Chapter 40

Quantum pinball

Semiclassical periodic orbit expansions are applied to the dynamics of a point particle scattering elastically off several disks in a plane. Fredholm determinants, zeta functions, and convergence of their cycle expansions are tested and applied to evaluation of quantum resonances. We demonstrate the utility of the periodic orbit description of chaotic motion by computing from a few periodic orbits highly accurate estimates of a large number of quantum resonances for the classically chaotic 3-disk scattering problem. The symmetry decompositions of the eigenspectra are the same for the classical and the quantum problem, and good agreement between the periodic orbit estimates and the exact quantum poles is observed. make a remark here

We shall here focus on an ideal quantum system, scattering off three (or more) disks in the plane. The system that we shall discuss here is simple, yet physical and instructive.

PREDRAG'S REMARK:
What was really done in the introductory lecture on billiards: The subject was develop to detect a cylinder by waves (ie submarine, by radar): Frantz, Keller, Maslov.

That 1 disk scattering resonances are known analytically; 2-disk not, but there is no chaos; 3-disk first example of chaos, known by semi-analytic methods only recently.

That repellers clean as purelly hyperbolic, trivial symbolic dynamics.

I explained that for elastodynamics Mark found a quartz fortune teller's ball from Madagascar, measured 500.000 resonaces, and theorists are happy to compute 100.

That there are almost no analytic solutions known (square, circle, parallelopiped, perhaps sphere in isotropic case).

That numerics can barely do anything else but a potato.

That hard ceramics gas valves and MEMS need new quality control

techniques, perhaps in frequency rather than time domain.
- END PREDRAG'S REMARK -

Our classical pinball system consists of a point particle and three identical circular disks in the plane (fig. 40.5.4a). The point particle is scattered elastically off the disks and moves freely between collisions. The dynamics with one or two disks is simple (there is either no or one trapped trajectory), but with three or more disks there are infinitely many trapped trajectories, forming a repeller. This repeller can be in principle observed by measurements such as irregularly fluctuating outgoing angles *vs.* impact parameter, but such measurements are difficult and very sensitive to small perturbations. Much more robust are the global averages such as the mean trapping time; resonances and the delay times.

We shall apply here the expansion (31.2) to evaluation of repeller escape rates. The classical repeller escape rate γ is determined by the largest zero of $1/\zeta(s)$ (s real) with each prime cycle weighted by

$$t_p(s) = \Lambda_p^{-1} e^{-sT_p}. \tag{40.1}$$

Here T_p is the period of the prime cycle p and $\mu_p = \ln(\Lambda_p)$ is its stability exponent, where Λ_p is the leading eigenvalue of the cycle Jacobian. The associated *quantum* amplitude is essentially the square root of the classical weight.

The logarithmic derivative of the infinite product of ζ functions $\det(\hat{H}-E)_{sc} = \prod_{j=0}^{\infty} \zeta_j^{-1}(k)$, where the weights of the prime cycles for the different ζ_j's are

$$t_p^{(j)} = e^{-\mu_p(1/2+j)+\frac{i}{\hbar}S_p(k)+i\pi\nu_p/2}, \tag{40.2}$$

where $S_p(k)$ is the action and ν_p the Maslov index, and k is the quantum wavenumber. The zeros of $\det(\hat{H}-E)_{sc}$ in the complex k plane determine the eigenvalues or resonances of the quantum system; here we shall compute only those closest to the real energy axis, which are given by the zeros of $1/\zeta_0(k)$.

We have chosen here the 3-disk scattering system because it captures the essential topology, stability and phase space structure of cycles in 2-d non-integrable potentials without the complications typical of motions in generic smooth potentials (pruning of the symbolic dynamics mixed phase space, intermittency effects due to marginally stable orbits. The billiard cycles are faster to compute than for arbitrary smooth potentials, and we were aided much by the availability of the exact spectra in checking our results.

point to remark

40.1 Spectral determinant for two-dimensional systems

spectral!determinant@“fd!2-dimensional

For Hamiltonian flows in two configuration dimensions the monodromy matrix M_p has two eigenvalues Λ_p and $1/\Lambda_p$, as explained in sect. 5.2. Isolated periodic orbits can be elliptic or hyperbolic. Here we discuss only the hyperbolic case, when the eigenvalues are real and not equal to one in magnitude. The determinant appearing in the trace formulas can be written in terms of the expanding eigenvalue as

$$|\det(1 - M_p^r)|^{1/2} = |\Lambda_p^r|^{1/2}\left(1 - 1/\Lambda_p^r\right) ,$$

and its inverse can be expanded as a geometric series

$$\frac{1}{|\det(1 - M_p^r)|^{1/2}} = \sum_{k=0}^{\infty} \frac{1}{|\Lambda_p^r|^{1/2}\Lambda_p^{kr}}.$$

restore links and exercises

With the 2-dimensional expression for the average density of states (36.9) the spectral determinant becomes

$$\begin{aligned}\det(\hat{H} - E)_{sc} &= e^{i\frac{mAE}{2\hbar^2}} \exp\left(-\sum_p \sum_{r=1}^{\infty}\sum_{k=0}^{\infty} \frac{e^{ir(S_p/\hbar - m_p\pi/2)}}{r|\Lambda_p^r|^{1/2}\Lambda_p^{kr}}\right) \\ &= e^{i\frac{mAE}{2\hbar^2}} \prod_p \prod_{k=0}^{\infty}\left(1 - \frac{e^{\frac{i}{\hbar}S_p - \frac{i\pi}{2}m_p}}{|\Lambda_p|^{1/2}\Lambda_p^k}\right) .\end{aligned} \qquad (40.3)$$

