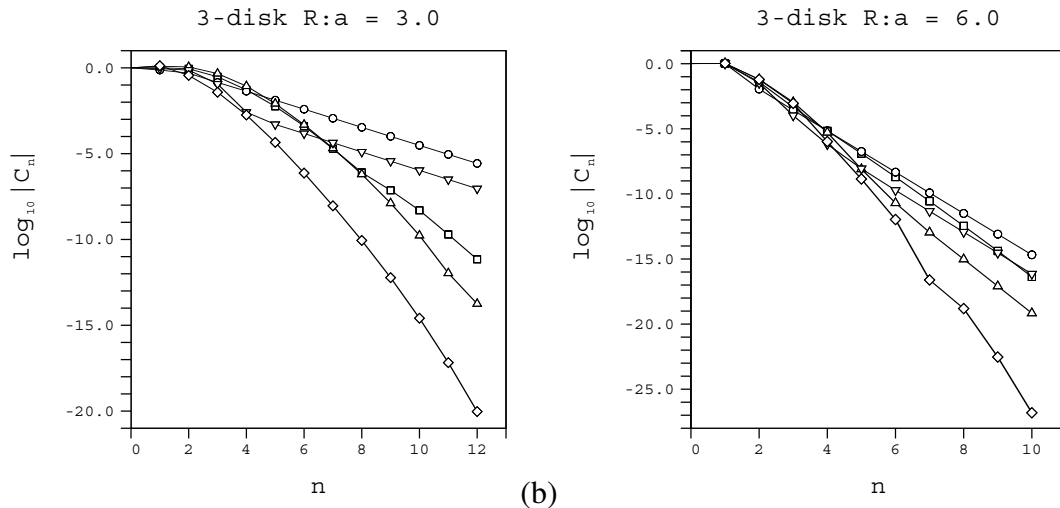


Figure 1: (a)  $\log_{10} |C_n|$ , the contribution of cycles of length  $n$  to the cycle expansion  $\sum C_n z^n$  for  $A_1$  symmetric subspace resonance for 3-disk repeller with center spacing - disk radius ratio  $R : a = 3 : 1$ , evaluated at the lowest resonance, wave number  $k = 7.8727 - 0.3847 i$ . Shown are: ( $\circ$ )  $1/\zeta_0$ , ( $\nabla$ ) the quantum Selberg zeta function, ( $\square$ )  $1/\zeta_0 \zeta_1^2$ , and ( $\triangle$ ) the quantum Fredholm determinant. Exponential falloff implies that  $1/\zeta_0$  and the quantum Selberg zeta 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  $C_n \approx \Lambda^{-n^{3/2}}$ . (b) Same as (a), 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 there is we have no estimate on the size of preasymptotic oscillations in cycle expansions, it is difficult to draw reliable conclusions from such numerics.

partition, then the Fredholm determinant (2) with classical weight (4) is entire [12]. In this case the cycle expansion coefficients (6) fall off asymptotically faster than exponentially [12, 14], as  $C_n \approx \Lambda^{-n^{3/2}}$ . This estimate is in agreement with numerical tests of ref. [12], as well as our and ref. [13] numerical results for the 3-disk repeller, see fig. 1 (a). However, as it is not known how quickly the asymptotics should set in, such numerical results can be misleading: for example, for a larger disk-disk spacing, preasymptotic oscillations are visible in fig. 1 (b). (Such oscillations can be observed already in simple 1-dimensional repellers).

On the basis of close analogy between the classical and the quantum zeta functions [16], it has been hoped [19] that for nice hyperbolic systems the quantum Selberg

zeta functions (3) should also be entire. However, it has not been possible to extend the classical Fredholm determinant proof [12] to the quantum case, essentially because the composition of the semiclassical propagators [3] is not multiplicative along the classical trajectory, but requires additional saddlepoint approximations. Indeed, Eckhardt and Russberg [13] have recently established by numerical studies that the 3-disk quantum Selberg zeta functions have poles.

In refs. [6, 20] 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 determinant entire. Eckhardt and Russberg have repeated this analysis for the  $1/\zeta_k$  terms in the quantum Selberg zeta function (3). They find numerically that  $1/\zeta_0$  has a double pole coinciding with the leading zero of  $1/\zeta_1$ . Consequently  $1/\zeta_0$ ,  $1/\zeta_0\zeta_1$  and  $Z$  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, fig. 1 (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, the theorem that establishes that the classical Fredholm determinant (2) 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. More explicitly,  $1/\zeta_k$  can be expressed in terms of weighted Fredholm determinants

$$F_k = \exp \left( - \sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(t_p/\Lambda_p^k)^r}{(1 - 1/\Lambda_p^r)^2} \right) \quad (7)$$

( $F_0 = F$  defined in (2)) by inserting 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 (1) of  $1/\zeta_k$ . This yields

$$1/\zeta_k = \frac{F_k F_{k+2}}{F_{k+1}^2}, \quad (8)$$

and we conclude that for 2-dimensional Hamiltonian flows the dynamical zeta function  $1/\zeta_k$  has a *double* leading pole coinciding with the leading zero of the  $F_{k+1}$  Fredholm determinant. It is easy to check that the infinite product  $\prod 1/\zeta_k^{k+1}$  collapses to  $F_0 = F$ .

