Resummation of classical and semiclassical periodic orbit formulas

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March 21, 2022

Abstract

The convergence properties of cycle expanded periodic orbit expressions for the spectra of classical and semiclassical time evolution operators have been studied for the open three disk billiard. We present evidence that both the classical and the semiclassical Selberg zeta function have poles. Applying a Padé approximation on the expansions of the full Euler products, as well as on the individual dynamical zeta functions in the products, we calculate the leading poles and the zeros of the improved expansions with the first few poles removed. The removal of poles tends to change the simple linear exponential convergence of the Selberg zeta functions
to an \( \exp\{-n^{3/2}\} \) decay in the classical case and to an \( \exp\{-n^2\} \) decay in the semiclassical case.

The leading poles of the \( j \)th dynamical zeta function are found to equal the leading zeros of the \( j + 1 \)th one: However, in contrast to the zeros, which are all simple, the poles seem without exception to be double. The poles are therefore in general not completely cancelled by zeros, which has earlier been suggested. The only complete cancellations occur in the classical Selberg zeta function between the poles (double) of the first and the zeros (squared) of the second dynamical zeta function.

Furthermore, we find strong indications that poles are responsible for the presence of spurious zeros in periodic orbit quantized spectra and that these spectra can be greatly improved by removing the leading poles, e.g. by using the Padé technique.

PACS: 05.45.+b, 03.65.Sq, 02.30.+g
1 Introduction

Trace formulas in chaotic dynamical systems relate phase space averages to sums over periodic orbits \[1, 2, 3, 4, 5, 6\]. Exponentiated trace formulas give rise to Selberg type zeta functions, named after corresponding expressions arising in studies of billiards on surfaces of negative curvature \[7, 8\]. Selberg zeta functions factorize further into products of dynamical zeta functions, each one being an infinite product over all primitive nonrepeated periodic orbits (ppo) of the system. Finally, the term cycle expansion refers to a certain expansion and truncation of (dynamical and Selberg) zeta functions into polynomials. Whereas the original trace formulas and the infinite products have the same convergence and analyticity properties, cycle expanded periodic orbit expressions typically converge much better \[3, 4\].

Calculations can be improved, if the pole structure is known \[9\]. Typically, dynamical zeta functions will have poles; for Selberg zeta functions, one can advance arguments \[3, 10\] that they should be entire and thus ideally suited for numerical purposes. We here present quantitative results on the analyticity properties of zeta functions for a 2d conservative dynamical system, a point particle elastically scattered off three disks placed symmetrically in the plane \[11, 12, 13, 14\]. This system is ideally suited for such an investigation since (for sufficiently separated disks) it is a hyperbolic system with a good symbolic coding (complete binary, once the symmetries are factored out). Periodic orbits can conveniently and accurately be computed.

We proceed with a formal definition of the objects investigated: Let \( p \) label all primitive non repeated periodic orbits, \( n_p \) their symbolic length, \( \mu_p \) the Maslov
index (in a billiard $\mu_p = 2n_p$), and $J_p$ the linearization perpendicular to the orbit with $\Lambda_p$ the eigenvalue of largest absolute value. For the two degree of freedom system considered here $J_p$ is a $2 \times 2$ matrix of determinant 1 so that the other eigenvalue is $1/\Lambda_p$. We then consider the classical Selberg zeta function [3]

$$Z(z) = \exp \left\{ - \sum_p \sum_{r=1}^{\infty} \frac{z^{rn_p}}{r} \frac{1}{|\det(1 - J_p)|} \right\} = \prod_{j=0}^{\infty} \left[ \zeta_j^{-1}(z) \right]^{j+1}$$ \hspace{1cm} (1)

with

$$\zeta_j^{-1}(z) = \prod_p \left( 1 - z^{n_p} |\Lambda_p|^{-1} \Lambda_p^{-j} \right),$$ \hspace{1cm} (2)

and the semiclassical Selberg zeta function [15, 16, 17]

$$Z(z) = \exp \left\{ - \sum_p \sum_{r=1}^{\infty} \frac{z^{rn_p} e^{-ir\mu_p \pi/2}}{r} \frac{1}{|\det(1 - J_p)|^{1/2}} \right\} = \prod_{j=0}^{\infty} \zeta_j^{-1}(z)$$ \hspace{1cm} (3)

with

$$\zeta_j^{-1}(z) = \prod_p \left( 1 - z^{n_p} e^{-i\mu_p \pi/2} |\Lambda_p|^{-1/2} \Lambda_p^{-j} \right),$$ \hspace{1cm} (4)

all as functions of $z$. We avoid use of additional labels distinguishing classical and semiclassical zeta functions and hope that it is clear from the context which one is meant. Straightforward formal manipulations allow to express each function (1)-(4) as a power series $\sum C_n z^n$ in $z$, which, when truncated, yields the cycle expansion. Where needed, we will abbreviate with $t_p$ the contributions of periodic orbits to the dynamical zeta function with $j = 0$ so that $\zeta_j^{-1} = \prod_p (1 - t_p \Lambda_p^{-j})$.

The above expressions are correct for maps, the periods of orbits being integers. For flows one would replace $z^{n_p}$ by $z^{n_p} \exp \{i\omega T_p \}$ in the classical case or by $z^{n_p} \exp \{iS_p(E)/\hbar \}$ in the semiclassical case, expand in a power series in $z$ and consider the final result as a function of frequency $\omega$ or energy $E$, respectively, for $z = 1$.

In billiards, the action is given by $S_p(E)/\hbar = L_p k(E)$, where $L_p$ is the geometrical
length of the ppo and \( k(E) = \sqrt{2mE/\hbar} \) is the wave number. In addition to Maslov phases there can be further phases due to symmetries \([18, 19, 20]\). For the case of the three disks, the above expressions are correct in the \( A_1 \)-representation; in the \( A_2 \)-representation there is an additional phase \( i\pi \) if \( n_p \) is odd.

Periodic orbits for the three disk system have been computed using Newton’s method on two different maps, one based on direct description (impact parameter, scattering cycle) of collisions with the disks and one based on stationarity of action. The computations were done for several values of the ratio \( \rho \equiv d/R \), where \( d \) is the disk separation and \( R \) the disk radius. Symmetry reduced orbits up to symbolic length 13 have been found in double precision numerics with relative accuracy \( 10^{-14} \). The exponential of (1) and (3) was computed using all orbits and repetitions satisfying \( n_p r \leq N \) and then expanded in a series \( \sum C_n z^n \) using the recurrence relations of Plemelj and Smithies \([21, 22, 23]\).