⇓PRELIMINARY

40.2 Semiclassical zeta function

add a section on the $k = 0$ zeta function part

40.3 Three-disk pinball

⇑PRELIMINARY

Here we shall illustrate the convergence of curvature expansions by computing the classical escape rates and quantum resonances for scattering off three disks. In this system the classical motion can be visualized as a pinball bouncing in a plane between three equally spaced disks of equal radius, and the quantum dynamics is described by wave functions which vanish on the boundaries of the disks. For billiard motion the momentum $vm = \hbar k = \sqrt{2E/m}$ is constant, the action $S_p(k)$ is given by $\hbar k L_p$, where L_p is the length of the cycle p, and the quantum amplitude (40.2) associated with the cycle p is simply $t_p = |\Lambda_p|^{-1/2} e^{ikL_p + in_p\pi}$. Here n_p is the number of bounces, and comes from the phase loss at every reflection (the boundary condition is $\psi|_{disk} = 0$).

point to remark

replace by back reference

The prerequisite for efficient use of curvature expansions is firm control of the symbolic dynamics. For sufficiently separated disks, the symbolic

refer to earlier text, rather than to refs. [40.2, 6.3] dynamics is a ternary dynamics with alphabet $\{1, 2, 3\}$ (the label of the disk the pinball bounces off) and a single pruning rule prohibiting consecutive repeats of the same symbol. The corresponding curvature expansion (31.2) is straightforward, and converges well. The C_{3v} point group invariance of the 3-disks problem simplifies and improves the curvature expansions in a rather beautiful way. The corresponding contributions to the Euler product (31.2) factorize as follows:

$$
\begin{aligned}
(1-t_p)^2 &= (1-t_p^{1/3})(1-t_p^{1/3})(1+t_p^{1/3}+t_p^{2/3})^2 \\
(1-t_p)^3 &= (1-t_p^{1/2})(1+t_p^{1/2})(1-(t_p^{1/2})^2)^2 \\
(1-t_p)^6 &= (1-t_p)(1-t_p)(1-t_p)^4 .
\end{aligned}
\tag{40.4}
$$

The three factors in this product contribute to the C_{3v} irreducible subclasses A_1, A_2 and E, respectively, and the 3-disk zeta function factorizes into $\zeta = \zeta_+ \zeta_- \zeta_E^2$. Due to the symmetry, any 3-disk cycle can be pieced together from segments passing through the *fundamental domain* (see Fig. ?1?). The $t_p^{1/2}$, $t_p^{1/3}$ weights in (40.4) have direct physical meaning: they are the weights of the corresponding cycles restricted to the fundamental domain.

Restriction to the fundamental domain also simplifies the symbolic dynamics: it becomes binary, with no restrictions on allowed sequences [6.1, 40.31, 6.3]. The ternary 3-disk $\{1, 2, 3\}$ labels are converted into the binary fundamental domain labels $\{0, 1\}$ by marking the backscatter by 0 and scatter to the third disk by 1. For ex., $\overline{23} = \ldots 232323 \ldots$ maps into $\ldots 000 \ldots = \overline{0}$ (and so do $\overline{12}$, $\overline{13}$), $\overline{123} = \ldots 12312 \ldots$ maps into $\ldots 111 \ldots = \overline{1}$, and so forth. (see Fig. ?1?).

The Euler product (31.2) on each irreducible subspace is easily evaluated using the factorization (40.4). On the symmetric A_1 and the antisymmetric A_2 subspaces, the ζ_+ and ζ_- are given by the standard curvature expansion for the binary dynamics:

$$
\begin{aligned}
1/\zeta_{\mp} &= (1 \pm t_0)(1-t_1)(1 \pm t_{10})(1-t_{100})(1 \pm t_{101})(1 \pm t_{1000}) \ldots \\
&= 1 \pm t_0 - t_1 \pm (t_{10} - t_1 t_0) - (t_{100} - t_{10} t_0) \pm (t_{101} - t_{10} t_1) \\
&\quad -(t_{1001} - t_1 t_{001} - t_{101} t_0 + t_{10} t_0 t_1) - \ldots \ldots
\end{aligned}
\tag{40.5}
$$

while for the mixed-symmetry subspace E the curvature expansion is given by

$$
\begin{aligned}
1/\zeta_E &= (1 + t_1 + t_1^2)(1 - t_0^2)(1 + t_{100} + t_{100}^2)(1 - t_{10}^2) \ldots \\
&= 1 + t_1 + (t_1^2 - t_0^2) + (t_{100} - t_1 t_0^2) + t_{1001} + (t_{100} - t_1 t_0^2) t_1 - t_{10}^2 \ldots
\end{aligned}
\tag{40.6}
$$

