Quantum Fluids and Classical Determinants

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Abstract. A "quasiclassical" approximation to the quantum spectrum of the Schrödinger equation is obtained from the trace of a quasiclassical evolution operator for the "hydrodynamical" version of the theory, in which the dynamical evolution takes place in the extended phase space $[q(t), p(t), M(t)] = [q_i, \partial_i S, \partial_i \partial_j S]$. The quasiclassical evolution operator is multiplicative along the classical flow, the corresponding quasiclassical zeta function is entire for nice hyperbolic flows, and its eigenvalue spectrum contains the spectrum of the semiclassical zeta function. The advantage of the quasiclassical zeta function is that it has a larger analyticity domain than the original semiclassical zeta function; the disadvantage is that it contains eigenvalues extraneous to the quantum problem. Numerical investigations indicate that the presence of these extraneous eigenvalues renders the original Gutzwiller-Voros semiclassical zeta function preferable in practice to the quasiclassical zeta function presented here. The cumulant expansion of the exact quantum mechanical scattering kernel and the cycle expansion of the corresponding semiclassical zeta function part ways at a threshold given by the topological entropy; beyond this threshold quantum mechanics cannot resolve fine details of the classical chaotic dynamics.

Introduction

What we shall describe here is very much in the spirit of early quantum mechanics, and were physicists of the period as familiar with classical chaos as we are today, this theory would have been developed in 1920's. The main idea is this: in the Bohr–de Broglie visualization of quantization, one places a wave instead of a particle on a Keplerian orbit around the hydrogen nucleus. The quantization condition is that only allowed orbits are those for which such wave is stationary; from this follows the Balmer spectrum, the old quantum theory, and the more sophisticated theory of Schrödinger and others. Today we are very aware of the fact that integrable systems are exceptional and that chaos is the rule. So, can the Bohr quantization be generalized to chaotic systems? The answer was provided by Gutzwiller in 1971; the trace of the quantum evolution operator for a chaotic system in a semiclassical approximation is given by the Gutzwiller trace formula, an oscillating sum over all periodic orbits of the system.

There is however a hidden intellectual challenge in Gutzwiller's derivation: the derivation is based on the semiclassical Van Vleck approximation $K(x, x', t)$

to the quantum propagator which does not satisfy the semigroup property

$$\int \mathrm{d}x''\, K(x,x'',t_1)K(x'',x',t_2) \neq K(x,x',t_1+t_2)\ . \tag{1}$$

In the literature this problem is usually sidestepped by saying that an equality holds if the integral is carried out by the saddle point method. Here we offer an alternative "quasiclassical" quantization scheme based on a quasiclassical evolution operator which is multiplicative along the flow. Our main result is the *quasiclassical trace formula* for the quantization of a Hamiltonian dynamical system. For a system of 2 degrees of freedom the quasiclassical trace formula takes the form

$$\mathrm{tr}\,\mathcal{L}^t(E) = \sum_p T_p \sum_{r=1}^{\infty} \frac{\delta(t-rT_p)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_p-ET_p)r-\mathrm{i}\pi\frac{m_p}{2}r}}{|\Lambda_p|^{r/2}(1-1/\Lambda_p^r)^2(1-1/\Lambda_p^{2r})}\ .$$

Throughout this paper we reserve the term "quasiclassical" to distinguish this class of formulae from the original Gutzwiller formulae which we shall refer to as "semiclassical".

Search for the above formula was motivated by the classical periodic orbit theory, where convergence of cycle expansions is under much firmer control than in the semiclassical quantizations. One of the main lessons of the classical theory is that the "exponential proliferation of orbits" in itself is not the problem; what limits the convergence of cycle expansions for generic flows is the proliferation of the grammar rules, or the "algorithmic complexity". Indeed, for nice hyperbolic flows a theorem of H. H. Rugh (1992) asserts that the appropriate spectral determinants are entire and that their cycle expansions converge superexponentially.

On the basis of close analogy between the classical and the quantum zeta functions, it has been hoped (Cvitanović 1992) that for nice hyperbolic systems the semiclassical zeta functions of Gutzwiller (1988) and Voros (1988) should also be entire. This hope was dashed by Eckhardt and Russberg (1992) who established that the semiclassical zeta functions for the 3-disk repeller have poles. Their result had in turn motivated guesses for spectral determinants with improved convergence properties by Cvitanović and Rosenqvist (1993) and Cvitanović et al. (1993), which eventually lead to the first derivation of the above trace formula by Cvitanović and Vattay (1993). In this paper we offer a different derivation and interpretation of this formula.

Improved analyticity has been very useful in sorting out the relative importance of the semiclassical, diffraction (Wirzba (1992), Wirzba (1993), Vattay, Wirzba and Rosenqvist (1994)) and quantum contributions (Gaspard and Alonso Ramirez (1992), Vattay (1996), Vattay (1994), Vattay and Rosenqvist (1996)). One had also hoped that improved analiticity would yield cycle expansions that would converge faster with the maximal cycle length truncation than the Gutzwiller-Voros type zeta functions. As is shown here, this is not the case. Improved analyticity comes at a cost; the quasiclassical zeta functions predicts extraneous eigenvalues which are purely classical and do not belong to the quantum spectrum, but their presence degrades significantly the convergence of the cycle expansions. Furthermore, the investigation of Wirzba (1996) has clarified the relationship between the cumulant expansion of the exact quantum mechanical scattering kernel and the cycle expansion of the semiclassical zeta function; the order of expansion at which the two part their ways is determined by the value of the topological entropy, and beyond this threshold quantum mechanics fails to resolve the arbitrarily fine details of the classical chaotic dynamics.

The paper is organized as follows: in Sect. 1 through Sect. 3 we develop the quasiclassical evolution operator formalism for a semiclassical approximation to the Schrödinger equation, and in Sect. 4 we derive the trace and zeta function formulae for quasiclassical quantization. In Sect. 5 we confront in numerical experiments the cycle expansions of the quasiclassical zeta functions with the cycle expansions of the more standard semiclassical zeta functions and dynamical zeta functions, as well as with the exact quantum mechanical results, and in Sect. 6 we explain the distinction between the asymptotic nature of quantum mechanical cumulant expansions and the convergence of semiclassical cycle expansions. Appendices contain some technical details as well as a discussion of the relation of the quasiclassical quantization to the Selberg zeta function.

1 Quantum Mechanics in Hydrodynamical Form

The Schrödinger equation for a particle in a d-dimensional potential V is

$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2}\Delta-V(q)\right)\psi(q,t)=0\ , \tag{2}$$

where $\psi(q,t)$ is the wave function, and we set the particle mass $m=1$ throughout. The ansatz

$$\psi=\varphi\mathrm{e}^{\mathrm{i}S/\hbar} \tag{3}$$

is as old as quantum mechanics itself. Schrödinger's first wave mechanics paper was submitted 27 January 1926. Submission date for Madelung (1926) "quantum theory in hydrodynamical form" paper, where this ansatz is interpreted as a fluid flow, was 25 October 1926.

Substituting the ansatz into (2), differentiating, and separating the result into the real and imaginary parts (under assumption that both φ and S are real functions) yields

$$\frac{\partial S}{\partial t}+\frac{1}{2}\left(\nabla S\right)^2+V(q)-\frac{\hbar^2}{2}\frac{\Delta\varphi}{\varphi}=0 \tag{4}$$

$$\frac{\partial\varphi}{\partial t}+\nabla S\nabla\varphi+\frac{1}{2}\Delta S\varphi=0\ . \tag{5}$$

The $\hbar^2$ term has many names and is called the "quantum potential" by Bohm (1952), "enthalpy" by Spiegel (1995), by fluid dynamics analogy, or "quantum pressure" by Feynman (1972). While Schrödinger in his 21 June 1926 paper noted that $\rho=\varphi\varphi^*$ satisfies the continuity equation, it was Born who (in a footnote of his 24 june 1926 paper) identified ρ as the probability density. Interpretations of quantum mechanics bifurcate here; keeping the $\hbar$ term in the potential (4) leads to the Madelung "fluid" theory. Shifting the $\hbar$ term into the second equation enforces that S satisfies the classical Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 + V(q) = 0 \ , \tag{6}$$

while the "diffusive" $\hbar$ term in the equation for the amplitude

$$\frac{\partial \varphi}{\partial t} + \nabla S \nabla \varphi + \frac{1}{2} \Delta S \varphi = \frac{i\hbar}{2} \Delta \varphi \ , \tag{7}$$

motivates the "stochastic" interpretation of Nelson (1985).

1.1 Semiclassical Approximation

Our goal here is to study the semiclassical approximation of quantum mechanics, with $\hbar$ small, and concentrate on the leading order expressions. This can be achieved by setting $\hbar$ formally zero in either the "hydrodynamic" or the "stochastic" picture. Either way we get

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S)^2 + V(q) = 0 \tag{8}$$

$$\frac{\partial \varphi}{\partial t} + \nabla S \nabla \varphi + \frac{1}{2} \Delta S \varphi = 0 \ . \tag{9}$$

As long as we concentrate on the leading semiclassical contribution, we can steer clear of the passions aroused by the differences between different interpretations of quantum mechanics, and follow the original Gutzwiller derivation of the semiclassical trace formula via Van-Vleck approximation to the quantum propagator, Gutzwiller (1971), Gutzwiller (1990).

Nevertheless, the procedure is unsatisfactory in the sense that in order to get an operator with the semigroup property we need to impose the saddle point condition. In order to overcome this problem we have to learn more about the technical details of the semiclassical dynamics first. This analysis will show that the semiclassical wave function evolution can be described as an evolution over an extended dynamical space.

2 Semiclassical Evolution as a Set of ODE's

We now examine the semiclassical approximation to the quantum wave evolution (a linear partial differential equation) and show that it can be reformulated in terms of a finite number of ordinary differential equations. We start by traversing a well trodden ground: Hamilton's 1823 formulation of wave mechanics.

2.1 Hamilton's Wave Mechanics

In the wave equation (2) q is *not* a variable; the variable is the wave function ψ that evolves with time, and one can think of ψ as an (infinite dimensional) vector where q plays a role of an index. $S(q,t)$ plotted as a function of the position q for two different times looks something like Fig. 1(a). A smooth "wavefront"

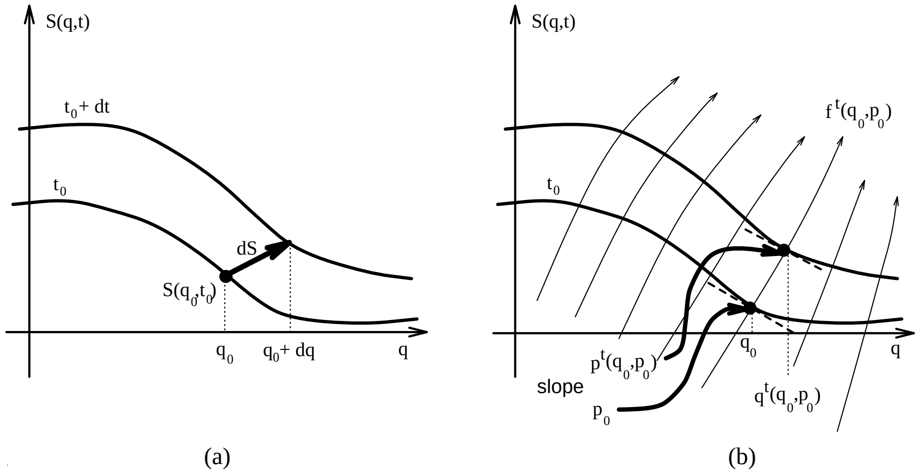


Fig. 1. (a) A wavefront $S(q,t)$ plotted as a function of the position q for two different times. (b) The phase of the wavefront $S(q,t)$ transported by a swarm of "particles"; Hamilton's equations (15) construct $S(q,t)$ by transporting $q_0 \to q(t)$ and p_0, the slope of $S(q_0,t_0)$, to $p_0 \to p(t)$.