Fig. 1 shows the results for the classical Selberg zeta function. An apparently faster than exponential decay is observed. In contrast, the semiclassical Selberg zeta function seems to decay faster than exponential for the first three or four terms, but then settles for an exponential decay, see Fig. 2. In the following we will explain this difference in behaviour, show its effects in calculations and demonstrate how this knowledge can be used to improve calculations.

We begin in section 2 with a detailed discussion of the convergence of cycle expanded zeta functions, including numerical results for the three disk system. In section 3 we turn to methods for identification and removal of poles. The effect of poles when calculating quantum resonances is discussed in section 4. We conclude
2 Convergence estimates

Some insight into the behaviour of the cycle expansions of (1) and (3) may be obtained by considering the special case of a complete binary code with $\Lambda_0 \sim \Lambda_1 \sim \Lambda$ and a factorization of the eigenvalues of the longer periodic orbits $\Lambda_p \sim \Lambda_0^{n_0} \Lambda_1^{n_1}$, where $n_0$ and $n_1$ are the numbers of zeros and ones in the symbolic description of $p$. Then the classical dynamical zeta functions take on the form

$$\zeta_j^{-1}(z) \sim \left(1 - 2z|\Lambda|^{-1}\Lambda^{-j}\right).$$  \hspace{1cm} (5)

Expanding the product on $j$ in a power series in $z$, one finds

$$Z(z) = \prod_j \left[\zeta_j^{-1}(z)\right]^{j+1} \sim \sum d_n z^n$$ \hspace{1cm} (6)

with $d_n \sim \Lambda^{-n^{3/2}}$ (see below). Similarly, in the semiclassical case one finds

$$\zeta_j^{-1}(z) \sim \left(1 - 2z|\Lambda|^{-1/2}\Lambda^{-j}\right)$$ \hspace{1cm} (7)

and

$$Z(z) = \prod_j \zeta_j^{-1}(z) \sim \sum d'_n z^n$$ \hspace{1cm} (8)

with $d'_n \sim \Lambda^{-n^2}$ (essentially due to the Euler product formula, see e.g. eq. (89.18.3) in Ref. [24]). Because of this rapid decay, these functions are free of poles.

In the general hyperbolic case, the expansion of dynamical zeta functions does not stop with the linear term but rather continues with exponentially decaying coefficients, $c_n \sim \beta^n$ with $|\beta| < 1$. Summing this geometrical series one finds a pole
at $z = \beta^{-1}$. In ref. [3, 10] $\beta$ has been related to the Lyapunov exponents which suggests that the poles of $\zeta_j^{-1}$ should be compensated by the zeros of $\zeta_{j+1}^{-1}$. To see what terms have to compensate in order to provide faster than exponential decay of the coefficients in the Selberg type zeta function, let us consider the classical and semiclassical cases in some more detail.

2.1 The semiclassical case

With each dynamical zeta function expanded in a power series in $z$, the semiclassical Selberg zeta function (3) looks like

$$Z(z) = \prod_j \zeta_j^{-1}(z)$$

$$= (1 - f_1^{(0)} z - c_6^{(0)} z^2 - c_9^{(0)} z^3 - \ldots)(1 - f_3^{(1)} z - c_10^{(1)} z^2 - \ldots)(1 - f_5^{(2)} z - c_{14}^{(2)} z^2 - \ldots) \ldots$$

As is often convenient for dynamical zeta functions we distinguish curvature terms $c_{in}$ of orbits grouped together with shorter shadowing orbits and fundamental contributions $f_i$ of the shortest orbits, which by definition are not approximated by other orbits. Superscript labels here indicate the order $j$ of the zeta function. Subscripts indicate the size of the terms in powers of $|\Lambda|^{-1/2}$, where $|\Lambda|$ is a typical instability of the shortest orbits (obviously, some uniformity in the Lyapunov exponents is assumed here). For instance, $f_1^{(0)}$ comes from terms of the form $|\Lambda_p|^{-1/2}e^{-i\mu_p\pi/2}$ in $\zeta_0^{-1}$, whence its subscript equals 1. Fundamentals $f_i^{(j)}$ with higher $j$ have additional powers $|\Lambda_p|^{-j}$ and thus $i = 1 + 2j$. The order of the curvature corrections $c_{in}^{(j)} z^n$ is determined by two factors: the typical size of the terms contributing (about $|\Lambda|^{-n/2-jn}$) and an additional factor $\sim \Lambda^{-n}$ due to exponential shadowing of long
orbits by short approximands, thus $i_n = (3 + 2j)n$.

To estimate the convergence behaviour, we will now expand (9) in $z$, $Z(z) = \sum C_n z^n$, and evaluate the leading order contributions in each coefficient $C_n$. One sees that there is a considerable difference in order of magnitude between the fundamental term and the first curvature correction, so to begin with one would expect to find significant contributions from fundamentals only. In the ideal two scale approximation $\Lambda_p = \Lambda_0^{n_0} \Lambda_1^{n_1}$ all curvatures are identically zero, $c^{(j)}_n = 0$, and the expansion looks as follows

$$Z(z) = (1 - f_1^{(0)} z) \left(1 - f_3^{(1)} z\right) \left(1 - f_5^{(2)} z\right) \ldots$$

$$= 1 - \left(f_1^{(0)} + f_3^{(1)} + f_5^{(2)} + \ldots\right) z$$

$$+ \left(f_1^{(0)} f_3^{(1)} + f_1^{(0)} f_5^{(2)} + f_1^{(0)} f_7^{(3)} + f_3^{(1)} f_5^{(2)} + \ldots\right) z^2$$

$$- \left(f_1^{(0)} f_3^{(1)} f_5^{(2)} + f_1^{(0)} f_3^{(1)} f_7^{(3)} + \ldots\right) z^3 + \ldots \equiv \sum_{n=0}^{\infty} d'_n z^n \ . \quad (10)$$

We notice that the leading terms grow in order $(I_n)$ like $I_1 = 1$, $I_2 = 1 + 3 = 4$, $I_3 = 1 + 3 + 5 = 9$, \ldots, i.e., $\log d'_n \sim I_n = \sum_{j=0}^{n-1} (1 + 2j) = n^2$, a quadratic exponential convergence.