Given the curvature expansions (40.5) and (40.6), the calculation is straightforward. We set the disk radius $a = 1$, fix the disk-disk center separation $R = 6$ (for the sample values listed here), compute the eigenvalues and lengths of prime cycles up to 5 bounces (total of 14 cycles), substitute them into the curvature expansions, and determine the complex zeros; some hundred quantum resonances are easily determined, with accuracy as good as 7 significant digits for the resonances closest to the real axis. In Table ?1? we list a few typical results, illustrate their convergence by computing them with different maximal length cycles, and compare them to the numerical solutions for poles of the exact quantum scattering matrix. The convergence of the curvature expansions is striking; they are many orders of magnitude more accurate than the estimates by other methods, and the gain in efficiency is dramatic: while the quantum scattering matrix requires computation of large truncations (of order of (70×70)) of infinite matrices with Bessel functions entries, the curvature expansions require evaluation of some dozen complex exponentials and a couple of sums and differences. The judicious use of symmetry helps considerably; for example, going to the fundamental domain often *doubles* the number of significant digits for a given cycle length. The estimates can be further improved by extrapolations and knowledge of the analyticity properties of $1/\zeta$, e.g. the positions of poles.

No poles of the infinite product can occur within the half-plane of absolute convergence [40.16]. This also leads to an upper bound on the resonance lifetimes. The abscissa of absolute convergence can be determined as the leading zero of (40.5) with t_p replaced by $|t_p|$; $\mathrm{Im}(k)$ for all zeros of $1/\zeta$ must lie below k_c (for the present a:R=1:6 example, $k_c = -0.121557\ldots$). The convergence of the curvature expansion is best near k_c (the longest lived resonances) and deteriorates as one moves further in the imaginary k direction. As Re k grows, the density of resonances increases. Implications for the curvature expansion are that a certain number of terms have to be included before two resonances are distinguished; thereafter one again observes rapid convergence. This is illustrated in table ?1? for the resonances k_2 and k_3, which have the same n=1 approximation.

The explicit curvature expansions like (40.5) and (40.6) perhaps make it easier to explain our claims about the exponential convergence of curvature expansions. A typical curvature expansion term involves a long cycle $\{ab\}$ minus its shadowing approximation by shorter cycles $\{a\}$ and $\{b\}$: insert tosect{} here

$$t_{ab} - t_a t_b = t_{ab}(1 - t_a t_b / t_{ab}) = t_{ab}(1 - e^{-\Delta\mu_{ab}/2 + ik\Delta S_{ab}})$$

where $\Delta\mu_{ab} = \mu_a + \mu_b - \mu_{ab}$ and $\Delta S_{ab} = S_a + S_b - S_{ab}$. The exponential fall off of curvatures is a consequence of the smallness of the term in the brackets; $\Delta\mu$ and ΔS are exponentially small for long orbits, typically $O(e^{-\mu_{ab}})$. Therefore, to resolve some scale Δk, one has to keep all *difference* actions $> 1/\Delta k$. Their number increases like $(\Delta k)^{h/\lambda}$, i.e., roughly linearly (if the topological entropy h equals the average Lyapunov exponent λ), and not exponentially, as one might expect naively.

Figure caption

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1. The scattering geometry for the disk radius/separation ratio $a : R = 1 : 2.5$. (a) the three disks, with $\overline{12}$, $\overline{123}$ and $\overline{121232313}$ cycles indicated.

Table caption: Representative classical escape rate and quantum resonance results, illustrating the convergence of the curvature expansions. The calculations listed here are for disks with ratio radius to separation $a : R = 1 : 6$. The first column gives the maximal cycle length used, the second the estimate of the classical escape rate from the full 3-disk cycle expansion, the third from the fundamental domain expansion. For comparison, numerical simulation [6.2] yields $\gamma = .410\ldots$, and the $n = 2, 3$ approximations of ref. [6.2]. yield 0.3102, 0.4508 respectively. The remaining columns illustrate convergence of "typical" quantum resonances from the A_1 subspace. For comparison, the exact quantum values [6.2, 40.19] are given in the last row; the $n = 3$ approximation of ref. [6.2] gives $k_1 = 8.354$–i0.342.

	quantum pole					
n	Re(k_1)	Im(k_1)	Re(k_2)	Im(k_2)	Re(k_3)	Im(k_3)
1	8.35954	−0.32103	27.36117	−0.15486	27.36117	−0.15486
2	8.26784	−0.28354	27.25948	−0.16044	27.68086	−0.36148
3	8.27549	−0.27576	27.25883	−0.15587	27.67331	−0.33837
4	8.27662	−0.27696	27.25922	−0.15561	27.67015	−0.33556
5	8.27640	−0.27712	27.25925	−0.15562	27.66956	−0.33531
exact	8.2611	-0.2749	27.2548	-0.1555	27.6661	-0.3340

40.4 Classical pinball

40.4.1 Symmetries of the system

We have already discussed the symmetries of the 3-disk pinball and its periodic orbits in sect. 22.1.1.

☞ sect. 22.1.1

40.4.2 Symbolic coding

We have already discussed the symbolic dynamics of the 3-disk pinball and its periodic orbits in sect. 1.4 and example 11.2.