$S(q,t_0)$ deforms smoothly with time into the "wavefront" $S(q,t)$ at time t. At this point one can ask: could we think of this front as a swarm of particles that move in such a way that if we know $S(q,t)$ and its slope $\partial S/\partial q$ at q at initial time $t=t_0$, we can construct a corresponding piece of $S(q,t)$ and its slope at time t, Fig. 1(b)? For notational convenience, define

$$p_i = p_i(q,t) := \frac{\partial S}{\partial q_i}, \quad i = 1,2,\ldots,d \ . \tag{10}$$

In the semiclassical approximation (4) reduces to the *Hamilton-Jacobi* equation

$$\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}\right) = 0 \ , \tag{11}$$

where $H(q,p)$ is the Hamiltonian, in this case

$$H = p^2/2m + V(q) \ . \tag{12}$$

For sake of simplicity we set $m = 1$ throughout. We shall also assume that the Hamiltonian is time independent (energy is conserved) and separable into a sum of kinetic and potential parts.

Infinitesimal variation of $S(q,t)$, Fig. 1(a), is given by

$$\mathrm{d}S = \mathrm{d}t\frac{\partial S}{\partial t} + \mathrm{d}q\frac{\partial S}{\partial q} \ .$$

Dividing through by $\mathrm{d}t$ and substituting (11) we obtain

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -H(q,p) + \dot{q}p \ . \tag{13}$$

The "velocity" $\dot{q}$ is arbitrary, and now comes Hamilton's idea: can we adjust $\dot{q}$ so that p is promoted to a variable *independent* of q? Take a $\frac{\partial}{\partial q}$ derivative of both sides of (13):

$$\frac{\partial}{\partial q}\frac{\mathrm{d}}{\mathrm{d}t}S = -\frac{\partial H}{\partial q} - \frac{\partial H}{\partial p}\frac{\partial p}{\partial q} + p\frac{\partial}{\partial q}\frac{\mathrm{d}}{\mathrm{d}t}q + \dot{q}\frac{\partial p}{\partial q} \ .$$

(remember that $H(q,p)$ depends on q also through $p(q,t) := \partial_q S$, hence the $\frac{\partial H}{\partial p}$ term in the above). Exchanging ∂_q and d/dt derivatives leads to

$$\dot{p} + \frac{\partial H}{\partial q} = \left(\dot{q} - \frac{\partial H}{\partial p}\right)\frac{\partial p}{\partial q} \ . \tag{14}$$

Now we use the freedom of choosing $\dot{q}$, and trade the $\frac{\partial p}{\partial q}$ dependence for a set of ordinary differential equations, the Hamilton's equations

$$\dot{q} = \frac{\partial H(q,p)}{\partial p} \ , \qquad \dot{p} = -\frac{\partial H(q,p)}{\partial q} \tag{15}$$

with the "wavefront" $S(q,t)$ replaced by the action increment $S^t(q_0,p_0)$, the integral of (13) evaluated along the phase space flow $(q_0,p_0) \to (q(t),p(t))$:

$$S^t(q_0,p_0) = \int_{t_0}^{t} \mathrm{d}\tau \ \{\dot{q}(\tau)\cdot p(\tau) - H(q(\tau),p(\tau))\} \ . \tag{16}$$

If the energy is conserved, $H(q(\tau),p(\tau)) = E$, and the second term is simply $(t_0 - t)E$.

To summarize: the Hamilton-Jacobi *partial* differential equation (11) for the evolution of a wave front can be reformulated as a finite number of *ordinary* differential equations of motion which increment the initial action $S(q_0,t_0)$ by the integral (16) along the phase space trajectory $(q(\tau),p(\tau))$. In order to obtain the full quasiclassical evolution we also have to deal with the amplitude evolution (9).

2.2 Amplitude Evolution

The amplitude evolution (9) now takes place in the velocity field given by

$$v(q,t) = \nabla S(q,t) \ . \tag{17}$$

We can define $q(t) = f^t(q)$ as a solution of the differential equation

$$\dot{q} = v(q,t) \tag{18}$$

with initial condition $q(0) = q$ at time $t = 0$. This solution will coincide with $q^t(q, \nabla S(q,0))$, which is the q solution of the Hamilton's equations with initial conditions $q' = q$ and $p' = \nabla S(q',0)$. We introduce the notation $\kappa(q,t) = \Delta S(q,t)$ and write (9) as

$$\left\{ \frac{\partial}{\partial t} + v(q,t) \cdot \nabla + \frac{1}{2}\kappa(q,t) \right\} \varphi(q,t) = 0 \ . \tag{19}$$

This is a linear equation in φ, so its solution can be written in terms of its Green's function as

$$\varphi(q,t) = \int \mathrm{d}q' \, \tilde{L}^t(q,q')\varphi(q',0) \tag{20}$$

where the kernel $\tilde{L}^t(q,q')$ is the special solution of (19) with initial condition $\tilde{L}^0(q,q') = \delta(q-q')$. It is easily checked by direct substitution into (20) and (19) that this Green's function is given by

$$\tilde{L}^t(q,q') = \exp\left\{ \frac{1}{2} \int_0^t \kappa(f^\tau(q'),\tau) \, \mathrm{d}\tau \right\} \delta(q - f^t(q')) \ , \tag{21}$$

where an extra negative contribution to (19) results from $v(q,t)\nabla\delta(q - f^t(q')) = -(\nabla v(q,t))\delta(q - f^t(q'))$ and $\nabla v(q,t) = \kappa(q,t)$.

2.3 Quasiclassical Evolution

The whole quasiclassical evolution procedure can now be summarized. First we take our initial wave function $\psi(q,0)$. We pick a function $S(q,t)$, a solution of (8), and compute the initial amplitude $\varphi(q,0) = \mathrm{e}^{-\mathrm{i}S(q,0)/\hbar}\psi(q,0)$. We evolve this amplitude for time t and put back the phase:

$$\psi(q,t) = \mathrm{e}^{\mathrm{i}S(q,t)/\hbar} \int \mathrm{d}q' \, \tilde{L}^t(q,q')\mathrm{e}^{-\mathrm{i}S(q',0)/\hbar}\psi(q',0) \ . \tag{22}$$

The whole evolution can be cast into the semiclassical evolution operator

$$\psi(q,t) = \int \mathrm{d}q' \, L^t(q,q',S)\psi(q',0) \ , \tag{23}$$

where

$$L^t(q,q',S) = \exp\left\{\frac{\mathrm{i}}{\hbar}(S(q,t)-S(q',0)) + \frac{1}{2}\int_0^t \kappa(f^\tau(q'),\tau)\,\mathrm{d}\tau\right\}\delta(q-f^t(q')) \ . \tag{24}$$

The functional dependence on $S(q',0)$ sounds somewhat discouraging; we have to see it in an explicit form in order to understand the machinery of this operator.

The most complicated looking object here is the function

$$\lambda(q',t) = \int_0^t \kappa(f^\tau(q'),\tau)\,\mathrm{d}\tau \ .$$

We do not need the full information about $S(q,t)$ in order to compute this integral of $\Delta S(q,t)$ along the trajectory; as we shall see, an ODE suffices to evaluate this function. Consider the curvature matrix

$$\mathbf{M}_{ij} = \frac{\partial^2 S(q,t)}{\partial q_i \partial q_j} \ . \tag{25}$$

The time evolution equation for this matrix is obtained by taking the second derivatives of (8):

$$\frac{\partial \mathbf{M}}{\partial t} + v(q,t)\cdot\nabla\mathbf{M} + \mathbf{M}^2 + \mathbf{D}^2 V = 0 \ , \tag{26}$$

where $\mathbf{D}^2 V$ is the second derivative matrix of the potential. The first two terms combine to the full time derivative, and the evolution of $\mathbf{M}$ along a trajectory is given by

$$\dot{\mathbf{M}} = -\mathbf{M}^2 - \mathbf{D}^2 V \ . \tag{27}$$

So in the extended dynamical space we do not only keep track of q and slope of S at q, but also the curvature of S at q, see Fig. 2. Let us denote the solution of this ODE along a trajectory with starting point (q,p) and an initial matrix $\mathbf{M}$ by $\mathbf{M}^t(q,p,\mathbf{M})$. The function $\lambda(q,t)$ now can be expressed as

$$\lambda(q,t) = \int_0^t \mathrm{d}\tau\,\mathrm{tr}\,\mathbf{M}^\tau(q,p,\mathbf{M}) \tag{28}$$

with p initialized as $p = \nabla S(q,0)$.

Another point where the “functional dependence” can be simplified is the phase term. We can make the replacement

$$S(q,t) - S(q',0) = S^t(q',p') \tag{29}$$

in the kernel (24), where S^t is the integral (16) with initial point $(q', p' = \nabla S(q',0))$ and $t_0 = 0$.

With these observations the kernel (24) can be written as

$$L^t(q,q',S) = \int \mathrm{d}p'\,\mathrm{d}\mathbf{M}'\,\mathrm{e}^{\mathrm{i}S^t(q',p')/\hbar + \frac{1}{2}\int_0^t \mathrm{d}\tau\,\mathrm{tr}\,\mathbf{M}^\tau(q',p',\mathbf{M}')} \times \\ \delta(q - q^t(q',p'))\,\delta(p' - \nabla S(q',0))\,\delta(\mathbf{M}' - \mathbf{D}^2 S(q',0)) \ , \tag{30}$$

where we have made the functional dependence explicit.

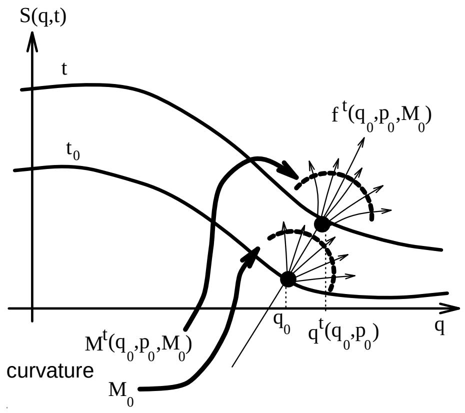


Fig. 2. The evolution of the curvature matrix M_{ij} of the wavefront $S(q,t)$ along the trajectory $[q(t),p(t),M(t)]$ in the extended dynamical space.

3 Quasiclassical Evolution Operator

If we write the time evolution of a wave function we get

$$\begin{aligned}\psi(q,t) &= \int \mathrm{d}q'\,\mathrm{d}p'\,\mathrm{d}\mathbf{M}'\,W^t(q',p',\mathbf{M}')\,\delta(q-q^t(q',p'))\\ &\times\psi(q',0)\,\delta(p'-\nabla S(q',0))\,\delta(\mathbf{M}'-\mathbf{D}^2S(q',0))\ ,\end{aligned} \tag{31}$$

where $W^t(q,p,\mathbf{M})$ is a short hand notation for the exponential in (30). We now make a new proposal: let us regard the last deltas $\delta(p'-\nabla S(q',0))\,\delta(\mathbf{M}'-\mathbf{D}^2S(q',0))$ as a part of the wave function. In other words, we think $\Psi(q',p',\mathbf{M}')=\psi(q',0)\,\delta(p'-\nabla S(q',0))\,\delta(\mathbf{M}'-\mathbf{D}^2S(q',0))$ as a function defined on the $(q,p,\mathbf{M})$ space. We can multiply (31) by $\delta(p-\nabla S(q,t))\,\delta(\mathbf{M}-\mathbf{D}^2S(q,t))$ and write the evolved function in the extended space as

$$\Psi(q,p,\mathbf{M}) = \int \mathrm{d}q'\,\mathrm{d}p'\,\mathrm{d}\mathbf{M}'\,\mathcal{L}^t(q,p,\mathbf{M}|q',p',\mathbf{M}')\,\Psi(q',p',\mathbf{M}')\ ,$$

where the kernel of this integral operator shall be referred to as the *quasiclassical evolution operator*

$$\begin{aligned}\mathcal{L}^t(q,p,\mathbf{M}|q',p',\mathbf{M}') &= \mathrm{e}^{\mathrm{i}S^t(q',p')/\hbar+\frac{1}{2}\int_0^t \mathrm{d}\tau\,\mathrm{tr}\,\mathbf{M}^\tau(q',p',\mathbf{M}')}\\ &\times\delta(q-q^t(q',p'))\,\delta(p-p^t(q',p'))\,\delta(\mathbf{M}-\mathbf{M}^t(q',p',\mathbf{M}'))\ .\end{aligned} \tag{32}$$

Here the quantities $\nabla S(q,t)$ and $\mathbf{D}^2S(q,t)$ are computed from their initial values and replaced with $p^t(q',p')$ and $\mathbf{M}^t(q',p',\mathbf{M}')$ using (29).