In the full evaluation of (9) we cannot expect the purely fundamental product terms to be leading forever. Arranging products like above according to the sum of the lower indices and calling the leading fundamental terms $F_{n2}$ we find the following expansion coefficients $C_n$:

$$C_0 = 1$$

$$C_1 = F_1 - f_3^{(1)} - f_5^{(2)} + O(7)$$

$$C_2 = F_4 + f_1^{(0)} f_5^{(2)} - c_6^{(0)} + f_1^{(0)} f_7^{(3)} + f_3^{(1)} f_5^{(2)} - c_9^{(0)} + O(10)$$
\[ C_3 = F_3 - c_9^{(0)} + f_3^{(1)} c_6^{(0)} - f_1^{(0)} f_3^{(1)} f_7^{(3)} + f_5^{(2)} c_6^{(0)} + f_1^{(0)} c_{10}^{(1)} + O(12) \]

\[ C_4 = -c_{12}^{(0)} + f_3^{(1)} c_9^{(0)} + f_5^{(2)} c_9^{(0)} - f_3^{(1)} f_5^{(2)} c_6^{(0)} + F_{16} + f_1^{(0)} c_{15}^{(1)} + \ldots + O(18) \]

\[ C_5 = -c_{15}^{(0)} + f_3^{(1)} c_{12}^{(0)} + f_5^{(2)} c_{12}^{(0)} - f_3^{(1)} f_5^{(2)} c_9^{(0)} + \ldots + F_{25} + \ldots + O(27) \quad (11) \]

e tc, where \( O(n) \) indicates terms of size \( \sim \Lambda^{-n} \). Up to and including \( n = 3 \) the convergence is unconditionally quadratic as in the ideal situation. At larger \( n \), however, due to the simple exponential decay of the pure curvatures, these as well as mixed curvature and fundamental cross product terms have outgrown the pure fundamental ones. Unless there now exist efficient additional cancellations within complexes of the form

\[ c_{3n}^{(0)} - f_3^{(1)} c_{3n-3}^{(0)} , \quad (12) \]

raising their order to at least \( n^2 \), a sudden change in the convergence behaviour of the semiclassical Selberg zeta function around \( n = 4 \) is to be expected. This is indeed what is observed in Figure 2.

### 2.2 The classical case

Following the procedure in the semiclassical treatment above we now analyse the slightly more complicated classical Selberg zeta function \([I]\),

\[ Z(z) = \prod_j \left[ \zeta_j^{-1}(z) \right]^{j+1} \]

\[ = (1 - f_1^{(0)} z - c_4^{(0)} z^2 - c_6^{(0)} z^3 - \ldots)(1 - f_2^{(1)} z - c_6^{(1)} z^2 - \ldots)^2(1 - f_3^{(2)} z - c_8^{(2)} z^2 - \ldots)^3 \ldots \]

Since in the classical case weights are proportional to powers of \(|\Lambda_p|^{-1}\), subscripts now indicate the size of the terms in powers of \(|\Lambda|^{-1}\) rather than \(|\Lambda|^{-1/2}\).
The convergence behaviour in the ideal case $c_i^{(j)} = 0$ is found as follows: From a straightforward expansion of

\[ Z(z) = \left(1 - f_1^{(0)} z\right) \left(1 - f_2^{(1)} z\right)^2 \left(1 - f_3^{(2)} z\right)^3 \ldots = \sum_{n=0}^{\infty} d_n z^n \quad (14) \]

one obtains the expansion coefficients

- $d_0 = 1$
- $d_1 = -f_1^{(0)} + \ldots = O(1)$
- $d_2 = 2f_1^{(0)} f_2^{(1)} + \ldots = O(3)$
- $d_3 = -f_1^{(0)} f_2^{(1)} f_2^{(1)} + \ldots = O(5)$
- $d_4 = 3f_1^{(0)} f_2^{(1)} f_2^{(1)} f_3^{(2)} + \ldots = O(8)$
- $d_5 = -3f_1^{(0)} f_2^{(1)} f_2^{(1)} f_3^{(2)} f_3^{(2)} + \ldots = O(11)$
- $d_6 = f_1^{(0)} f_2^{(1)} f_2^{(1)} f_2^{(1)} f_3^{(2)} f_3^{(2)} + \ldots = O(14)$
- $d_7 = -4f_1^{(0)} f_2^{(1)} f_2^{(1)} f_2^{(1)} f_3^{(2)} f_3^{(2)} f_4^{(2)} + \ldots = O(18) \quad (15)$

etc. The growth rule should be obvious: From the $j$th zeta function (counting $\zeta_0^{-1}$ as the 1st), there are $j$ consecutive contributions to the leading order terms, each increasing the order of magnitude by an amount $j$, i.e., $j = j_n$ grows by one over an interval of length $\Delta n = j_n$ and the total growth in order $I_n$ is $\Delta I_n = I_n + \Delta n - I_n = j_n^2$. For large $n$ one thus ends up with the following differential equations:

\[ \frac{dn}{dj} = j \quad (16) \]
\[ \frac{dI}{dn} = j \quad . \quad (17) \]
Eq. (16) gives $j_n = n^{1/2}$, which is inserted into Eq. (17). The solution of the resulting equation is the sought for asymptotic relation $I_n \sim n^{3/2}$.