☞ sect. 1.4
☞ example 11.2

40.4.3 Periodic orbits

There is only one length scale in the system, the ratio of the center-to-center separation to the disk radius $d : R$. The energy is a quadratic function of momenta, $H = p^2/2m$, so motion at different energies E and E_0 is related by the scaling $p_E \to p_0\sqrt{E/E_0}$ for momenta, $t_E \to t_0\sqrt{E_0/E}$ for times, and

$$S(E) = L\sqrt{2mE} = S(E_0)\sqrt{E/E_0} \qquad (40.7)$$

for the actions, where L is the geometrical length of the orbit. The eigenvalues of the Jacobian transverse to a periodic orbit (see below) are invariant under the above energy rescaling. These observations will be useful below in the semiclassical context where the (34.15) will combine with $\hbar$ to the relevant quantum variable, the wavenumber $k = \sqrt{2mE}/\hbar$.

Each map has a fixed point, corresponding to the orbits $\overline{0}$ and $\overline{1}$. Longer periodic orbits are fixed points of sequences of maps, e.g.

$$T_0 T_0 T_1 T_0 T_1 x_{10100} = x_{10100} \,, \tag{40.8}$$

check if incorporated?: (note that in our convention the maps are applied in reverse order compared to the symbolic sequence).

The Jacobian of the single collision map is given by The sign of the eigenvalue depends of the number of collisions along the cycle. For the '0' symbol there are two bounces in the fundamental domain: one with the disk and one with the reflecting wall. Since the wall can be regarded as a disk of infinite radius, the trace changes sign two times and thus the eigenvalues are positive. Symbol '1' corresponds to one bounce with the disk but two wall bounces and hence the eigenvalues of the '1'-cycle are negative. For an arbitrary fundamental domain cycle, the eigenvalue sign is given by $(-1)^{n_1}$, where n_1 is the number of '1's in the binary string corresponding to the cycle.

link

add pointer

8.1
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The exact lengths and eigenvalues of $\overline{0}$, $\overline{1}$ and $\overline{10}$ cycles follow from elementary geometrical considerations, and are left to the reader as exercises. Longer cycles require numerical evaluation by methods such as the multipoint shooting or orbit length minimization. A typical set of the periodic orbit data, for $d : R = 6$ and length ≤ 6, is listed in table ?2?.

8.2
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add pointers

40.5 Quantum pinball

For the three disk system, the explicit expressions of the outgoing waves in terms of the ingoing waves using the quantum scattering matrix S have been given by Gaspard and Rice. Resonances are related to complex zeros of $\mathrm{tr}\, S^\dagger \frac{dS}{dE}$, the generalization of the concept of the density of states to scattering systems. We shall first evaluate these complex zeros in the semiclassical approximation, and then compare them with the exact quantum-mechanical resonances.

40.5.1 The semiclassical density of states

The group theoretic weights associated with reducing the dynamics to irreducible representations of the discrete symmetry group can sometimes also be absorbed into the phase indices. In the A_1 representation, one has only reflections at the disks, none at the boundaries of the fundamental domain. Therefore, $\mu_p = 2n_p$, since the symbol string length counts the number of the disk collisions. For the A_2 representation, the wave function is antisymmetric under reflections at the symmetry lines, and one can associate one additional reflection with each occurence of the symbol 0, and two reflections with each occurence of the symbol 1. The net effect is an additional overall minus sign, if the number of 0's in the symbol string of the orbit is odd. Furthermore, special attention should be paid to the orbits that run along the borders of the fundamental domain. The 3-disk system studied here does not have boundary orbits, but the 4-disk system, for example, does have such orbits.

link section

As mentioned above one can replace $S_p(E)/\hbar = L_p k$, where L_p is the geometric length of the orbit, and k is the wavenumber.

$$\rho(k) = -\mathrm{Im}\frac{1}{\pi}\frac{\partial}{\partial k}\log Z(k) \tag{40.9}$$

where $Z(k)$ is

$$Z(k) = \prod_{j=0}^{\infty}\prod_{p}(1 - e^{iL_p k - i\mu_p\pi/2}|\Lambda_p|^{-1/2}\Lambda_p^{-j})\,. \tag{40.10}$$

The quantum Selberg zeta function can also be expressed as a product over dynamical zeta functions,

$$Z(k) = \prod_{j=0}^{\infty} 1/\zeta_j\,, \tag{40.11}$$

this time with cycles weighted by semiclassical weights

$$t_p = z^{n_p} e^{iS_p/\hbar - i\mu_p\pi/2}/|\Lambda_p|^{1/2}\;. \tag{40.12}$$

Thousands of semiclassical and exact quantum resonances in the three symmetry subspaces A_1, A_2 and E have been computed; some of them are listed in table ?4? and plotted in fig. 40.5.4. The accuracy and numerical convergence of the semiclassical estimates cames as a surprise.

40.5.2 "Quantum escape rate"

The region of absolute convergence of the Gutzwiller trace formula in the $k = \kappa - is$ complex plane is determined by the convergence of the sum of absolute values of the terms in the series (**??**). The sum converges absolutely for $s < s_c$, where s_c is called the abscissa of absolute convergence. Since s_c is the value of s for which the sum

$$\tilde{\Omega}(s) = \sum_p \frac{T_p}{|\det(\mathbf{1} - \mathbf{J}_p)|^{1/2}} e^{sT_p}\,, \tag{40.13}$$

diverges, one can, by analogy to the determination of the classical escape rate by the divergence of the sum , interpret the abscissa of absolute convergence s_c as a "quantum escape rate". In fact, s_c is only a lower bound on the escape rate; the correct rate of a decay of a given initial wave function is given by a superposition of complex resonances evaluated below. Within the same short cycles truncations as in the classical case, one finds the s_c curves shown in the lower half of fig. 40.5.4.

ref

upper?

recheck?