So, what does this mean? We have constructed an evolution operator which acts on functions of the $(q,p,\mathbf{M})$ space. Because of the three delta functions the evolution operator has the semigroup property. However, there will be a price to pay: while a wave function can be embedded into the enlarged space, not all the functions living in the enlarged space represent functions in the old space. The spectrum of the quasiclassical operator will contain the semiclassical spectrum, but as we shall see in Sect. 5, it will also contain extraneous eigenvalues without quantum mechanical counterpart.

3.1 Wave Packet Evolution

There is also an easy way back from the extended space to the original one. If the function $\Psi(q,p,\mathbf{M})$ is a representation of a q space wave function or represents a linear combination of such functions, the delta function dependence on p and $\mathbf{M}$ insures that a q dependent wave function can be recovered by

$$\psi(q,t) = \int \mathrm{d}p\,\mathrm{d}\mathbf{M}\,\Psi^t(q,p,\mathbf{M}) \ . \tag{33}$$

The quasiclassical evolution introduced here is closely related to the Gaussian wave packet evolution theories of Heller (1975), Heller, Tomsovic and Sepúlveda (1992). There a wave packet

$$\psi(q,0) = A_0 \mathrm{e}^{\mathrm{i}p_0(q-q_0)/\hbar + \frac{\mathrm{i}}{2\hbar}(q-q_0)\mathbf{M}_0(q-q_0)} \tag{34}$$

is "launched" at $t=0$, with the parameters $(q_0,p_0,\mathbf{M}_0)$ evolving in time according to the equations we have for q, p and $\mathbf{M}$, and with the amplitude evolving as

$$A^t = A_0 \mathrm{e}^{\mathrm{i}S^t(q_0,p_0)/\hbar - \frac{1}{2}\int_0^t \mathrm{d}\tau\,\mathrm{tr}\,\mathbf{M}^\tau(q_0,p_0,\mathbf{M}_0)} \ . \tag{35}$$

Initial wave functions can be decomposed into a linear combination of wave packets and the pieces can be evolved separately. Each packet is characterized by a phase point in the $(q,p,\mathbf{M})$ phase space and evolves according to (15) and (27), with clouds of points representing initial wave packets evolving as in the Heller, Tomsovic and Sepúlveda (1992) picture.

3.2 A Classical Motivation for the Extended Dynamical Space

The above discussion might lead the reader to believe that the extended dynamical phase space is a peculiarity of quantum quasiclassics. However, what we have done is an example of a much more general procedure for constructing multiplicative evolution operators in settings where the multiplicative property seems to have been lost.

The problem can be illustrated by the Ruelle (1987) "thermodynamic" evolution operator of form

$$\mathcal{L}^t(x,x') = \mathrm{e}^{h^t(x')}\,\delta(x - f^t(x'))\,\frac{1}{|\Lambda^t(x')|^{\beta-1}} \ ,$$

with $\Lambda^t(x)$ an eigenvalue of the Jacobi matrix $\mathbf{J}^t(x)$ (see Appendix A) and $h^t(x)$ is a weight additive along the trajectory $f^t(x)$. For one-dimensional maps this operator is multiplicative, but *not* so for flows with two or more transverse dimensions, for the simple reason that the eigenvalues of successive stability matrices are in general not multiplicative

$$\Lambda_{ab} \neq \Lambda_a \Lambda_b \ .$$

Here $\mathbf{J}_{ab} = \mathbf{J}_b \mathbf{J}_a$ is the Jacobian matrix of the trajectory consisting of consecutive segments a and b, $\mathbf{J}_a$ and $\mathbf{J}_b$ are the stability matrices for these segments separately, and Λ's are their leading eigenvalues. It was this lack of multiplicative property for Λ's that had for long time frustrated attempts to construct evolution operators whose spectrum contains the semiclassical Gutzwiller spectrum, until the method presented here was developed.

The main idea, extending the dynamical system to the tangent space of the flow, is suggested by one of the standard numerical methods for evaluation of Lyapunov exponents; instead of computing eigenvalues of linearized stability matrices, one monitors the growth rate of separation between nearby trajectories, i.e. one adjoins the d-dimensional tangent space $\xi \in TU_x$ to the d-dimensional dynamical evolution space $x \in U \subset \mathbb{R}^d$. The dynamics in the $(x, \xi) \in U \times TU_x$ space is governed by the system of equations of variations, Arnold (1978):

$$\dot{x} = \mathbf{v}(x) \,, \quad \dot{\xi} = \mathbf{D}\mathbf{v}(x)\xi \ .$$

Here $\mathbf{D}\mathbf{v}(x)$ is the derivative matrix of the flow. We write the solution as

$$x(t) = f^t(x_0) \ , \quad \xi(t) = \mathbf{J}^t(x_0) \cdot \xi_0$$

with the tangent space vector ξ transported by the transverse stability matrix $\mathbf{J}^t(x_0) = \partial x(t)/\partial x_0$. Multiplicative evolution operators and the corresponding trace and determinant formulae for such flows are given in Cvitanović and Vattay (1993) and Pollner and Vattay (1996).

4 Quasiclassical Trace and Determinant Formulae

Determination of the approximate eigenvalues of the Schrödinger operator (2) is now reduced to the computation of the eigenvalues of the quasiclassical evolution operator (32). But before we do this, a warning is in order. The spectrum of the new operator *contains* the semiclassical spectrum, i.e. we might find eigenvalues beyond those found in quantum mechanics. Optimally these extraneous eigenvalues should be filtered out, but at present we know of no practical technique for doing this, other than comparison with the exact quantum mechanical spectrum.

We shall determine the eigenvalues of our operator by first deriving the classical trace formula (Cvitanović and Eckhardt (1991), Cvitanović et al. (1996)), and then determining the zeros of the associated Fredholm determinant, in this context called the quasiclassical zeta function. The (p, q) integrations can be carried out first, and yield a weighted sum over primitive periodic orbits p and their repetitions r

$$\mathrm{tr}\,\mathcal{L}^t(E) = \sum_p T_p \sum_{r=1}^{\infty} \frac{\delta(t-rT_p)\,\mathrm{e}^{\frac{\mathrm{i}}{\hbar}(S_p-ET_p)r}}{|\det(1-\mathbf{J}_p^r)|} \Delta_{p,r} \ . \tag{36}$$

By the periodicity condition $\delta(t-rT_p)$ the $\mathbf{M}$ trace is restricted to a transverse Poincaré section of the flow, evaluated at a prime cycle completion $t = T_p$, or its r-th repeat

$$\Delta_{p,r} = \int \mathrm{d}\mathbf{M}\,\delta\big(\mathbf{M} - \mathbf{M}^{rT_p}(q,p,M)\big)\,\mathrm{e}^{\frac{r}{2}\int_0^{T_p}\mathrm{d}\tau \mathrm{tr}\,\mathbf{M}^{\tau}(q,p,\mathbf{M})} \ . \tag{37}$$

The integration of this part requires some skill and it is left for Appendix A. It turns out that this last integral can also be expressed in terms of the eigenvalues of the full phase space Jacobian matrix $\Lambda_1, \Lambda_2, \cdots, \Lambda_{d+1}{=}1/\Lambda_1, \cdots, \Lambda_{2d}{=}1/\Lambda_d$. Putting all ingredients together we get the *quasiclassical trace formula* for the quantization of a Hamiltonian dynamical system in $(d+1)$ configuration dimensions, i.e. restricted to the fixed energy shell in the $2(d+1)$ phase space:

$$\mathrm{tr}\,\mathcal{L}^t(E) = \sum_p T_p \sum_{r=1}^{\infty}\prod_{i=1}^{d} \frac{\delta(t-rT_p)\,\mathrm{e}^{(\frac{\mathrm{i}}{\hbar}(S_p-ET_p)-\mathrm{i}\pi m_p/2)r}}{|\Lambda_{p,i}|^{r/2}(1-1/\Lambda_{p,i}^r)^2(1-1/\Lambda_{p,i}^{2r})} \ . \tag{38}$$

Here $T_p(E) = \oint dt$ is the p-cycle period, $S_p(E) = \oint pdq$ the cycle action evaluated along the periodic orbit on the energy surface $H = E$, m_p the Maslov index, and $\Lambda_{p,1}, \Lambda_{p,2}, \cdots, \Lambda_{p,d}$ are the d expanding eigenvalues of the transverse Jacobian matrix of the flow belonging to the p-cycle. The period is related to the action through $T_p(E) = \frac{\partial}{\partial E} S_p(E)$. The associated quasiclassical zeta function is given by

$$Z_{\mathrm{qc}}(E) \ = \ \exp\left\{ -\sum_{p,r} \frac{1}{r} \prod_{i=1}^{d} \frac{|\Lambda_{p,i}|^{-r/2}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_p(E)r - \mathrm{i}\pi\frac{m_p}{2}r}}{(1-1/\Lambda_{p,i}^r)^2(1-1/\Lambda_{p,i}^{2r})} \right\} \tag{39}$$

(see for ex. Cvitanović et al. (1996) for the trace $\leftrightarrow$ zeta functions relationship). This *quasiclassical zeta function* is our main result. The zeros of $Z_{\mathrm{qc}}(E)$ yield the spectrum of the "quasiclassical" evolution operator.

4.1 The Semiclassical Zeta Function

The formulae derived above differ from those of the semiclassical periodic orbit theory for hyperbolic flows as originally developed by Gutzwiller (1971) in terms of traces of the Van Vleck semiclassical Green's functions. The *semiclassical Gutzwiller trace formula* has topologically the same structure as the quasiclassical trace formula (38):

$$\mathrm{tr}\,G(E) = \overline{g}(E) + \frac{1}{\mathrm{i}\hbar}\sum_p T_p \sum_{r=1}^{\infty} \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S_p(E)r - \mathrm{i}\pi\frac{m_p}{2}r}}{|\det\left(\mathbf{1}-\mathbf{J}_p^r\right)|^{\frac{1}{2}}} \ . \tag{40}$$

The Gutzwiller trace formula differs from the quasiclassical trace formula in two aspects. One is the volume term $\overline{g}(E)$ in (40) which is a missing from our version of the classical trace formula. While an overall pre-factor does not affect the location of zeros of the determinants, it plays a role in relations such as the zeta function functional equations of Berry and Keating (1990). The other difference is that the quantum kernel leads to a square root of the cycle Jacobian $1/\sqrt{\det(1-\mathbf{J}_p)}$, a reflection of the relation probability = (amplitude)^2. This difference does not effect the leading eigenvalues (which coincide for the semi- and quasiclassical quantizations), but has a dramatic effect on the convergence of respective zeta functions.

The precise relation between the semiclassical zeta functions and the quasiclassical zeta functions is given in Appendix C.

In the remainder of the paper we shall investigate the relative merits of the quasiclassical quantization compared to the Gutzwiller semiclassics and the exact quantum mechanics.

5 Numerical Convergence of Cycle Expansions and Extraneous Eigenvalues

A 3-disk repeller is one of the simplest classically completely chaotic scattering systems and provides a convenient numerical laboratory for testing both the ideas about chaotic dynamics and for computing exact quantum mechanical spectra, see Eckhardt (1987), Gaspard and Rice (1989a)-(1989c), Cvitanović and Eckhardt (1989). The 3-disk repeller consists of a free point particle moving in the two-dimensional plane and scattering specularly off three identical disks of radius a centered at the corners of an equilateral triangle of side length R. The discrete C_{3v} symmetry reduces the dynamics to motion in a fundamental domain, and the spectroscopy to irreducible subspaces A_1, A_2 and E. All our computations are performed for the fully symmetric subspace A_1.