The full evaluation of Eq. (13) gives

$$C_0 = 1$$

$$C_1 = F_1 - 2f_2^{(1)} - 3f_3^{(2)} + O(4)$$

$$C_2 = F_3 - c_4^{(0)} - f_2^{(1)} f_2^{(1)} + 3f_1^{(0)} f_3^{(2)} + 6f_2^{(1)} f_3^{(2)} + 4f_1^{(0)} f_4^{(2)} + O(6)$$

$$C_3 = F_5 - c_6^{(0)} + 2f_2^{(1)} c_4^{(0)} - 6f_1^{(0)} f_2^{(1)} f_3^{(2)} + 2f_1^{(0)} c_6^{(1)} + 3f_3^{(2)} c_4^{(0)} - \ldots + O(8)$$

$$C_4 = F_7 - c_8^{(0)} + 2f_2^{(1)} c_6^{(0)} - f_2^{(1)} f_2^{(1)} c_4^{(0)} - 2f_1^{(0)} f_2^{(1)} c_6^{(1)} + 3f_3^{(2)} c_6^{(0)} + \ldots + O(10)$$

$$C_5 = -c_{10}^{(0)} + 2f_2^{(1)} c_8^{(0)} - f_2^{(1)} f_2^{(1)} c_6^{(0)} + F_{11} + \ldots + O(12)$$

(18)

etc. The leading order terms in each $C_n$ which have to compensate in order to get the faster than exponential convergence $n^{3/2}$ are now of the form

$$c_{2n}^{(0)} - 2f_2^{(1)} c_{2n-2}^{(0)} + f_2^{(1)} f_2^{(1)} c_{2n-4}^{(0)} .$$

(19)

Things work out nicely until order 4; beginning from order 5 additional cancellations are needed. As figure 1 shows, these seem to occur in the classical case.

### 2.3 Numerical estimate of curvatures

A rather crude estimate of the individual curvature terms, $c_p^{(j)} \sim t_p \Lambda_p^{-(j+1)}$, where $t_p = |\Lambda_p|^{-1}$ in the classical and $t_p = |\Lambda_p|^{-1/2}$ in the semiclassical case, was used above to obtain the correct order of magnitude for the full curvatures $c_{i_n}^{(j)}$, each of which being a sum over individuals with the same symbol length. One would be able to benefit more from the results of the preceding sections if there were a
better estimate of the individual curvatures \( c_p^{(0)} \) in \( \zeta_0^{-1} \). Consider again a system with binary symbolic dynamics:

First note that due to uncertainty in the building of complexes like \( c_{00011}^{(0)} = t_{00011} - t_{0001} - t_0 t_{0011} + t_0 t_{011} \) and \( c_{00101}^{(0)} = t_{00101} - t_{001} t_0 t_{11} \) it appears necessary to collect curvatures with the same number of zeros and ones into a single term

\[
c_{nm} \equiv \sum_p \delta_{n,n_0} \delta_{m,n_1} c_p^{(0)} \, ,
\]

where the Kronecker \( \delta \)'s select primitive periodic orbits with number of symbols \( n_0 = n \) and \( n_1 = m \). After this precaution one may make the following ansatz,

\[
c_{n_0n_1} \equiv \alpha_{n_0n_1} \left( t_0 \Lambda_0^{-1} \right)^{n_0} \left( t_1 \Lambda_1^{-1} \right)^{n_1} \, ,
\]

hoping that the essential stability dependence has been correctly extracted, so that the prefactors \( \alpha_{n_0n_1} \) depend only weakly on stability. We aim at finding an approximation for the prefactors \( \alpha_{n_0n_1} \) better than \( \alpha_{n_0n_1} \sim 1 \).

We have calculated the prefactors \( \alpha_{n_0n_1} \) up to symbol length 6 for the open three disk system, with values of \( \rho (= d/R) \) ranging from 2.5 to 6.0, and with weights given by \( t_p = |\Lambda_p|^{-D} \). The results of the calculations are presented in Table 1 \((D = 1/2, \text{semiclassical case})\) and Table 2 \((D = 1, \text{classical case})\). The values for \( D = 1 \) are roughly twice those for \( D = 1/2 \) and some variation in parallel with the instabilities \( \Lambda_0 \) and \( \Lambda_1 \) are noticable. The dependence on \( n_0 \) and \( n_1 \) seems to be roughly binomial with an additional factor \( n_0 + n_1 \); we conclude that the data in Tables 1 and 2 should be more or less well approximated by the following formula:

\[
\alpha_{n_0n_1} \approx D \hat{h}_D(\Lambda_0(\rho), \Lambda_1(\rho)) (n_0 + n_1) \begin{pmatrix} n_0 + n_1 - 2 \\ n_0 - 1 \end{pmatrix} = D \hat{h}_D(\rho) B_{n_0n_1} \, ,
\]
where $h_D$ captures the dependence on the separation ratio $\rho$. Fig. 3 shows the rescaled prefactors $\alpha_{n_0 n_1}/DB_{n_0 n_1}$ as a function of $\rho$, together with the linear fits of the data:

$$\tilde{h}_1(\rho) \approx -0.584 + 0.378\rho \quad (23)$$

$$\tilde{h}_{1/2}(\rho) \approx -0.506 + 0.376\rho \quad . \quad (24)$$

The relative deviations from the linear fits are rather large for small values of $\rho$, but shrink with increasing $\rho$; at $\rho = 6$ the maximum relative error is less than 10% (semiclassical case). The ansatz $h_D(\Lambda_0, \Lambda_1) \approx \kappa_D \times |\Lambda_0 \Lambda_1|^{1/2}$ with $\kappa_1 \approx \kappa_{1/2} \approx 0.2$ is another simple and relatively accurate estimate.

Eq. (22) gives us information with sufficient detail that we may now return to the question whether there exist additional cancellations in the classical and semiclassical cycle expansions for the open three disk problem. The estimate of the full curvatures becomes

$$c^{(0)}_{i_n} \approx nDh_D \sum_{n_0=1}^{n-1} \binom{n-2}{n_0-1} \lambda_0^{n_0} \lambda_1^{n-n_0}$$

$$= nDh_D \lambda_0 \lambda_1 (\lambda_0 + \lambda_1)^{n-2} = nDh_D \lambda_0 \lambda_1 f_D^{n-2} , \quad (25)$$

where $f_D$ refers to $f_2^{(1)}$ in the classical and $f_3^{(1)}$ in the semiclassical case, respectively. For short, we have written $\lambda_0 \equiv t_0 \Lambda_0^{-1}$ and $\lambda_1 \equiv t_1 \Lambda_1^{-1}$. The perhaps surprising observation to emerge from Eq. (23) is that the leading pole of $\zeta^{-1}_0(z)$ has to be double:

$$\sum_n c^{(0)}_{i_n} z^n = Dh_D \lambda_0 \lambda_1 f_D^{-1} z \sum_n n (f_D z)^{n-1} \sim \frac{z}{(1 - f_D z)^2} . \quad (26)$$
If now (25) is inserted into the semiclassical complexes (12),
\[ c_n^{(0)} - f_D c_{n-1}^{(0)} \approx [n-(n-1)] Dh_D \lambda_0 \lambda_1 f_D^{n-2} = Dh_D \lambda_0 \lambda_1 f_D^{n-2} \neq 0 \text{ , (27)} \]
the terms do not cancel; there still remains a rest of (roughly) the order \(O(3n)\), building up a (simple) pole at \(z_p = 1/f_3^{(1)} = \left(|\Lambda_0|^{-1/2} \Lambda_0^{-1} + |\Lambda_1|^{-1/2} \Lambda_1^{-1}\right)^{-1}\). This is in line with our earlier numerical findings that the semiclassical Selberg zeta function is not free of poles. However, if we insert the same expression (25) into the classical complexes (19),
\[ c_n^{(0)} - 2 f_D c_{n-1}^{(0)} + f_D^2 c_{n-2}^{(0)} \approx [n-2(n-1) + (n-2)] Dh_D \lambda_0 \lambda_1 f_D^{n-2} = 0 \text{ , (28)} \]
the additional cancellations are there.

Note that the qualitative results above are independent of the choice of weight (i.e., the value of \(D\)); the different results for the classical and the semiclassical Selberg zeta function are entirely due to the difference in the power of \(\zeta_1^{-1}\). The double pole of \(\zeta_0^{-1}\) occurs at \(z_p \approx f_D^{-1}\), which is identical to the lowest order approximation of the leading zero of \(\zeta_1^{-1}(z)\). By taking the square of \(\zeta_1^{-1}(z)\) as in the classical Selberg zeta function one doubles the leading zero, which then precisely cancels the double pole of \(\zeta_0^{-1}\). In the semiclassical case the simple zero of \(\zeta_1^{-1}\) cancels only one pole with a simple pole remaining [Eq. (27)]. We study this point further below.

The conjecture \[3\] that the position of the poles of the dynamical zeta function \(\zeta_j\) is given by the zeros of \(\zeta_{j+1}\) remains valid, but the order of the poles is not simple but double. Returning to the arguments of Artuso et al. \[3, 10\] one notes that they are rather liberal with the prefactors; and it is precisely in the prefactors that the difference between a simple and a double pole resides.
3 Identification and removal of poles

In the case of maps, phase space averages can be related to zeros of zeta functions $Z(z) = \sum_{n=0}^{\infty} C_n z^n$. Practical calculations estimate such zeros from a truncation of the series, $F_N(z) = \sum_{n=0}^{N} C_n z^n$. In ideal situations, exponential \[3, 4\] or even faster than exponential convergence \[9\] is obtained. The presence of poles destroys faster than exponential convergence and makes it more difficult to calculate the exact positions of the zeros; consider a simple case where there is one zero and one pole:

$$F(z) = \frac{1 - az}{1 - bz} = (1 - az) \left(1 + b z + b^2 z^2 + \ldots \right) = 1 - (a - b) z - (a - b) b z^2 - \ldots = \sum_{n=0}^{\infty} C_n z^n.$$ (29)

We assume that $0 < b < a$. A truncation after the linear term gives a value of the zero $z'_0 = (a - b)^{-1}$. This is obviously a bad estimate of the true value $z_0 = a^{-1}$ if $a$ and $b$ are of the same order of magnitude. The inclusion of higher order terms only slowly improves $z'_0$, the error being $\sim (b/a)^N$ asymptotically. Furthermore, additional “ghost” zeros appear: The number of these unwanted zeros equals $N - 1$ and they do not vanish to infinity as $N$ grows large – they cluster around the circle $|z| = b^{-1}$, which borders the region of absolute convergence. To see this, consider the function

$$\tilde{F}_N(z) = \frac{(1 - az)(1 - (bz)^N)}{1 - bz} = (1 - az) \sum_{j=0}^{N-1} (bz)^j ,$$ (30)

which differs from $F_N(z)$ only in the coefficient $C_N$. It clearly has $N - 1$ additional zeros on the circle $|z| = b^{-1}$. 

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For $b > a > 0$ the situation is still worse; there is no zero of $F_N(z)$ converging to $z_0 = a^{-1}$.

If on the other hand the pole were absent, one would have a polynomial $1 - az$, which “converges” to its exact form already after the first term in the “expansion”; the zero $z_0 = a^{-1}$ is at once correctly determined. By estimating the value of $b$ from the asymptotic behavior of the coefficients $C_n$, we could remove the effect of the pole: Assume an estimate $\tilde{b}$ close to $b$ with $|b - \tilde{b}| = |\varepsilon| \ll a$. Then the function

$$
(1 - \tilde{b}z)F(z) = 1 - (a - \varepsilon)z - \varepsilon (a - b) z^2 \left[ 1 + bz + b^2 z^2 + \ldots \right]
$$

has already in the linear approximation a zero $\tilde{z}_0 = (a - \varepsilon)^{-1}$ close to $z_0$. The position of the ghost zeros may be estimated from the function (cf. Eq. (30))

$$
(1 - \tilde{b}z)\tilde{F}_N(z) = (1 - az)(1 + \varepsilon/b) \sum_{j=1}^{N} (bz)^j ;
$$

for large $z$, it is dominated by the highest power of $z$, so that its zeros lie on the circle $|z| \sim (\varepsilon/b)^{-1/N}b^{-1}$. They tend to infinity as $\varepsilon \to 0$.

Are several poles present, as e.g. in a rational function

$$
F(z) = \frac{P(z)}{Q(z)} ,
$$

with polynomials $P$ and $Q$, the zeros $|z_1| \ll |z_2| \ll |z_3| \ll \ldots$ of $Q$ being different from the zeros of $P$, the removal of the leading pole $z_1$ leaves a function where $z_2$ determines the convergence. In the special case $P(z) = (1 - az)$ and $Q(z) = (1 - b_1 z)(1 - b_2 z)$ with $0 < b_2 \ll b_1 < a$, the removal of $z_1 = b_1^{-1}$ pushes the ghost zeros to the neighborhood of $|z| = b_2^{-1}$ and the error in the linear estimate of $z_0$ shrinks from $b_1 [a (a - b_1)]^{-1}$, which may be larger than $a^{-1}$, to $b_2 [a (a - b_2)]^{-1} \ll$
If \( z_2 \) in the last example is not much larger than \( z_1 \), but close in magnitude, the improvement is of course only marginal. Thus, if two (or \( n \)) leading poles are close in magnitude, one has to remove both (all \( n \)) before any considerable improvement takes place.