Since the trace formulas are convergent in the domain of absolute convergence, one cannot have zeros of the zeta function or resonances of the S-matrix in that domain. In particular, for sufficiently large $d : R$, all resonances will stay a finite distance from the real axis. In contrast to the classical case, for $d : R$ less than about 2.8 the bound s_c actually becomes negative. As we shall see below, the semiclassical resonances do lie below the real axis, as they should; but this serves as a reminder that the resonances (and the energy eigenvalues for bound systems) are being evaluated in a region where cycle expansions are only conditionally convergent, and one has to be very careful in ordering terms in such expansions.

The same absolute convergence arguments can be applied to the dynamical zeta functions. Their logarithmic derivatives correspond to sums over orbits of form

$$-\frac{\partial}{\partial k}\ln\zeta_j = i\sum_p L_p \frac{e^{iL_p k - i\mu_p\pi/2}}{|\Lambda_p|^{1/2}\Lambda_p^j}\,. \tag{40.14}$$

Due to the extra powers of Λ_p's present in $1/\zeta_j$ cycle weigths, the corresponding abscissas of absolute convergence form an ordered sequence $s_j < s_{j-1} < \cdots < s_0$. The resonances closest to the real axis - which will be noticable as the sharpest resonances - should be due to zeros in $1/\zeta_0$ since the leading zeros of other $1/\zeta_j$ have larger imaginary parts. We find it often convenient to use this fact and restrict our numerical work to the leading zeros of $1/\zeta_0$ rather than the full Selberg zeta functions.

40.5.3 Quantum resonances

> If the same -Vedic mantra- is chanted loudly ("Vedaghosa") it will give divine joy to the listeners even if they do not understand its meaning. Such a sound has the power to make mankind happy.
> Guru Pujyasri Chandrasekharendra Sarasvati Svami,
> *"Hindu Dharma: The Universal Way of Life"*

We evaluate the exact quantum mechanical resonances by the method described in refsect{??}. A comparison of resonances obtained from cycle expansions truncated to the 14 cycles of periods ≤ 5 with the exact quantum values is given in table 5?. and in fig. 40.5.4, together with the difference between the semiclassical and quantum resonances $\delta = \sqrt{|k_{QM} - k_{sc}|}$.

Numerically this difference seems to decrease with increasing Re k, i.e., with approach to the semiclassical limit. As the semiclassical approximation ignores terms of higher order in $\hbar$, one expects on general grounds this difference to approach a non-zero constant. Our data are insufficient to estimate the asymptotic behaviour and to bound it away from zero.

Also shown in fig. 40.5.4 is the abscissa of absolute convergence s_c. No semiclassical resonance lies above it. Two of the lowest exact quantum resonances, for which the semiclassical approximation error is largest, do lie above s_c, but that is acceptable as the bound is semiclassical.

40.5.4 Poles of dynamical zeta functions

The exponential decay of the coefficients for $1/\zeta_0$ indicates the presence of a 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 (**??**) is entire implies that the poles in $1/\zeta_j$ must have right multiplicities in order that they be cancelled in the $F = \prod 1/\zeta_j$ product. More explicitely, $1/\zeta_j$ can be expressed in terms of weighted Fredholm determinants

$$F_j = \exp\left(- \sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{(t_p/\Lambda_p^j)^r}{(1 - 1/\Lambda_p^r)^2} \right) \tag{40.15}$$

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 of $1/\zeta_j$. This yields

$$1/\zeta_j = \frac{F_j F_{j+2}}{F_{j+1}^2} \,, \tag{40.16}$$

and we conclude that for 2-dimensional Hamiltonian flows the dynamical zeta function $1/\zeta_j$ has a *double* leading pole coinciding with the leading zero of the F_{j+1} Fredholm determinant.

The effect of such convergence properties of the coefficients on the calculation of classical and quantum escape rates is demonstrated in table 5? and figure 40.5.4.

	n	. Z_{qm}	. $1/\zeta_0$
	1	0.11	0.119
	2	0.12153	0.12152
	3	0.1215574	0.121556
$d:R=6$	4	0.121557625	0.12155760
	5	0.1215576283	0.121557627
	6	0.1215576284	0.1215576284
	7	0.1215576284	0.1215576284
	1	-0.076	0.019
	2	0.041	0.038
	3	0.04052	0.0403
	4	0.040575	0.04054
$d:R=3$	5	0.0405789	0.040575
	6	0.04057935	0.040578
	7	0.040579405	0.0405793
	8	0.0405794102	0.04057940
	9	0.0405794108	0.0405794099
	10	0.0405794108	0.0405794107

Table 4?. Quantum escape rates computed from the Fredholm determinant F_{cl} (??), the quantum Selberg zeta function Z_{qm} (40.10), and the dynamical zeta function $1/\zeta_0$, as function of the maximal cycle length. Due to the presence of the same pole in both quantum zeta functions, the convergence of the quantum Selberg zeta function is not significantly better than the convergence of the dynamical zeta function. See also fig. 40.5.4.