In this section we address the following question: which of the three approximate quantization zeta functions is the best in predicting the exact quantum mechanical scattering resonances

(a) the semiclassical zeta function of Gutzwiller (1988) and Voros (1988)

$$Z_{\mathrm{sc}}(z;k) = \exp\left\{-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{z^{rn_p}\, t_p^r}{1-1/\Lambda_p^r}\right\} = \prod_p \prod_{j=0}^{\infty} \left(1 - \frac{z^{n_p} t_p}{\Lambda_p^j}\right) \tag{41}$$

(b) the dynamical zeta function of Ruelle (1987), the $j=0$ part of the semiclassical zeta function

$$\zeta^{-1}(z;k) = \exp\left\{-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} z^{rn_p}\, t_p^r\right\} = \prod_p \left(1 - z^{n_p} t_p\right) \tag{42}$$

(c) or the quasiclassical zeta function (39)

$$Z_{\mathrm{qc}}(z;k) = \exp\left\{ - \sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{z^{rn_p}\, t_p^r}{\left(1-1/\Lambda_p^r\right)^2 \left(1-1/\Lambda_p^{2r}\right)} \right\}$$
$$= \prod_p \prod_{j=0}^{\infty} \prod_{l=0}^{\infty} \left(1 - \frac{z^{n_p} t_p}{\Lambda_p^{j+2l}}\right)^{j+1} \quad ? \tag{43}$$

Here

$$t_p = \mathrm{e}^{\mathrm{i}kL_p - \mathrm{i}m_p\pi/2} / |\Lambda_p|^{\frac{1}{2}} \tag{44}$$

is the weight of the p^{th} prime cycle, n_p its topological length and z a book-keeping variable for keeping track of the topological order in cycle expansions — the above zeta functions are Taylor-expanded in z around $z=0$ up to a given cycle expansion order and only then z is set to $z=1$ (see also (51) below). L_p is the length of the p^{th} cycle, m_p its Maslov index together with the group theoretical weight of the studied C_{3v} representation, and Λ_p its stability (the expanding eigenvalue of the p^{th} Jacobian matrix).

The results of comparing finite cycle expansion truncations of the above zeta functions with each other and with the exact quantum mechanical results computed with the methods outlined in Sect. 6 are summarized in Figs. 3 and 4. Resonances are plotted as the real part of the resonance wavenumber (resonance "energy") vs. the imaginary part of the wavenumber (resonance "width"). We have computed several thousands of exact quantum mechanical as well as approximate A_1 resonances for the 3-disk repeller with center-to-center separation $R=6a$. Further and considerably more detailed numerical results are available from Wirzba and Henseler (1995).

Some of the features of the resonance spectra have immediate interpretation. The mean spacing of the resonances is approximately $2\pi/\bar{L}$, where $\bar{L}$ is the average of the lengths L_0 and L_1 of the two shortest cycles of topological length one. The data also exhibit various beating patterns resulting from the interference of cycles of nearly equal lengths; e.g. the leading beating pattern is of order $2\pi/\Delta L$, where ΔL is the difference of the lengths L_1 and L_0.

In Fig. 3 the cycle expansion includes cycles up to topological length four. Already at this order the four leading resonance bands are well approximated by the semiclassical zeta function (41) (in fact, for $\mathrm{Re}\, k \lesssim 75/a$ already cycles up to length two suffice to describe the first two leading resonance bands). Neither the quasiclassical zeta function (43) nor the dynamical zeta function (42) perform quite as well. The reason is that the quasiclassical as well as the dynamical zeta function predict extra resonances which are absent in the exact quantum mechanical calculation. The accessible resonances close to the real axis can in this regime be parameterized by 16 measured numbers, i.e. 8 cycle lengths and stabilities, together with the 8 Maslov indices. It turns out that the subleading bands remain completely shielded all the way up to $\mathrm{Re}\, k \approx 950/a$ where they start mixing with the four leading ones.

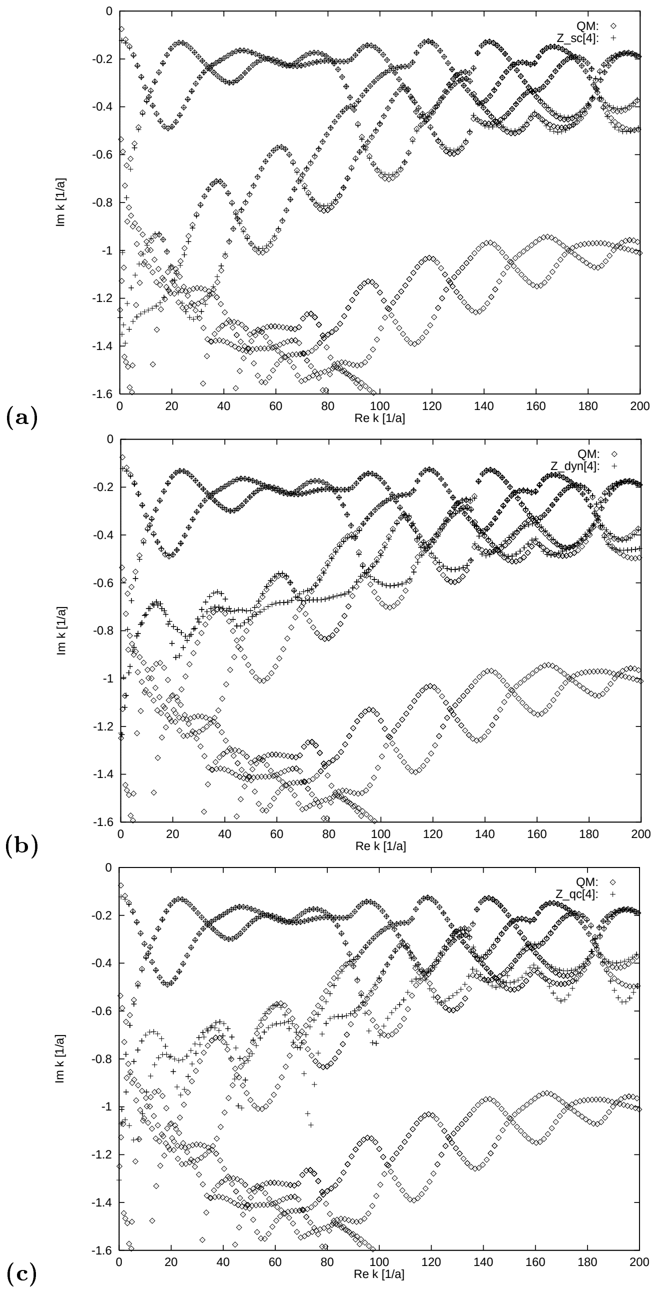


Fig. 3. The A_1 resonances of the 3-disk repeller with $R = 6a$. The exact quantum mechanical data are denoted by diamonds. The semiclassical ones are calculated up to 4^{th} order in the cycle expansion and are denoted by crosses. **(a)** semiclassical zeta function (41), **(b)** dynamical zeta function (42), **(c)** quasiclassical zeta function (43).

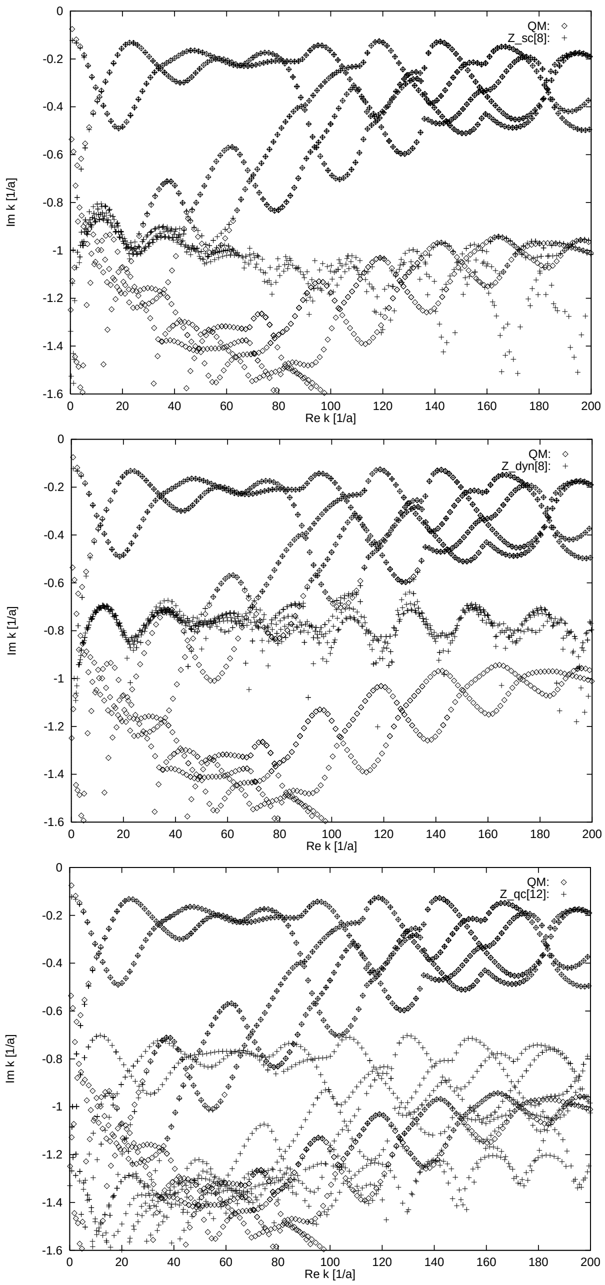
In Figs. 4a-c the comparison is made up to eight, respectively twelfth cycle expansion order. The border of convergence of the semiclassical zeta function has now moved (in the plotted region) above the fifth and sixth band of the exact quantum resonances. The dynamical zeta function exhibits a sharp accumulation line of resonances, the border of convergence controlled by the location of the nearest pole of the dynamical zeta function (Eckhardt and Russberg (1993), Cvitanović et al. (1993)). With cycles up to length 12 the quasiclassical zeta function resolves the exact quantum fifth and sixth bands of subleading resonances, but at the cost of many extraneous resonances, see Fig. 4(c). At these high cycle expansion orders the quasiclassical zeta function has convergence problems for large negative imaginary k values (especially for low values for $\mathrm{Re}\,k$), in agreement with the expected large cancellations in the cycle expansion at high cycle expansion orders, Wirzba and Henseler (1995). There is the further caveat that the quasiclassical zeta function finds the lowest subleading resonances just barely at the 12^{th} order in the cycle expansion. Therefore cycles of larger topological length would be needed to confirm this success.

The extraneous eigenvalues are not without a meaning; they belong to the spectra of classical evolution operators, such as those that describe the escape from a classical 3-disk repeller, plotted in Cvitanović et al. (1993). The problem is that we now know, by comparing them to the exact quantum mechanical spectra, that they have nothing to do with quantum mechanics. As far as quantum mechanics is concerned, they are "extraneous".

Another distinctive feature of the exact quantum mechanical spectra is the *diffractive* band of resonances from $k \approx (0. - \mathrm{i}0.5)/a$ to $k \approx (100. - \mathrm{i}1.6)/a$. As shown by Vattay, Wirzba and Rosenqvist (1994) and Rosenqvist, Vattay and Wirzba (1996), the diffractive band of resonances can be accounted for by inclusion of creeping periodic orbits, omitted from the calculations undertaken here.

Qualitatively, the results can be summed up as follows. The semiclassical zeta function (41) does well above the line of convergence defined by the dynamical zeta function (42), already at very low cycle expansion orders where the other two zeta functions still have problems. Below this line of convergence the semiclassical zeta function works only as an asymptotic expansion; when it works, it works very well and very efficiently. The dynamical zeta function does eventually as well for the leading resonances as the semiclassical one. As experimentally these are the only resonances accessible, one can – for practical purposes – limit the calculation just to this zeta function. The quasiclassical zeta function finds all known subleading quantum resonances, but at a high expense: the rate of convergence is poor compared to the semiclassical zeta function, as most of the information provided by longer cycles is used to determine the extraneous resonance bands, with no quantum counterpart. Without a quantum calculation, one could not tell the extraneous from the real resonances.