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

$$\mathcal{L}_k^t(y, x) = \Lambda^t(x)^{-k} \phi^t(x) \delta(y - f^t(x)) , \quad (9)$$

where  $\Lambda^t(x)$  is the expanding eigenvalue of the Jacobian transverse to the flow, and  $\phi^t(x)$  is any smooth weight multiplicative along the trajectory.

The numerical results of ref. [13] suggest that the *quantum Fredholm determinant*, i.e. the Fredholm determinant (2) with the *quantum weights* (5) may be entire, and that, in the spirit of the thermodynamical formalism [1, 21, 22], the quantum evolution operator should be approximated by a classical transfer operator with a quantum weighting factor:

$$\mathcal{L}^t(y, x) = \sqrt{|\Lambda^t(x)|} e^{-iS^t(x)/\hbar + \nu_p} \delta(y - f^t(x)) . \quad (10)$$

The difference between the two infinite products (2) and (3) can be traced to the quantum  $1/\sqrt{|\det(1 - J_p)|}$  weight that arises in the saddle point expansion derivation of the Gutzwiller trace formula; the delta-function transfer operator (10) leads to the cycle weight  $1/|\det(1 - J_p)|$  instead. Both the quantum Fredholm determinant and the quantum zeta function yield the same leading zeros, given by  $1/\zeta_0$ . They presumably differ in nonleading zeros (with larger imaginary part of the complex energy), but as the quantum Selberg zeta function (3) is the leading term of a semiclassical approximation, with the size of corrections unknown, the physical significance of these nonleading zeros remains unclear.

The transfer operator (10) is problematic as it stands, because it is not multiplicative along the trajectory. While for the Jacobians  $J_{ab} = J_a J_b$  for two successive segments  $a$  and  $b$  along the trajectory, the corresponding expanding eigenvalues are *not* multiplicative,  $\Lambda_{ab} \neq \Lambda_a \Lambda_b$ , and consequently (10) does not satisfy the assumptions required by the theorem of ref. [12]. Nevertheless, such transfer operators have been routinely used in, for ex., evaluation of partial dimensions [23]. Our numerical results support the conjecture that  $\Lambda^k$  weighted determinant has enlarged domain of convergence.

In conclusion, we have proposed and tested numerically a new approximation to the quantum determinant, and conjectured that it has better analyticity properties than the commonly used quantum Selberg zeta function. The quantum Fredholm determinant suggests a starting approximation to the quantum propagator different from the usual used Van Vleck semiclassical propagator. The new determinant is expected to be of practical utility as for nice hyperbolic systems its convergence is superior to that of the quantum Selberg zeta functions.

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## References

- [1] D. Ruelle, *Statistical Mechanics, Thermodynamic Formalism* (Addison-Wesley, Reading MA, 1978).
- [2] A. Grothendieck, "La théorie de Fredholm", *Bull. Soc. Math. France* **84**, 319 (1956).
- [3] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York 1990).
- [4] A. Voros, *J. Phys.* **A 21**, 685 (1988).
- [5] R. Artuso, E. Aurell and P. Cvitanović, *Nonlinearity* **3**, 325 (1990).
- [6] F. Christiansen, G. Paladin and H.H. Rugh, *Phys. Rev. Lett.* **65**, 2087 (1990).
- [7] D. Wintgen, K. Richter and G. Tanner, *CHAOS* **2**, 19 (1992).
- [8] P. Cvitanović, ed., *Periodic Orbit Theory - theme issue*, *CHAOS* **2**, 1-158 (1992).
- [9] P. Cvitanović, *Phys. Rev. Lett.* **61**, 2729 (1988).
- [10] D. Ruelle, *Inventiones math.* **34**, 231 (1976).
- [11] D. Fried, *Ann. Scient. Éc. Norm. Sup.* **19**, 491 (1986).
- [12] H.H. Rugh, *Nonlinearity* **5**, 1237 (1992).
- [13] B. Eckhardt and G. Russberg, *Phys. Rev.* **E**, to appear.
- [14] P. Cvitanović, *Physica D* **51**, 138 (1991).
- [15] P. Gaspard and S.A. Rice, *J. Chem. Phys.* **90**, 2225 (1989); **90**, 2242 (1989); **90**, 2255 (1989).
- [16] P. Cvitanović and B. Eckhardt, *Phys. Rev. Lett.* **63**, 823 (1989).
- [17] P. Cvitanović and B. Eckhardt, *J. Phys. A* **24**, L237 (1991).
- [18] M.C. Gutzwiller, *J. Phys. Chem.* **92**, 3154 (1984).
- [19] P. Cvitanović, *CHAOS* **2**, 1 (1992).
- [20] R. Artuso, E. Aurell and P. Cvitanović, *Nonlinearity* **3**, 361 (1990).
- [21] Ya. G. Sinai, *Russ. Math. Surveys* **166**, 21 (1972).
- [22] R. Bowen, *Equilibrium states and the ergodic theory of Anosov-diffeomorphisms*, Springer Lecture Notes in Math. **470** (1975).
- [23] See sect. 9 of ref. [5] and sect. 5 of ref. [20].