The scattering geometry for the disk radius : separation ratio $R : d = 1 : 2.5$. (a) the three disks, with $\overline{12}$, $\overline{123}$ and $\overline{121232313}$ cycles indicated. (PC: REFRE BACK TO THE FIGURE)

Some examples of 3-disk cycles: (a) $\overline{12123}$ and $\overline{13132}$ are mapped into each other by σ_{23}, the flip across 1 axis; this cycle has degeneracy 6 under C_{3v} symmetries. (PC: REFER BACK TO THE FIGURE)

	Re k_{QM}	Im k_{QM}	Re k_{zeta}	Im k_{zeta}
A_1	0.69800	-0.07497	0.75831	-0.12282
	2.23960	-0.11880	2.27427	-0.13305
	3.76270	-0.14756	3.78787	-0.15412
	4.13165	-0.61702	4.15179	-0.66591
	5.27569	-0.18325	5.29607	-0.18678
	6.77609	-0.22750	6.79366	-0.22986
	8.26114	-0.27492	8.27663	-0.27698
	9.73452	-0.13880	9.74826	-0.32121
	10.33819	-0.37371	10.34656	-0.37834
	11.20210	-0.35823	11.21361	-0.36168
	11.90760	-0.33223	11.91448	-0.33488
	12.66760	-0.39467	12.67500	-0.39841
	13.47692	-0.29412	13.48266	-0.29623
	14.13370	-0.42883	14.13680	-0.42956
	15.04170	-0.25552	15.04705	-0.25762
	16.59706	-0.21700	16.60244	-0.21889
	18.14115	-0.18280	18.14647	-0.18426
	19.67567	-0.15653	19.68084	-0.15761
	21.20308	-0.13958	21.20807	-0.14032
	22.72484	-0.13187	22.72966	-0.13235
	24.24120	-0.13284	24.24588	-0.13311
	25.75156	-0.14130	25.75605	-0.14153
A_2	7.93363	-0.15129	7.94561	-0.15526
	9.45604	-0.13196	9.46661	-0.13458
	10.97616	-0.12325	10.98563	-0.12504
	12.49347	-0.12432	12.50215	-0.12550
	14.00693	-0.13468	14.01501	-0.13534
	15.51469	-0.15329	15.52229	-0.15368
	17.01453	-0.17810	17.02178	-0.17836
	18.50574	-0.20544	18.51273	-0.20573
	19.99011	-0.23236	19.99681	-0.23275
	20.54565	-0.31325	20.54989	-0.31495
	21.46993	-0.25775	21.47596	-0.25817
	22.10098	-0.28557	22.95261	-0.28199
	22.94703	-0.28164	23.66203	-0.26365
E	18.85038	-0.17271	18.56037	-0.17350
	19.44833	-0.25471	19.45385	-0.25454
	20.37203	-0.17461	20.37745	-0.17502
	20.94214	-0.28849	20.94718	-0.28767
	21.88904	-0.19045	21.89438	-0.19059

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Table 5. Several subsets of semiclassical and quantum resonances for $d : R = 6$. The A_1 subspace resonances are plotted in Fig. 40.5.4.

Classical escape rates and bounds on quantum escape rates, *ie.* the zeros of the zeta functions (**??**) and (40.10) with absolute weights (40.13), as function of the disk-disk separation. The top two curves show the classical escape rate. Zeros computed from fixed points alone are shown as dotted lines, zeros from fixed points and period two orbits as full lines, and the Monte Carlo estimates of classical escape rates are marked by diamonds. The classical escape rate should approach 0 as $R : d \to 0.5$; in this limit cycle expansions are expected to converge poorly due to pruning and intermittency effects. The two lower curves show s_c, the abscissa of absolute convergence of the Gutzwiller trace formula, which serves as a crude lower bound on the imaginary part of the semiclassical quantum resonances. Though this bound becomes negative near $R : d \approx 0.33$, the semiclassical resonances do remain below the real energy axis, see fig. 40.5.4.

Semiclassical scattering resonances (diamonds) compared with the exact quantum scattering resonances (crosses). The lines in the upper half of the diagram indicate the (geometrical) difference between the semiclassical and quantum resonances for all resonances with $\mathrm{Im}\, k > -0.4$, magnified by a factor 10. The dotted line at $k_c = -0.121556$ indicates the semiclassical abscissa of convergence; all semiclassical resonances lie below this line, but the first two quantum resonances lie above it. For the semiclassical calculation, all orbits up to symbolic length 5 have been used in the cycle expansion for ζ_0^{-1}.

Energy dependence of the cycle expansion coefficients for $d : R = 6$. Shown are (from top to bottom) the absolute values of the coefficients C_4, C_6, C_8, C_{10} and C_{12} (barely visible in the lower right corner) as a function of the wavenumber k.