As a by-product of this calculation we can state an empirical rule of thumb: Each new cycle expansion or cumulant order is connected with a new line of subleading resonances. This rule relates the cycle expansion truncations limit,



(a)

(b)

(c)

Fig. 4. The A_1 resonances of the 3-disk repeller with $R = 6a$. The exact quantum mechanical data are denoted by diamonds, the semiclassical ones by crosses. **(a)** semiclassical zeta function (41) up to 8^{th} order in the cycle expansion, **(b)** dynamical zeta function (42) up to 8^{th}, **(c)** quasiclassical zeta function (43) up to 12^{th} order.

$n \to \infty$ (where n is defined below in (51)), and the limit $\mathrm{Im}\, k \to -\infty$. Numerics supports the claim that the cycle expansion limit $n \to \infty$ and the semiclassical limit $\mathrm{Re}\, k \to \infty$ do not commute deep down in the lower complex k plane, a point that we shall return to in Sect. 6.

5.1 Exact Versus Semiclassical Cluster Phase Shifts

In the above we compared the exact and semiclassical resonances of the 3-disk repeller in the A_1 representation. As the deviations are most pronounced for the subleading resonances which are shielded by the leading ones, one could argue that experimentally it does not matter which of the three zeta functions are used to describe the measured data, as all three give the same predictions for the leading resonances.

Nevertheless, as we shall now show, the three approximate quantizations can be told apart (Wirzba (1995)), even experimentally.

The exact and semiclassical expressions for the determinant of the S-matrix for the non-overlapping 3-disk repeller are given by

$$\begin{aligned} \det \mathbf{S}^{(3)}(k) &= \left(\det \mathbf{S}^{(1)}(ka)\right)^3 \frac{\det \mathbf{M}_{A1}(k^*)^\dagger}{\det \mathbf{M}_{A1}(k)} \frac{\det \mathbf{M}_{A2}(k^*)^\dagger}{\det \mathbf{M}_{A2}(k)} \frac{\left(\det \mathbf{M}_E(k^*)^\dagger\right)^2}{(\det \mathbf{M}_E(k))^2} \\ &\xrightarrow{\text{s.c.}} \left(\mathrm{e}^{-\mathrm{i}\pi N(k)}\right)^6 \left(\frac{Z_{1\text{-disk(l)}}(k^*)^*}{Z_{1\text{-disk(l)}}(k)} \frac{Z_{1\text{-disk(r)}}(k^*)^*}{Z_{1\text{-disk(r)}}(k)}\right)^3 \times \\ &\qquad \times \frac{Z_{A1}(k^*)^*}{Z_{A1}(k)} \frac{Z_{A2}(k^*)^*}{Z_{A2}(k)} \frac{Z_E(k^*)^{*2}}{Z_E(k)^2} \ . \end{aligned} \tag{45}$$

(See Wirzba and Henseler (1995) for details and notation.) For the A_1 representation of the 3-disk repeller the quantum mechanical kernels and the semiclassical zeta functions (41) are related by

$$\frac{\det \mathbf{M}_{A1}(k^*)^\dagger}{\det \mathbf{M}_{A1}(k)} \xrightarrow{\text{s.c.}} \frac{Z_{A1}(k^*)^*}{Z_{A1}(k)} \tag{46}$$

Both sides of (45) and (46) respect unitarity, and if the wave number k is real, both sides can be written as $\exp\{\mathrm{i}2\eta(k)\}$ with a real *phase shift* $\eta(k)$. We define the total phase shift for the coherent part of the 3-disk scattering problem (here always understood in the A_1 representation) for the exact quantum mechanics as well as for the three approximate quantizations by:

$$\begin{aligned} \mathrm{e}^{2\mathrm{i}\eta_{\mathrm{qm}}(k)} &:= \frac{\det \mathbf{M}(k^*)^\dagger}{\det \mathbf{M}(k)} \qquad & \mathrm{e}^{2\mathrm{i}\eta_{\mathrm{sc}}(k)} &:= \frac{Z_{\mathrm{sc}}(k^*)^*}{Z_{\mathrm{sc}}(k)} \\ \mathrm{e}^{2\mathrm{i}\eta_{\mathrm{dyn}}(k)} &:= \frac{\zeta^{-1}(k^*)^*}{\zeta^{-1}(k)} \qquad & \mathrm{e}^{2\mathrm{i}\eta_{\mathrm{qc}}(k)} &:= \frac{Z_{\mathrm{qc}}(k^*)^*}{Z_{\mathrm{qc}}(k)} \ . \end{aligned} \tag{47}$$

This phase shift definition should be compared with the cluster phase shift given in section 4 of Lloyd and Smith (1972). The important point here is that the coherent or cluster phase shift of $\det \mathbf{S}(k)$ is in principle experimentally accessible: one just has to construct the elastic scattering amplitude from the measured cross sections, and subtract the single disk contributions.

So, $\eta_{\rm qm}(k)$ is a "measurable" quantity, useful to us as a different method for discriminating between the various zeta functions. An example is given in Fig. 5 where the zeta functions in the numerators as well as in the denominators in (47) have been expanded up to cycles of topological length 12. The phase shifts are compared in the window $104/a \le k \le 109/a$, a typical window sufficiently narrow to resolve the rapid oscillations, with k sufficiently big that the diffraction effects are unimportant. The performance of the original semiclassical zeta func-

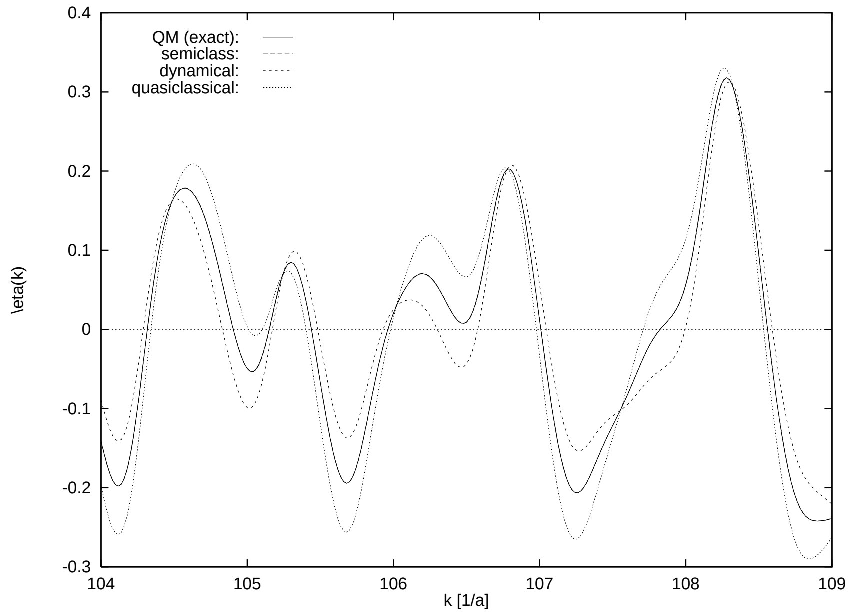


Fig. 5. The coherent cluster phase shifts of the 3-disk scattering system in the A_1 representation with $R = 6a$. The exact quantum mechanical data compared to the predictions of the semiclassical zeta function (41), the dynamical zeta function (42) and the quasiclassical zeta function (43) calculated up to $12^{\rm th}$ order in the cycle expansion. The semiclassical zeta function and the exact quantum mechanical data coincide within the resolution of the plot.

tion is again the best. We stress that in contrast to the subleading resonances studied in Sect. 5 (which are completely shielded from experimental detection by the leading resonances), phase shifts are *hard* data, in principle extractable from measured cross sections.

In conclusion: One can tell the three candidate zeta functions apart even experimentally. We have again confirmed that the semiclassical zeta function is the best.

6 Semiclassics Versus Asymptotic $\hbar$ Expansion

So far we have tested various approximate quantization proposals against each other and against exact quantum mechanics. Now we turn to a deeper question: how seriously should we take these cycle expansions in the first place? We will show here, following Wirzba (1996), that the semiclassical zeta function is approximating its quantum mechanical counterpart, the "characteristic KKR determinant" (Kohn and Rostoker (1954), Lloyd and Smith (1972), Berry (1981)) as an asymptotic series and therefore makes sense only as a truncated series.

Let $\det \mathbf{M}(k) = \det(\mathbf{1} + \mathbf{A}(k))$ be the characteristic KKR determinant of the 3-disk repeller in the A_1 representation, where the pertinent kernel $\mathbf{A}(k)$ expressed in the angular momentum basis relative to the half-disk in the fundamental domain reads (see Gaspard and Rice (1989c))

$$\begin{aligned}\mathbf{A}(k)_{m,m'} = d(m)d(m')\frac{J_m(ka)}{H^{(1)}_{m'}(ka)} \Big\{ &\cos\left(\frac{\pi}{6}(5m-m')\right) H^{(1)}_{m-m'}(kR) \\ &+(-1)^{m'}\cos\left(\frac{\pi}{6}(5m+m')\right) H^{(1)}_{m+m'}(kR)\Big\}\end{aligned} \tag{48}$$

with $0 \le m, m' < \infty$ and

$$d(m) := \begin{cases} \sqrt{2} \text{ for } & m>0 \\ 1 \text{ for } & m=0 \ . \end{cases}$$

Let $Q_m(k)$ denote the m^{th} cumulant of $\det \mathbf{M}(k)$, i.e. the coefficient of z^m in the Taylor expansion of $\det(\mathbf{1} + z\mathbf{A}(k))$. $Q_m(k)$ satisfies the Plemelj-Smithies recursion relation (Wirzba and Henseler (1995))

$$\begin{aligned} Q_m(k) &= \frac{1}{m}\sum_{j=1}^{m}(-1)^{j+1} Q_{m-j}(k)\,\mathrm{Tr}(\mathbf{A}^j(k)) \quad \text{for } m \ge 1 \\ Q_0(k) &\equiv 1 \ , \end{aligned}$$

where $\mathrm{Tr}(\mathbf{A}^j(k))$ is the trace of the j^{th} power of the kernel $\mathbf{A}(k)_{m,m'}$ evaluated in the angular momentum basis, $\{|m\rangle\}$, relative to the half-disk in the fundamental domain.

The semiclassical analog of the characteristic determinant $\det(\mathbf{1} + z\mathbf{A}(k))$ is the semiclassical zeta function (41). More precisely, the cycle expansion of the semiclassical zeta function truncated at the topological order n is the semiclassical analog of the quantum cumulant expansion of $\det(\mathbf{1} + z\mathbf{A}(k))$ truncated at the same order. Thus $c_m(k)$, the corresponding semiclassical m^{th} order cycle expansion term of $Z_{\rm sc}(k)$, is constructed from the semiclassical equivalent of the Plemelj-Smithies recursion relation:

$$c_m(k) = \frac{1}{m}\sum_{j=1}^{m}(-1)^{j+m+1}c_{m-j}(k)\sum_{p,r} n_p \frac{\delta_{n_p r,j}{t_p}^r}{1-1/\Lambda_p^r} \qquad \text{for } m \geq 1 \qquad (49)$$
$$c_0(k) \equiv 1 \ ,$$

with t_p defined in (43). The cycle expansion (Cvitanović (1988)) follows from the semiclassical limit

$$\mathrm{Tr}(\mathbf{A}^j(k)) \ \stackrel{\text{s.c.}}{\longrightarrow} \ (-1)^j \sum_{p,r} n_p \frac{\delta_{n_p r,j}{t_p}^r}{1-1/\Lambda_p^r} \ + \text{diffractive creeping orbits} \ . \qquad (50)$$

In summary, the $n^{\rm th}$ order truncated cumulant and cycle expansions are given by

$$\det \mathbf{M}(k)|_n = \sum_{m=0}^{n} Q_m(k)\,, \qquad Z_{\rm sc}(k)|_n = \sum_{m=0}^{n} c_m(k) \qquad (51)$$

where the notation $\cdots|_n$ indicates that the corresponding determinant or zeta function has been truncated at cumulant/cycle expansion order n. The following facts are known:

1. The cumulant sum
$$\lim_{n\to\infty} \det \mathbf{M}(k)|_n = \lim_{n\to\infty} \sum_{m=0}^{n} Q_m(k) = \det \mathbf{M}(k)$$
is absolutely convergent, $\sum |Q_m(k)| < \infty$, because of the trace class property of $\mathbf{A}(k) \equiv \mathbf{M}(k) - \mathbf{1}$ for non-overlapping, non-touching n-disk repellers (Wirzba and Henseler (1995)).
2. The semiclassical cycle expansion sum converges above an accumulation line (which runs below and approximately parallel to the real wave number axis, see Fig. 4(a)) given by the leading poles of the leading dynamical zeta function, $\zeta^{-1}(k)$, or the leading zeros of the subleading zeta function, $\zeta_1^{-1}(k)$ (Eckhardt and Russberg (1993), Cvitanović et al. (1993), Cvitanović and Vattay (1993)).
3. The *truncated* semiclassical cycle expansion sum $Z_{\rm sc}(k)|_n$ can approximate the quantum mechanical result as an asymptotic series even below the semiclassical zeta function border of convergence, Wirzba and Henseler (1995).