To remove a certain number of poles in a consistent way, one may use a Padé approximation [25]: Assume that \( N + 1 \) coefficients \( C_n \) of the function \( F(z) = P(z)/Q(z) = \sum_{n=0}^{N} C_n z^n \) are known and that one wants to know the power series expansion of the unknown functions \( P_M(z) = \sum_{n=0}^{M} A_n z^n \) and \( Q_L(z) = \sum_{n=0}^{L} B_n z^n \).

With the normalization \( B_0 = 1 \), one has to determine \( M + 1 + L \) coefficients \( A_n, B_n \), so that \( N = M + L \) is required. The coefficients are determined from \( Q_L(z) F_N(z) = P_{N-L}(z) \), i.e.,

\[
\sum_{n=0}^{N} \sum_{n'=0}^{L} \theta(N-n-n')C_n B_{n'} z^{n+n'} = \sum_{n=0}^{N-L} A_n z^n ; \quad \theta(x) \equiv \begin{cases} 0 & x < 0 \\ 1 & x \geq 0 \end{cases} .
\tag{34}
\]

By identifying terms of equal power in \( z \), one finds altogether \( N + 1 \) equations for the \( M + L + 1 = N + 1 \) unknowns.

Once the coefficients are known, the solution of \( Q_L(\tilde{z}_p) = 0 \) gives approximately the position(s) of the dominant pole(s). If the computed value \( \tilde{z}_p \) converges for increasing \( L \) (and \( N \)), one may feel confident about really having identified a pole. Similarly, solutions of \( P_M(\tilde{z}_0) = 0 \) that converge for increasing \( L \) and \( N \) should give improved estimates of the zeros of the full function \( F(z) \). (Calculating poles is in general much more difficult than finding good values for the zeros; even the leading pole requires large \( N \).)

We have applied this to the three disk system. An approximation with linear
denominator $Q_1(z)$ already gave good results, confirmed and stabilized by computations for quadratic and higher order denominators. The positions of the leading zeros and poles of the full Selberg zeta function and of the three first dynamical zeta functions are listed in Tables 3-6. The data clearly confirm the conclusion drawn at the end of the last section that the poles of $\zeta_j^{-1} \approx$ coincide with zeros of $\zeta_j^{-1}$. The poles appeared in the computations either as pairs of nearby real values or as pairs of complex conjugate values with small imaginary parts; a strong indication that they are double. Assuming that they are all real and double, the identification of poles could in some cases be done with up to seven digits precision, applying an extrapolation scheme on the results given by different orders of approximations $N$ and $L$.

The improvement in the decay of the coefficients is apparent from Fig. 4, where we show the the behaviour of the coefficients $A_n$ in the $P_{N-1}(z)/Q_1(z)$ approximation of the semiclassical Selberg zeta function; in line with the above discussion we have approximated the denominator by $Q_1(z) = 1 - z/z_1$, where $z_1$ is the leading zero of $\zeta_1^{-1}$. With the leading pole gone, the faster than exponential decay now continues beyond $n = 4$ out to $n = 5$ or 6.

In the classical Selberg zeta function we were not able to identify any pole with the Padé technique ($N \leq 13$), which would imply that they are all cancelled by zeros of higher order dynamical zeta functions. As our numerical results show, however, the (leading) poles of the dynamical zeta functions are double; it is evident that the double zeros of $\zeta_1^{-2}$ do cancel the double poles of $\zeta_0^{-1}$, as was also shown in the preceding section, but the poles of $\zeta_1^{-2}$ are then quadruple and too many to be
completely cancelled by the triple zeros of $\zeta_2^{-3}$. Thus we expect the classical Selberg zeta function to have poles as well, the leading ones arising not from $\zeta_0^{-1}$ as in the semiclassical case, but from $\zeta_1^{-1}$. Since the magnitude of these poles is rather large, we have not been able to extract them directly from a Padé approximation to $Z(z)$.

## 4 Real and spurious zeros in quantum spectra

As mentioned in the introduction most calculations require the zeta functions not as functions of $z$ but rather as functions of frequency $\omega$ and energy $E$ or wavenumber $k$. Consider therefore a case similar to the one above, but with “energy” dependent coefficients, $C_n = C_n(E)$. Put $a = 1$, $b = e^{-\delta}$, and replace $z$ in Eq. (29) by $e^{iE}$ to obtain a function

$$F(E) = \frac{1 - e^{iE}}{1 - e^{iE-\delta}};$$

it mimics the behaviour of zeta functions in the case of a bounded system. We assume $\delta > 0$, consistent with $0 < b < a$ above. The function $F(E)$ has zeros $E_n = 2\pi n$, $n \in \mathbb{N}$ along the real axis and poles $E_n' = 2\pi n' - i\delta$, $n' \in \mathbb{N}$ along the line $\text{Im}(E) = -\delta$, defining the abscissa of absolute convergence in the complex $E$-plane.

We are interested in the properties of a finite order expansion of $F$ and introduce therefore a generalized function $\hat{F}(E, z)$ with the property $F(E) = \hat{F}(E, 1)$,

$$\hat{F}(E, z) = \frac{1 - e^{iE}z}{1 - e^{iE-\delta}z} = 1 - (1-e^{-\delta})e^{iE}z - (1-e^{-\delta})e^{2iE}z^2 - \ldots = \sum_{n=0}^{\infty} C_n(E)z^n. \quad (36)$$

The expansion in $z$ is only formal; at the end one puts $z = 1$. All results of the former section concerning zeros, poles, etc. can now be used, replacing $z$ by $e^{iE}$, $z_0$,
by $e^{iE_0}$, etc., and relating them to the complex $E$-plane rather than the $z$-plane. For a finite order expansion of $F(E)$ one may therefore immediately state the following:

(i) Any truncation of the power series puts the zeros of $F(E)$ off the real axis; in the linear approximation we obtain $e^{iE} = \left(1 - e^{-\delta}\right)^{-1}$, with solutions $E'_n = E_n - i\epsilon$, where $\epsilon = -\log(1 - e^{-\delta})$; for $\delta$ sufficiently large $\epsilon \approx e^{-\delta}$. The imaginary part of the energy vanishes with increasing $N$ like $\epsilon \sim e^{-\delta N}$. Large $N$ are required if the poles lie close to the real axis.