The coefficients of the cycle expansion for the quantum Selberg zeta function $Z_{qm}(z)$ (connected with lines) and for $1/\zeta_0$ (not connected) for ratios $d : R = 6$ (diamonds), 3 (squares) and 2.5 (triangles). Note that the asymptotic slope for the quantum Selberg zeta functions and the dynamical zeta functions is the same; the double pole present in the dynamical zeta function persists as a single pole in the Selberg product.

The coefficients of the cycle expansion for the quantum Selberg zeta function $Z_{qm}(z)$ after multiplication with $(1 - z/z_1)$ where z_1 is the zero of $\zeta_1^{-1}(z)$. The coefficients still decay only exponentially but with much steeper slope, indicating the presence of yet another pole.

Convergence of zeros of zeta functions towards the asymptotic values as more and more orbits are included. Shown are the convergence of the classical Fredholm determinant escape rate estimates, the quantum Selberg zeta function lowest resonance estimates, and the quantum $1/\zeta_0$ lowest resonance estimates for ratios $d : R = 6$ and $d : R = 3$. The zero obtained for $n = 14$ has been taken as the asymptotic value. Note the faster than exponential convergence for the classical Fredholm determinant, and the exponential approach for the quantum zeta functions.

40.5.5 3-disk numerical resonances

inte remark: refs. [6.3, 18.11, 6.2, 6.4]

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 chapter 17. For billiards the cycle weight t_p required for evaluation of the classical escape rates and correlation spectra is given by (**??**). 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 (40.12) is given by

$$t_p = (-1)^{n_p} \frac{e^{-ikT_p}}{\sqrt{|\Lambda_p|}} z^{n_p} \,, \tag{40.17}$$

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

Cycle expansion (**??**) coefficients $|C_n|$ for different determinants and zeta functions are plotted in figs. 40.1 and 40.2 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 semiclassical spectral 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 semiclassical spectral determinant enables us to uncover a larger part of the quantum resonances than what was hitherto accessible by means of the dynamical zeta functions. 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 semiclassical spectral determinants, fig. 40.3, reveal complicated patterns of resonances, with the classical and the semiclassical resonance patterns surprisingly similar. It is known [6.3] that the leading semiclassical resonances are very accurate approximations to the exact quantum resonances; the semiclassical resonances further down in the s complex plane in fig. 40.3 have not yet been compared with the exact quantum values. It would be of interest to check whether also all semiclassical spectral determinant resonances correspond to the true quantum resonances.

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An interpretation of the resonance spectrum of the semiclassical spectral determinant is given in ref. [6.4], 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 [11.17] $f = 2\pi/(T_1 - T_0)$ is clearly visible in fig. 40.3. A rough measurement of the period of the beats in fig. 40.3 yields some 23.7 units along the real k axis, to be compared to $2\pi/(T_1 - T_0) = 23.4$.

defer this to diffraction

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 semiclassical zeta function.

Contour plots are also helpful in comparing the domain of convergence of the spectral determinant to that of the semiclassical zeta function. As can be seen from fig. 40.4, the semiclassical spectral determinant can be continued considerably farther down in the complex k plane, in contrast to the dynamical zeta function scans. While the zeta functions clearly exhibit a finite radius of convergence, in agreement with the arguments of sect. ??, both the semiclassical spectral determinant and the semiclassical spectral determinant behave as entire functions. We compute the abscissa of absolute convergence for the semiclassical zeta function by means of (**??**); 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. 40.4 shows that no feature of the semiclassical zeta function countor plot below k_c is significant. Interestingly enough, the apparent border of semiclassical zeta function convergence in fig. 40.4 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. (**??**).

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 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 semiclassical spectral determinant (see fig. 40.3), 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. **??**.

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. **??**. 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 semiclassical cycle expansions; while semiclassical intuition implies that the semiclassical zeta function should be applicable for large $\mathrm{Re}(k)$, in practice the semiclassical cycle expansions work best for the bottom of the spectrum.

In conclusion, we have tested numerically the semiclassical spectral determinant.

Note: Vattay *et al.* have succeeded in constructing a multiplicative evolution operator for semiclassical quantum mechanics, whose Fredholm determinant is

$$F(\beta, E) = \exp\left(-\sum_{p,r} \frac{1}{r} \frac{|\Lambda_p|^{-r\beta} e^{i(S_p(k)/\hbar+\nu_p\pi/2)r}}{(1-1/\Lambda_p^r)^2(1-1/\Lambda_p^{2r})}\right) . \qquad (40.18)$$

This determinant is entire for the Axiom A flows. In particular, the semiclassical spectral 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. **??**, 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 semiclassical spectral determinant can be continued almost a factor 2 down in the complex k plane beyond the region of applicability of the semiclassical zeta function. This explains why for all practical purposes the semiclassical spectral determinants behave as entire functions: only careful numerics reveals the difference between the semiclassical spectral determinant and the Vattay determinant in higher order terms in cycle expansions. The difference is illustrated by fig. 40.5; the suspicious straight section visible in the semiclassical spectral determinant ($\triangle$) in fig. 40.2 turns out to indeed indicate a pole, while the Vattay determinant converges super-exponentially.