We have checked numerically that the following formulae relate the $m^{\rm th}$ cumulants and cycle expansion terms on the real k-axis with the corresponding quantities inside the complex k plane — at least as long as the condition $|\mathrm{Im}\, k| \ll |\mathrm{Re}\, k|$ is satisfied: for the quantum mechanical cumulants of order m we have the approximate leading order relation (under assumption that the diffraction effects are negligible)

$$Q_m(\mathrm{Re}\, k + \mathrm{i Im}\, k) \sim Q_m(\mathrm{Re}\, k)\, \mathrm{e}^{-m\bar{L}\mathrm{Im}\, k} \ . \qquad (52)$$

$\bar{L} \approx R - 2a$ is the average length of the cycles of topological length one. We have also checked numerically that the corresponding relation for the semiclassical cycle expansion terms of order m is also approximately valid:

$$c_m(\mathrm{Re}\, k + \mathrm{i}\mathrm{Im}\, k) \sim c_m(\mathrm{Re}\, k)\, \mathrm{e}^{-m\bar{L}\mathrm{Im}\, k} \quad . \tag{53}$$

Furthermore, on the basis of Fig. 6 we conjecture that for arbitrary values of the

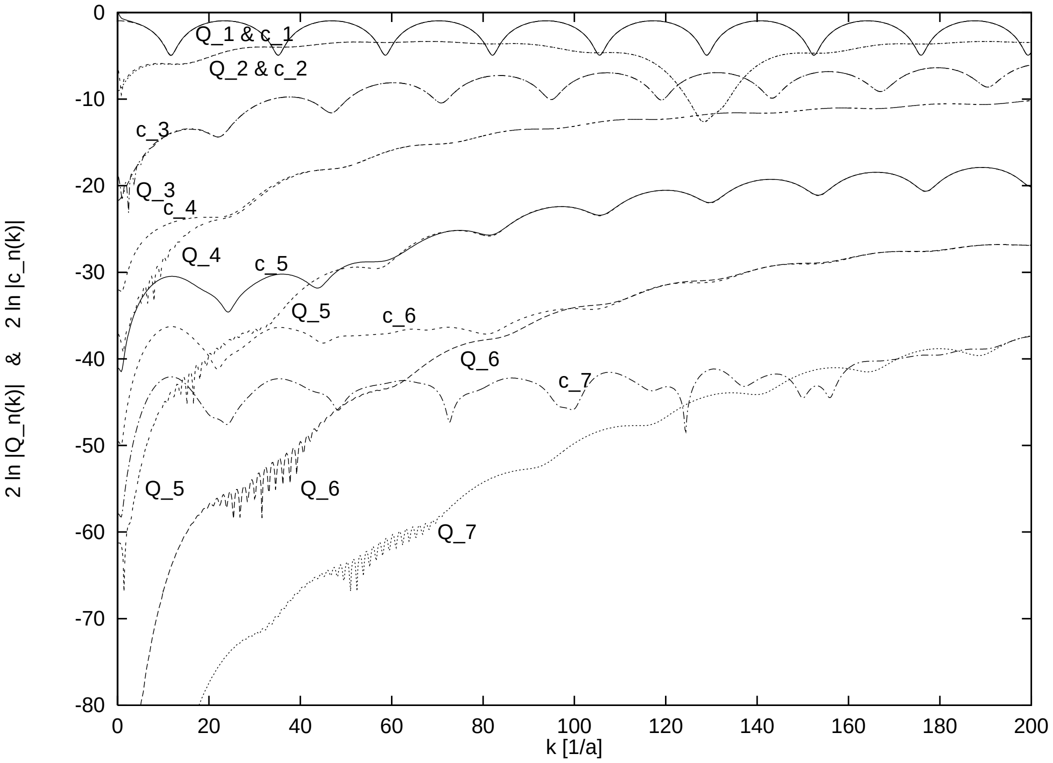


Fig. 6. Comparison of the absolute values of the first seven quantum mechanical cumulant terms, $|Q_n(k)|^2$, with the corresponding semiclassical cycle expansion terms, $|c_n(k)|^2$, of the semiclassical zeta function (41) evaluated on the real wave number axis k. Note that the deviations between quantum mechanics and semiclassics decrease with increasing $\mathrm{Re}\, k$, but increase with increasing cycle expansion order n. The value of $\mathrm{Re}\, k$ where the quantum mechanical and semiclassical curves join is approximately given by $\mathrm{Re}\, ka \sim 2^{n+1}$ where n is the order of the cumulant/cycle expansion term and a is the radius of the disk. A_1 3-disk repeller with center-to-center separation $R = 6a$.

center-to-center separation R of the non-overlapping 3-disk repeller $(R > 2a)$

the following relations hold on the real wave number axis (k real):

$$c_m(k) \approx Q_m(k) \quad \text{with} \quad 1 \gg |c_m(k)| \qquad \text{if} \quad ka \gtrsim 2^{m-1}\frac{\bar{L}}{a}\ , \tag{54}$$

$$1 \gg |c_m(k)| \gg |Q_m(k)| \qquad \text{if} \quad ka \lesssim 2^{m-1}\frac{\bar{L}}{a}\ . \tag{55}$$

6.1 The Meaning of It All

Where is the boundary $ka \approx 2^{m-1}\bar{L}/a$ coming from?

This boundary follows from a combination of the uncertainty principle with ray optics and the non-vanishing value for the topological entropy of the 3-disk repeller. When the wave number k is fixed, quantum mechanics can only resolve the classical repelling set up to the critical topological order n given by (54). The quantum wave packet which explores the repelling set has to disentangle 2^n different sections of size $d \sim a/2^n$ on the "visible" part of the disk surface (which is of order a) between any two successive disk collisions. Successive collisions are separated spatially by the mean flight length $\bar{L}$, and the flux spreads with a factor $\bar{L}/a$. In other words, the uncertainty principle bounds the maximal sensible truncation in the cycle expansion order by the highest quantum resolution attainable for a given wavenumber k.

The upper limit n for which $c_m(k)$ with $m \leq n$ approximates $Q_m(k)$ is increasing with increasing $\mathrm{Re}\, k$. For $n > m(\mathrm{Re}\, ka)$, defined in (55), the cycle expansion terms and cumulant terms deviate so much from each other, that beyond this order the contributions of longer cycle expansions have nothing to do with quantum mechanics. The fact that $Z_{\mathrm{sc}}(k)|_n$ – even in its convergence regime – is a good approximation to quantum mechanics *only* up to a finite n is usually not noticed, as the terms in (55) are exponentially small on or close to the real axis and sum therefore to a tiny quantity. In other words, for $n > m(\mathrm{Re}\, ka)$ and close to the real k axis, the absolute error $|c_n(k) - Q_n(k)|$ is still small, the relative error $|c_n(k)/Q_n(k)|$ on the other hand is tremendous. With increasing negative $\mathrm{Im}\, k$, however, using the scaling rules (52) and (53), the deviations (55) are blown up, such that the relative errors $|c_n(k)/Q_n(k)|$ eventually become visible as absolute errors $|c_n(k) - Q_n(k)|$ (see e.g. the resonance calculation of Wirzba and Henseler (1995)). For $\mathrm{Im}\, k$ above the boundary of convergence these errors still sum up to a finite quantity which might, however, not be negligible any longer. Below the convergence line these errors sum up to infinity.

So, the value of $\mathrm{Im} k$ where — for a given n — the $Z_{\mathrm{sc}}(k)|_n$ sum deviates from $\det \mathbf{M}(k)|_n$ is governed by the real part of k and the scaling rules (52) and (53). It has nothing to do with the boundary of convergence of $Z_{\mathrm{sc}}(k)$, as a good approximation is given by the *finite* sum of terms satisfying (54). Therefore, the truncated semiclassical expansion can describe the quantum mechanical resonance data even *below* the line of convergence of the infinite cycle expansion series, as we have already noted in Sect. 5.

On the other hand, the boundary line of the convergence regime of the semiclassical expansion is governed by $c_m(k)$, $m \to \infty$, terms which have nothing to do with the quantum analog $Q_m(k)$, i.e. solely by terms of type (55). The reason is that the convergence property of an infinite sum is governed by the *infinite* tail and not by the first few terms. Whether a semiclassical expansion converges or not is a separate issue from the question whether the quantum mechanical data are described well or not. The *convergence property* of a semiclassical zeta functions on the one hand and the *approximate description of quantum mechanics* by these zeta functions are therefore two different issues. It could happen that a zeta function is convergent, but not equivalent to quantum mechanics, as we have seen was the case with the extraneous resonances in the quasiclassical calculation. Or that it is not convergent in general, but its finite truncations nevertheless approximate well quantum mechanics, as is the case for the Gutzwiller-Voros semiclassical zeta function(41).

We conclude that the exponential rise of the number of cycles with increasing cycle expansion order n is the physical reason for the breakdown of the cycle expansion of the semiclassical zeta function(41) with respect to the exact quantum mechanical cumulant expansion.

Summary and Conclusions

In conclusion, we have constructed a classical evolution operator for the quasiclassical wave function evolution, and derived the corresponding trace and determinant formulae for periodic orbit quasiclassical quantization of chaotic dynamical systems.

Improved analyticity has been very useful in sorting out the relative importance of the semiclassical, diffraction and quantum contributions. However, one hope for consequence of the superexponential convergence of the cycle expansions of the new Fredholm determinant was that they would converge faster with the maximal cycle length truncation than the more familiar Gutzwiller-Voros and Ruelle type zeta functions. As is shown here, this is not the case. Improved analyticity comes at cost; extraneous eigenvalues are purely classical and do not belong to the quantum spectrum, but their presence degrades significantly the convergence of the cycle expansions.

The analysis sheds new light on the differences between the classical and semiclassical spectra; in particular, we have made explicit for the case of n-disk repellers the quantum limitations on the phase space resolution by classical orbits, in the spirit of Bogomolny (1992) analysis of the finite resolution of phase space for the bound systems.

In spite of its laggard performance as a putative competitor to the semiclassical quantization, the mere fact that there exists an alternative "quasiclassical" quantization that follows directly from the Schrödinger equation without recourse to path integrals and saddle points is of intellectual interest. It is still possible that a more ingeniously constructed "classical" evolution operator would also perform better than the semiclassical zeta function in practice.