(ii) Ghost zeros of $F(E)$ will be found in the neighborhood of the line $\text{Im}(E) = -\delta$: There are $N - 1$ of them distributed more or less evenly around the circle $|e^{iE}| = e^{\delta}$; they satisfy $e^{iE} = e^{i\phi_j + \delta_j}$ with $\delta_j \approx \delta$, $0 \leq \phi_j < 2\pi$, $j = 1, 2, \ldots, N - 1$, i.e., $E = E_{n,j} = E_n + \phi_j - i\delta_j$. The ghost zeros converge towards the abscissa of absolute convergence and their number goes to infinity with $N$.

One may remove poles in the same manner as before; the formal expansion $\hat{F}(E, z) = \sum C_n(E)z^n$ is approximated with the Padé technique, $z$ is put to 1, and left is a power series approximation of the part of $F(E)$ containing the zeros. The energy dependent analogue of the two-pole example in the former section demonstrates the general tendency:

(iii) Removing leading poles has the following effect: Ghost zeros are pushed down in the negative imaginary direction; main zeros having small imaginary part approach the real axis.

The numerical investigations in this paper were performed for an open hyperbolic system, and property (i) has no relevance. Properties (ii)–(iii) are not restricted to bounded systems, though. We present numerical evidence that the removal of the
leading pole does indeed push what seems to be ghost zeros in the open three disk system far down in the negative complex energy plane: Fig. 5a shows the lower part of the spectrum of the \( N = 8 \) approximation of the semiclassical Selberg zeta function together with an improved spectrum where the leading pole has been removed (Padé, \( L = 1 \)). The original spectrum displays, in addition to the main zeros which lie relatively close to the real axis, a whole band of lower lying zeros. When plotting spectra with higher \( N \), one obtains main zeros at the positions of the old ones, but the zeros in the band seem not to stabilize and their number increases with \( N \). In the improved spectrum in Fig. 5a a few zeros in the band remain with approximately unchanged or even larger imaginary part, while most of the others are pushed away; in a certain range around \( \text{Re}(k) \approx 13 \), however, no such improvement of the spectrum can be noted.

To find out whether the remaining zeros correspond to real resonances, we can compare Padé improved spectra for different \( N \). Fig. 5b shows improved (\( L = 1 \)) spectra for \( N = 6 \) and \( N = 8 \). Except for the zeros in the interval \( \text{Re}(k) \approx 10 - 16 \) most remaining zeros in the \( N = 8 \) approximation correspond also to a nearby zero in the \( N = 6 \) approximation and thus seem to be stable. One exception is the zero at \( k \approx 24.4 - i1.5 \) – we have checked with the \( N = 10 \) approximation though and have found a corresponding zero very close to that position.

To see the correlation between the quantum spectra in Fig. 5a and the position of the leading poles, we have plotted the absolute values of the two lowest zeros of \( \zeta^{-1}_1(E, z) \) [assuming that they equal the poles of \( \zeta^{-1}_0(E, z) \) and \( Z(E, z) \)] as a function of \( \text{Re}(k) \) with \( \text{Im}(k) = -2.5 \) fixed, see Fig. 6. At low values of \( \text{Re}(k) \) the magnitude
of the second pole is much larger than the leading one, so that the removal of the leading pole has a large effect on the spectrum, which is also observed in Fig. 5a. Around \( \text{Re}(k) \approx 13 \) the two poles are very close in magnitude, which explains why the removal of just one pole only marginally affects the spectrum. For increasing \( \text{Re}(k) \) the number of leading poles with comparable magnitude increases; it becomes more and more difficult to improve the spectrum.

5 Summary and discussion

We have presented numerical evidence that the classical and semiclassical Selberg zeta functions for the open three disk system have poles. This shows that results for 1-d maps \[1, 26\] cannot be transferred immediately to higher dimensional systems, such as the three disk system. In the classical case at least this is somewhat surprising, since the system under consideration is an almost ideal hyperbolic 2d system (complete binary symbolics, highly unstable periodic orbits with \( |\Lambda_p| \gg 1 \), no intermittency). In the semiclassical case it was clear already from a simple plot of the expansion coefficients that the convergence soon settles for a simple exponential decay. This was confirmed by
(1) a numerical determination of zeros and poles of dynamical zeta functions, showing that the leading poles of $\zeta_j^{-1}$ equal the leading zeros of $\zeta_{j+1}^{-1}$, but are double and therefore not completely cancelled;

(2) a numerical estimate of the curvature corrections of $\zeta_0^{-1}$, showing that the leading pole is double;

(3) an analysis of the explicit terms in the expansion of $Z(z)$, which with use of (2) showed that necessary cancellations between cross terms, in addition to those present within the curvatures, do not occur, causing a transition in the convergence rate at around $n = 4$;

(4) the fact that stable poles could be extracted from $Q_L(z)$, the denominator of a Padé approximation, $Z(z) \approx P_{N-L}(z)/Q_L(z)$, and that the numerator $P_{N-L}(z)$ showed improved convergence.

A plot of the expansion coefficients of the classical Selberg zeta function shows seemingly a faster than exponential decay. This is not in contradiction to (2)–(4) above as explained at the end of section 2.3: The poles of $\zeta_0^{-1}$ are cancelled by the zeros of $\zeta_1^{-1}$, but there are not enough zeros from $\zeta_2^{-1}$ to cancel the poles in $\zeta_1^{-1}$. Nevertheless, we have not been able to locate a pole in the classical Selberg product by Padé analysis and the tests of Cvitanović and Rosenqvist [27] are also consistent with an $\exp\{-n^{3/2}\}$ scaling. The presence or absence of a pole in the classical Selberg zeta function thus remains an open question.