Figure 40.1: $\log_{10}|C_n|$, 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 semiclassical zeta function, ($\Box$) $1/\zeta_0\zeta_1^2$, and ($\triangle$) the semiclassical spectral determinant. Exponential falloff implies that $1/\zeta_0$ and the semiclassical zeta function have the same leading pole, cancelled in the $1/\zeta_0\zeta_1^2$ product. For comparison, ($\Diamond$) the semiclassical spectral determinant coefficients are plotted as well; cycle expansions for both spectral 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, wavenumber $k = 7.8727 - 0.3847\, i$, maximal cycle length $n = 8$.

Figure 40.2: Same as fig. 40.1, but with $R : a = 6 : 1$. This illustrates possible pitfalls of numerical tests of asymptotics; the semiclassical spectral 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 semiclassical spectral determinant abscissa of absolute convergence.

Figure 40.3: Leading resonances in the 3-disk repeller A_1 subspace, (a) for the semiclassical spectral determinant, and (b) the 952 leading resonances of the semiclassical spectral determinant F_{qm}. Ratio $R : a = 6 : 0$, cycle expansions truncated at cycle length $n = 8$.

Figure 40.4: Complex s plane countor plot comparison of (a) the semiclassical zeta function $\log|\det(\hat{H} - E)_{sc}(s)|$ with (b) the semiclassical spectral determinant $\log|F_{qm}(s)|$. The border of the convergence of the semiclassical 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 semiclassical spectral 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 $n = 8$.

Figure 40.5: Same parameter values 3-disk system as fig. 40.1: ($\circ$) the semiclassical spectral determinant compared with ($\Box$) the Vattay determinant. While the semiclassical spectral 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 40.1: The "quantum" eigenvalues obtained from the semiclassical zeta function $\det(\hat{H}-E)_{sc}(s)$ and the semiclassical spectral 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.

k	$\det(\hat{H}-E)_{sc}(s)$ Real part	$F_{qm}(s)$ 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

Commentary

Remark 40.1 Our hopes. Quite generally, despite considerable progress (see for example the periodic orbit theory theme issue of CHAOS [11.18]), the semiclassical quantization of bounded systems is still not a routine calculation: all known bounded systems have either pruning, marginally stable periodic orbits and/or accumualting sequences of orbits, and the quantum Selberg zeta functions have poles that degrade the converegence of cycle expansions. We remain optimistic, and believe that not so long in the future many of these problems will be overcome.

Remark 40.2 Poles of dynamical zeta functions. Numerical investigations [40.21] of both the classical and the quantum dynamical $1/\zeta_j$ functions for 2-dimensional Hamiltonian flows indicate that a $1/\zeta_j$ function has a *double* pole coinciding with the leading zero of $1/\zeta_{j+1}$. Consequently $1/\zeta_0$, $1/\zeta_0\zeta_1$ and the quantum Selberg zeta function all have the same leading pole, and coefficients in their cycle expansions fall off exponentially with the same slope, fig. 40.5.4. Multiplying the quantum Selberg zeta function with $(1 - z/z_1)$, where z_1 is the leading zero of $1/\zeta_1(z)$, one obtains faster, but still exponential decay in the coefficients, indicating further poles down in the complex plane (see fig. 40.5.4).

Résumé

To summarize, we have demonstrated that the curvature expansions are a very efficient way of evaluating the semiclassical periodic orbit sums. The essential ingredient for this success has been the physical insight that the dynamical zeta functions expanded this way utilize the shadowing of arbitrarily long orbits by shorter cycles; the technical prerequisite for implementing this shadowing is a good understanding of the symbolic dynamics of the classical dynamical system. Exploiting the symmetries of the problem, we are able to compute accurately a large number of resonances, using as input the actions and eigenvalues of as few as 2–14 prime cycles.

We conclude with three more general comments on the relation of classical and quantum chaotic dynamics:

1. The curvature expansion approach presented here applies to strongly chaotic (non-integrable) systems, and is thus a quantization scheme for a class of systems complementary to those amenable to torus quantization.

2. The symmetry factorization (40.4) of the dynamical zeta function is intrinsic to the classical dynamics, and not a special property of quantal spectra

3. For the strange sets studied in refs. [18.1, 40.2], the curvature expansion is believed to be the *exact* perturbation expansion for classical chaotic averages: even though each cycle carries with it only its linearized neighborhood (analogue of the stationary phase approximation in the derivation of the quantum Gutzwiller sum), the union of the periodic points captures the invariant content of the full underlying smoothly curved dynamics.

As we have shown in the above, the three disk system is an ideal system for tests of periodic orbit expansions in hyperbolic systems, not only in the classical but also in the semiclassical context. With a little bit of geometry one can obtain very good estimates for the classical and quantum escape rates as a function of the separation : radius ratio (fig. 40.5.4), demonstrating the accuracy of approximating the repeller by a few scales. With numerically obtained periodic orbits up to periods 14 one can test the analyticity properties of quantum Selberg zeta functions and Fredholm determinants; to our surprise we found that quantum Selberg zeta functions have poles. Their presence spoils the faster than exponential convergence typical of the classical Fredholm determinants; whether their analyticity can be improved is still being investigated. In the case of sufficiently separated three disks, this may not seem to be terribly important (one already has good exponential convergence), but also the more poorly converging cycle expansions for spectra of bounded systems also seem to have poles.

This success points to the most serious problem in classical chaos, namely the problem of Mandelbrot. (still with no solution in sight).

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