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A Calculation of Trace M

In this appendix we calculate the trace (37). The equations of motion for a time independent Hamiltonian (15) can be written as

$$\dot{x}_m = \omega_{mn}\frac{\partial H}{\partial x_n} \ , \qquad \omega = \begin{bmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{bmatrix} , \qquad m,n = 1,2,\ldots,2d \ , \tag{56}$$

where $x = [q,p]$ is a phase space vector, $\mathbf{I} = [d \times d]$ unit matrix, and ω the $[2d \times 2d]$ symplectic form $\omega_{mn} = -\omega_{nm}$, $\omega^2 = -1$. The linearized motion in the vicinity of a phase space trajectory $x(t) = [q(t), p(t)]$ is given by the Jacobian matrix

$$\delta x(t) = \mathbf{J}^t(x)\,\delta x(0) \ , \qquad J^t(\xi)_{ij} = \frac{\partial x_i(t)}{\partial \xi_j} \ , \qquad \xi = x(0) \ .$$

The equations of motion of $\mathbf{J}$ follow from (56)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{J}^t(x) = \mathbf{L}(x,t)\,\mathbf{J}^t(x) \ , \qquad \text{with} \qquad \mathbf{L}(x,t)_{mn} = \omega_{mk}H_{kn}(x)|_{x(t)} \ . \tag{57}$$

where $H_{kn} = \partial_k\partial_n H$ is the matrix of second derivatives of the Hamiltonian. $\mathbf{L}$ is infinitesimal generator of symplectic (or canonical) transformations which leaves ω invariant

$$\mathbf{L}^T\omega + \omega\mathbf{L} = 0 \ . \tag{58}$$

$\mathbf{J}$ is a symplectic matrix, as it preserves the symplectic bilinear invariant ω:

$$\mathbf{J}^T\omega\mathbf{J} = \omega \ . \tag{59}$$

From this follows that $\det\mathbf{J} = 1$, and that the transpose $\mathbf{J}^T$ and the inverse $\mathbf{J}^{-1}$ are also symplectic; $\mathbf{J}^{-1} = -\omega\mathbf{J}^T\omega$. Hence if Λ is an eigenvalue of $\mathbf{J}$, so are $1/\Lambda$, Λ^* and $1/\Lambda^*$.

Let $\mathbf{j}$ be the *configuration* space Jacobian matrix

$$\mathbf{j}^t_{ij}(x) := \frac{\mathrm{d}q_i(t)}{\mathrm{d}q_j(0)} \ , \qquad j^t(x) := \det\mathbf{j}^t(x) \ , \tag{60}$$

and j the *configuration* space Jacobian evaluated on the q-space projection of the phase-space trajectory $x(t)$ passing through the $t=0$ initial point $x=(q,p)$. The curvature matrix (25) is related to the configuration space Jacobian matrix (60) by

$$M_{ij}(x,t) = \frac{\partial v_i}{\partial q_j} = \frac{\partial q_k(0)}{\partial q_j(t)}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial q_i(t)}{\partial q_k(0)} = \left(\frac{1}{\mathbf{j}^t}\right)_{kj}\left(\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{j}^t\right)_{ik} \quad ,$$

so the configuration space Jacobian matrix satisfies

$$\frac{d}{dt}\mathbf{j}^t = \mathbf{M}\,\mathbf{j}^t \tag{61}$$

and is given by the exponentiated time-ordered integral of the trace of $\mathbf{M}$

$$\det \mathbf{j}^t(x) = \mathrm{T}\mathrm{e}^{\int_0^t \mathrm{d}\tau\, \mathrm{tr}\, \mathbf{M}^\tau} \quad . \tag{62}$$

The *full phase space* Jacobian matrix $\mathbf{J}$ is given by

$$\begin{bmatrix}\delta\mathbf{q}' \\ \delta\mathbf{p}'\end{bmatrix} = \mathbf{J}\begin{bmatrix}\delta\mathbf{q} \\ \delta\mathbf{p}\end{bmatrix} = \begin{bmatrix}\mathbf{J}_{qq} & \mathbf{J}_{qp} \\ \mathbf{J}_{pq} & \mathbf{J}_{pp}\end{bmatrix}\begin{bmatrix}\delta\mathbf{q} \\ \delta\mathbf{p}\end{bmatrix} \quad , \tag{63}$$

where $\delta\mathbf{q}$, $\delta\mathbf{p}$ are d-dimensional infinitesimal tangent space vectors, and $\mathbf{J}_{qq}$, $\mathbf{J}_{qp}$, $\mathbf{J}_{pq}$ and $\mathbf{J}_{pp}$ are the $[d \times d]$ submatrices of the full $[2d \times 2d]$ Jacobian matrix. (To save paper, we suppress the t, q, p dependence for the time being). Take a derivative $\partial/\partial\delta q_i$ of both sides of (63), keeping terms to linear order in δq. This expresses the configuration Jacobian matrix $\mathbf{j}$ and the curvature matrix (25) $\mathbf{M}'$ in terms of the $\mathbf{J}$ and the initial $\mathbf{M}$

$$\begin{bmatrix}\mathbf{j} \\ \mathbf{M}'\,\mathbf{j}\end{bmatrix} = \mathbf{J}\begin{bmatrix}\mathbf{I} \\ \mathbf{M}\end{bmatrix} \quad . \tag{64}$$

Using (61) we see that $\mathbf{J}$ evolves the configuration Jacobian matrix and its time derivative

$$\begin{bmatrix}\mathbf{j}^t \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{j}^t\end{bmatrix} = \mathbf{J}\begin{bmatrix}\mathbf{j}^0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{j}^0\end{bmatrix} \quad ,$$

where the initial condition for $\mathbf{j}^0 = \mathbf{1}$ for $t=0$.

To spell it out: for a given initial set of $\delta\mathbf{q}$'s and $\delta\mathbf{p}$'s, the projection of the phase space volume onto the configuration space is given by the configuration space Jacobian matrix $\mathbf{j}$

$$\mathbf{j} = \mathbf{j}^t(q,p,\mathbf{M}) := \mathbf{J}_{qq} + \mathbf{J}_{qp}\mathbf{M} \quad , \tag{65}$$

and the matrix of curvatures $\mathbf{M}'$ is evolved recursively by

$$\mathbf{M}' = \mathbf{M}^t(q_0,p_0,\mathbf{M}_0) := (\mathbf{J}_{pq} + \mathbf{J}_{pp}\mathbf{M})\,\frac{1}{\mathbf{J}_{qq} + \mathbf{J}_{qp}\mathbf{M}} \quad , \tag{66}$$

where the q, p, t dependence is hidden in $\mathbf{J}$. We also note that transposing (64), multiplying from the right by $\omega\mathbf{J}$, and using the symplectic invariance (59) yields an alternative formula for the configuration space Jacobian matrix

$$\left(\frac{1}{\mathbf{j}}\right)^T = \mathbf{J}_{pp} - \mathbf{M}'\mathbf{J}_{qp} \ . \tag{67}$$

Evaluation of the trace (37) requires a first variation in all of the dynamical space coordinates X, including $\delta\mathbf{M}'$. From (66) together with (67) we obtain

$$\delta\mathbf{M}' = \mathbf{J}_{pp}\,\delta\mathbf{M}\,\frac{1}{\mathbf{j}} - \mathbf{M}'\,\mathbf{J}_{qp}\,\delta\mathbf{M}\frac{1}{\mathbf{j}} = \left(\frac{1}{\mathbf{j}}\right)^T \delta\mathbf{M}\,\frac{1}{\mathbf{j}} \ , \tag{68}$$

so the trace (37) is simply reinstated

$$\Delta_{p,r} = \sum \frac{(\det \mathbf{j}_p)^{r/2}}{\left|\det\left(\mathbf{1} - \frac{\partial}{\partial\mathbf{M}}\mathbf{M}^{T_p r}(M)\right)\right|} = \sum \frac{(\det \mathbf{j}_p)^{r/2}}{\left|\det\left(\mathbf{1} - \mathbf{j}_p^{-r}\otimes\mathbf{j}_p^{-r}\right)\right|} \ . \tag{69}$$

The sum is over all $\mathbf{M}$ that satisfy the fixed point condition

$$\mathbf{M}^{T_p}(q,p,M) = \mathbf{M} \ . \tag{70}$$

Consider now $\mathbf{j}$ for a periodic orbit p; $\mathbf{j}$ is a $[d\times d]$ matrix with eigenvalues and eigenvectors

$$\mathbf{j}\,\mathbf{e}_i = \Lambda_i\mathbf{e}_i \ , \qquad i = 1,2,\cdots,d \ .$$

Multiply (64) from the right by the $2d$-dimensional vector $[\mathbf{e}_i, \mathbf{e}_i]$; we see that an eigenvalue of $\mathbf{j}$ is also an eigenvalue of the $[2d\times 2d]$ phase space Jacobian matrix:

$$\Lambda_i \begin{bmatrix} \mathbf{e}_i \\ \mathbf{M}\mathbf{e}_i \end{bmatrix} = \mathbf{J} \begin{bmatrix} \mathbf{e}_i \\ \mathbf{M}\mathbf{e}_i \end{bmatrix} \ ,$$

Furthermore, transposing this equation, multiplying it from right by $\Lambda_i^{-1}\omega\mathbf{J}$, and using the symplectic condition (59) yields the associated left eigenvector with eigenvalue $1/\Lambda_i$,

$$[\mathbf{e}_i^T, \mathbf{e}_i^T\mathbf{M}]\,\omega\Lambda_i^{-1} = [\mathbf{e}_i^T, \mathbf{e}_i^T\mathbf{M}]\,\omega\mathbf{J} \ .$$

In this way the $(\Lambda_i, 1/\Lambda_i)$ pairs of eigenvalues of the $[2d\times 2d]$-dimensional phase space Jacobian matrix correspond the d eigenvalues of the d-dimensional $\mathbf{j}$. As the d eigenvalues of $\mathbf{j}$ generate the d pairs of eigenvalues of $\mathbf{J}$, the sum (69) gets 2^d contributions $\Lambda_1^{\pm 1}\Lambda_2^{\pm 1}\cdots\Lambda_d^{\pm 1}$. Each of these is expanding on its own $\mathbf{M}$ subspace, and the dominant one is the most expanding one, so we keep from (69) only the modulus of the leading term (the phase will be treated in the next section)

$$\left|\widetilde{\Delta}_{p,r}\right| = \prod_{i=1}^{d} \frac{|\Lambda_{p,i}|^{r/2}}{1 - 1/\Lambda_{p,i}^{2r}} \ . \tag{71}$$

The dynamics in the tangent space can be restricted to a unit eigenvector neighborhood corresponding to the largest eigenvalue of the Jacobian matrix. On this neighborhood the largest eigenvalue of the Jacobian matrix is the only fixed point, and the quasiclassical zeta function obtained by keeping only the largest term in the $\Delta_{p,r}$ sum in (69) is also entire, Cvitanović and Vattay (1993).

So, (very pleasantly) as Λ_i are also eigenvalues of the configuration space Jacobian matrix $\mathbf{j}$, the extra trace over $\mathbf{M}$ is coming for free; we have *already* computed the eigenvalue set $\{\Lambda_1, 1/\Lambda_1, \cdots, \Lambda_d, 1/\Lambda_d\}$ for every full (q, p) phase space cycle p.