Since the zeros of dynamical zeta functions are relatively easy to compute, one may also quite easily identify the poles, provided there is a 1:1 (here rather 2:1) correspondence between poles and zeros of neighbouring dynamical zeta functions.
Our numerical findings give evidence that this is most probably the case for the leading zeros and poles. With the precision of our investigations, we were not able to identify stable next to leading poles from $Q_L(z) = 0$ more than in a few cases and then only with 1–2 digits precision; in these cases there did exist a next to leading zero within the uncertainty of the pole.

There are several ways to remove poles. The Padé numerator $P_M(z)$ directly gives an approximation of $Z(z)$ or $\zeta^{-1}_0(z)$. One may also first compute leading pole estimates $\tilde{z}_n$ from zeros of dynamical zeta functions and then multiply $\prod_n (1 - z/\tilde{z}_n)$ into the expansion of $Z(z)$. Furthermore, the classical Selberg zeta function can be used with semiclassical weights to improve the convergence for semiclassical zeros; the poles of $\zeta^{-1}_0$ will then be gone. If, finally, there actually is a $m : 1$ correspondence between the poles of $\zeta^{-1}_j$ and the zeros of $\zeta^{-1}_{j+1}$ for all $j$, the following construction,

$$\tilde{Z}(z) \equiv \prod_j \left[ \zeta^{-1}_j \right]^{m^j}(z) = \exp \left\{ - \sum_p \sum_r \frac{z^{rnp}}{r} \frac{t^r_p}{1 - m\Lambda^p r} \right\},$$  \hspace{1cm} (37)

is free of poles and has zeros which equal the zeros of $\zeta^{-1}_0(z)$ and $Z(z)$. A numerical test for the three disk system ($m = 2$) shows that this zeta function (classical or semiclassical weights) really has faster than exponential convergence all the way out to the largest $n$ considered (=13). Eq. (37) and related forms require further investigations.

Recently, quantum spectra of bounded chaotic systems have been computed from expansions of the semiclassical Selberg zeta function \[28, 29, 30\]. Despite some success, the calculations were made difficult by slow convergence, no clear indication that the zeros of the Selberg zeta function approach the real axis as $N \to \infty$, missing quantum levels, and presence of spurious zeros (i.e., zeros of $Z(E)$
not associated with exact quantum eigenvalues). The pole induced properties (i)–(ii) of the preceding section are here recognizable. We therefore suggest a relation, similar to the simple example above, between the position of poles and the distance from the real axis of the zeros of $Z(E)$ [or $\zeta^{-1}_0(E)$] in bounded systems. In the calculations for the anisotropic Kepler problem and the closed three disk system, there is one obvious pole, connected with an orbit not realized by the dynamics, but for which heteroclinic orbits of arbitrary length exist. This pole has been removed in the calculations reported in [29]. But the present investigation suggests that there are further poles, not so simply identified. We suspect that they are at least partially responsible for the bad convergence of the zeros of $Z(E)$ (in bounded systems there are many other sources of trouble, like intermittency and stable islands). Spurious zeros present in cycle expanded spectra could be (in many cases at least) nothing but the ghost zeros connected to the poles. Improved spectra should therefore be obtained by removing the leading poles, as done here for the open three disk system.

6 Acknowledgments

This work has been performed with financial support (to G. Russberg) from the Alexander von Humboldt-Stiftung.
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Figure captions

Figure 1: Expansion coefficients $C_n$ of the classical Selberg zeta function (1) for different $d/R$ in the open three disk system. ($A_1$-representation.)

Figure 2: Expansion coefficients $C_n$ of the semiclassical Selberg zeta function (3) for different $d/R$ in the open three disk system. ($A_1$-representation.)

Figure 3: Rescaled semiclassical (boxes) and classical (crosses) curvature prefactors, $\alpha_{n_0n_1}/DB_{n_0n_1}$, for different $\rho (= d/R)$ in the $A_1$-representation. The straight lines are the corresponding linear approximations (Eq. (24)): $\tilde{\hbar}_{1/2}(\rho)$ in the semiclassical case (broken line), and $\tilde{\hbar}_1(\rho)$ in the classical case (continuous line).

Figure 4: Improved convergence is achieved in the semiclassical Selberg zeta function (3) after removal of the leading pole: The figure shows the expansion coefficients of $(1 - z/z_1)Z(z)$ where $z_1$ is the leading zero of $\zeta_1^{-1}(z)$. The data are for the $A_1$-representation.

Figure 5: Semiclassical resonances for the open three disk system for $d/R = 3$, computed using Selberg’s zeta function in the $A_2$-representation. The energy is expressed in terms of $k = k(E) \equiv \sqrt{2mE}/\hbar$. (a) Spectrum in the $N = 8$ approximation, without
removal (boxes) and with removal (crosses) of the leading pole.

(b) Spectrum with the leading pole removed, in the $N = 8$ (boxes) and $N = 6$ (crosses) approximation.

**Figure 6:** The magnitude of the leading and next to leading zero of the semiclassical $\zeta_1^{-1}(E, z)$ as a function of $\text{Re}(k)$ with $\text{Im}(k) = -2.5$. The zeros are assumed to equal the leading and next to leading pole of $Z(E, z)$. ($d/R = 3$, $A_2$-representation.)
Table captions

Table 1: Semiclassical curvature prefactors $\alpha_{n_0,n_1}$ of $\zeta^{-1}_0$ (eq. (4)) for the open three disk system ($A_1$-representation).

Table 2: Classical curvature prefactors $\alpha_{n_0,n_1}$ of $\zeta^{-1}_0$ (eq. (2)) for the open three disk system ($A_1$-representation).

Table 3: Leading zeros and poles of the semiclassical Selberg zeta function (3) and of the three lowest order dynamical zeta functions (4) in the $A_1$-representation, determined from different Padé approximations of the respective functions ($N \leq 13$).

Table 4: Zeros and poles of the semiclassical zeta functions in the $A_2$-representation. (Cf. Table 3.)

Table 5: Zeros and poles of the classical zeta functions in the $A_1$-representation. Ellipses in column two indicate that no pole could be determined from the Padé approximation. (Cf. Table 3.)

Table 6: Zeros and poles of the classical zeta functions in the $A_2$-representation. Ellipses in column two indicate that no pole could be determined from the Padé approximation. (Cf. Table 3.)