B Maslov Indices

The square root of the configuration space Jacobian (62) is also a time ordered integral

$$\left(\det \mathbf{j}^t(x)\right)^{\frac{1}{2}} = \mathrm{T}\exp\left\{\frac{1}{2}\int_0^t \mathrm{d}\tau\,\mathrm{tr}\,(\mathbf{M}^\tau)\right\} \quad . \tag{72}$$

$\mathbf{M}$ diverges at caustics; for example, for $d = 1$ Poincaré sections (such as for billiards) $\mathbf{M} = \partial p/\partial q$ diverges whenever a trajectory points in the p-axis direction. Close to a singularity, where

$$\mathbf{M}(t \to t^c) = \infty \quad ,$$

we can neglect the non-leading terms from (27) and use the solution of

$$\dot{\mathbf{M}} = -\mathbf{M}^2 \quad , \tag{73}$$

after the symmetric matrix $\mathbf{M}$ had been transformed into a diagonal form. The time ordered integral close to the singularity is dominated by

$$\left(\det\left\{\frac{\mathrm{d}q_i(t_+^c)}{\mathrm{d}q_j(t_-^c)}\right\}\right)^{1/2} = \exp\left(\frac{1}{2}\int_{t_-^c}^{t_+^c}\frac{R}{\tau + \mathrm{i}\epsilon - t_c}\mathrm{d}\tau\right) \quad ,$$

where $t_\pm^c = t^c \pm \eta$ are infinitesimally close to t^c and the integration variable τ is shifted to $\tau + \mathrm{i}\epsilon$, because the corresponding wave packet should start out with a positive phase before it encounters the first singularity. This integral can be computed by taking the limit $\epsilon \to 0$,

$$\left(\det\left\{\frac{\mathrm{d}q_i(t_+^c)}{\mathrm{d}q_j(t_-^c)}\right\}\right)^{1/2} = \exp(-\mathrm{i}\pi(R/2))\left|\det\left\{\frac{\mathrm{d}q_i(t_+^c)}{\mathrm{d}q_j(t_-^c)}\right\}\right|^{\frac{1}{2}} \quad . \tag{74}$$

Note that the phase only results from the delta function part of the integrand, whereas the principle value contributes just to the modulus which has been already calculated in (71). Between two singular points the time ordered integral is positive and gives the absolute value of the volume ratio. R counts the number of rank reductions of the matrix $\mathbf{M}$ along the classical path, and it is a function of the initial condition $\mathbf{M}_0$; for a periodic orbit it is an invariant property of the cycle.

C Gutzwiller Trace Formula vs. Quasiclassics

Consider a generalization of the quasiclassical zeta function (39), weighted by extra powers of $\Lambda_{p,i}$:

$$F_n(k) = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \prod_{i=1}^{d} \frac{|\Lambda_{p,i}|^{-r/2}\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar} S_p(k) r - \mathrm{i}\pi \frac{m_p}{2} r}}{\Lambda_{p,i}^{nr}(1-1/\Lambda_{p,i}^{r})^2(1-1/\Lambda_{p,i}^{2r})}\right) . \qquad (75)$$

The weight $1/(1-x)$, $x = 1/\Lambda_{p,i}^r$ of p-th term in the exponent of the semiclassical zeta function (41) can be related to the quasiclassical zeta function cycle weight $1/(1-x)^2(1-x^2)$ in (75) by multiplying it by

$$1 = \frac{1}{(1-x)(1-x^2)} - \frac{x}{(1-x)(1-x^2)} - \frac{x^2}{(1-x)(1-x^2)} + \frac{x^3}{(1-x)(1-x^2)} .$$

From this it follows that the semiclassical zeta function function (41) for Axiom A flows is meromorphic in the complex k plane, as it can be written as a ratio of entire functions; for 2-dimensional Hamiltonian systems

$$Z_{\mathrm{sc}}(k) = \frac{F_0(k)F_3(k)}{F_1(k)F_2(k)} , \qquad (76)$$

where $F_k(k)$ includes only (71), the first term in the $\Delta_{p,r}$ sum (69). The zeros of the semiclassical zeta function coincide with the ones obtained from $F_0(k) = Z_{\mathrm{qc}}(k)$, and the leading poles should arise from $F_1(k)$. In two dimensions, i.e. $d = 1$, (75) can be resummed as

$$F_n(k) = \prod_p \prod_{j=0}^{\infty} \prod_{l=0}^{\infty} \left(1 - \frac{t_p}{\Lambda_p^{n+j+2l}}\right)^{j+1} , \qquad (77)$$

where t_p is defined in (44).

D Selberg Zeta Function

The question that arises naturally in discussing semiclassical quantization is following: if the usual semiclassical evolution is not multiplicative, why does it anyway yield the *exact* quantization in the case of the Selberg trace formula? And what does the quasiclassical quantization yield for flows on surfaces of constant negative curvature?

The Selberg (1956) zeta function for geodesic flows on surfaces of constant negative curvature is exceptional: in this very special case the multiplicativity is guaranteed by the Bowen-Series (1979) map, which reduces the two-dimensional flow to a direct product of 1-dimensional maps, and makes it possible to construct the associated transfer operators in terms of one variable, Mayer (1990).

The essence of the construction is the following: In the Poincaré halfplane representation the dynamics is described by the free Hamiltonian

$$\hat{H} = \frac{1}{2y^2}(p_x^2 + p_y^2) \tag{78}$$

whose classical trajectories are circle segments. The centers of the circles always lie on the $y = 0$ axis, and any free trajectory can be characterized by x_f and x_b, the forward and backward intersection points of its circle with the $y = 0$ axis. The polygonal billiards in the x, y plane are defined in terms of walls which themselves are geodesics, hence also characterized by their footpoints x_1, x_1', x_2, x_2' ... (see Fig. 7). A reflection off a wall changes the direction of the particle,

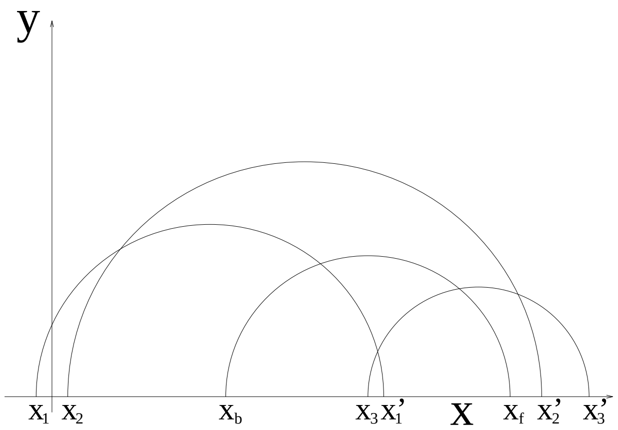

Fig. 7. A typical arrangement on the Poincaré halfplane. The half circles with footpoints (x_i, x_i'), $i = 1, 2, 3$ are the billiard walls. The forward and backward footpoints (x_b, x_f) represent a trajectory.

with the new trajectory characterized by a new pair of footpoints x_f' and x_b'. The new forward footpoint will be the image of the old footpoint with respect to an inversion transformation on the circle of the wall. For example, a reflection off the wall x_n, x_n' of radius $R_n = |x_n - x_n'|/2$ and center $x_n^c = (x_n + x_n')/2$ is described by

$$x_f' = f_n(x_f) = x_n^c + R_n^2/(x_f - x_n^c) \ .$$

The forward footpoint and the index of the wall determine uniquely the next forward footpoint. The footpoint of a periodic orbit reflected off walls $\epsilon_1\epsilon_2...\epsilon_{n_p}$ respectively is determined by the equation

$$x_p = F_{\epsilon_1\epsilon_2\ldots\epsilon_{n_p}}(x_p) = f_{\epsilon_{n_p}}(f_{\epsilon_{n_p-1}}(...f_{\epsilon_1}(x_p)...)) \ . \tag{79}$$

The hyperbolic length of this periodic orbit is $l_{\epsilon_1\epsilon_2\ldots\epsilon_{n_p}} = \log|F'_{\epsilon_1\epsilon_2\ldots\epsilon_{n_p}}(x_p)|$, and its stability eigenvalue is also given by the derivative $F'_{\epsilon_1\epsilon_2\ldots\epsilon_{n_p}}(x_p)$. The stability is the product of derivatives evaluated along the orbit

$$F'_{\epsilon_1\epsilon_2\ldots\epsilon_{n_p}} = \prod_{i=1}^{n_p} F'_{\epsilon_i} \ ,$$

and is multiplicative without any need for further manipulations. This property makes the polygonal billiards on surfaces of constant negative curvature unique and atypical.

The Fredholm determinant of the 1-dimensional Perron-Frobenius operator

$$\mathcal{L}(y,x,k) = |f'(x)|^{1/2+\mathrm{i}k}\delta(y-f(x)) \ ,$$

where f is the appropriate footpoint mapping and $k = \sqrt{E-1/4}$ is the wave number, is precisely the Gutzwiller-Voros semiclassical zeta function for this problem, $Z_{\mathrm{sc}}(E) = \det(1-\mathcal{L}_0)$. Unlike the generic situation discussed in this paper, the semiclassical zeta function is in this case an entire function. However, the spectrum of the quasiclassical zeta function $Z_{\mathrm{qc}}(E)$ defined in this paper contains spurious zeroes in the complex plane in addition to the true zeroes on the real k axis. These spurious zeroes are the eigenvalues of weighted operators of type

$$\mathcal{L}_m(y,x,k) = |f'(x)|^{1/2+m+\mathrm{i}k}\delta(y-f(x)) \ , \tag{80}$$

where m is an integer number. Since the $F_n(k)$'s (see (77)) can be expressed in terms of the Fredholm determinants of these operators as

$$F_n(k) = \prod_{l=0}^{\infty}\left\{\det\left(1-\mathcal{L}_{n+l}\right)\,\det\left(1-\mathcal{L}_{n+l+1}\right)\right\}^{l+1} \ , \tag{81}$$

$Z_{\mathrm{sc}}(k) = \det(1-\mathcal{L}_0)$ results under the relation (76), too.

References

Arnold V. I. (1978): *Ordinary Differential Equations* (MIT Press, Cambridge, Mass.)

Artuso R., Aurell E., Cvitanović P. (1990): Recycling of strange sets: I. cycle expansions. Nonlinearity **3**, 325–359

Berry M. V. (1981): Quantizing a Classically Ergodic System: Sinai's Billiard and the KKR Method. Ann. Phys. (N.Y.) **131**, 163–216

Berry M. V., Keating J. P. (1990): A rule for quantizing chaos? J. Phys. **A 23**, 4839–4849

Bogomolny E. B. (1992): On dynamical zeta function. CHAOS **2**, 5–14

Bohm D. (1952): A suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I. Phys. Rev. **85**, 166

Born M. (1926): Z. f. Physik **37**, 863

Bowen R., Series C. (1979): Publ. Math. Inst. Hautes Etud. Sci. **50**, 153–170

Cvitanović P. (1988): Invariant measurement of strange sets in terms of cycles. Phys. Rev. Lett. **61**, 2729–2733

Cvitanović P., ed. (1992): *Periodic Orbit Theory - theme issue*, CHAOS **2**, 1–158

Cvitanović P., Eckhardt B., Rosenqvist P. E., Russberg G., Scherer P. (1995): *Pinball Scattering*, in *Quantum chaos between order and disorder*, Casati G. and Chirikov B. eds. (Cambridge University Press, Cambridge), 405–433

Cvitanović P., Rosenqvist P. E., Rugh H. H., Vattay G. (1993): A Fredholm determinant for semi-classical quantization. CHAOS **3**, 619–636

Cvitanović P., et al., (1996): *Classical and Quantum Chaos: A Cyclist Treatise*, http://www.nbi.dk/~predrag/QCcourse/

Cvitanović P., Eckhardt B. (1989): Periodic-Orbit Quantization of Chaotic Systems. Phys. Rev. Lett. **63**, 823–826

Cvitanović P., Eckhardt B. (1991): Periodic orbit expansions for classical smooth flows. J. Phys. **A 24**, L237–L241

Cvitanović P., Rosenqvist P. E. (1993): *A new determinant for quantum chaos*, in *From Classical to Quantum Chaos*, Dell'Antonio G. F., Fantoni S., Manfredi V. R., eds., Soc. Italiana di Fisica Conf. Proceed. **41** (Ed. Compositori, Bologna), 57–64

Cvitanović P., Vattay G. (1993): Entire Fredholm determinants for evaluation of semi-classical and thermodynamical spectra. Phys. Rev. Lett. **71**, 4138–4141

Eckhardt B. (1987): Fractal properties of scattering singularities. J. Phys. **A**: Math. Gen. **20**, 5971–5979

Eckhardt B., Russberg G. (1993): Resummations of classical and semi-classical periodic orbit expressions. Phys. Rev. **E 47**, 1578–1588

Feynman R. P. (1972): *Statistical Mechanics - a set of lectures*, (W. A. Benjamin, Mass.)

Gaspard P., Alonso Ramirez D. (1992): Ruelle classical resonances and dynamical chaos: The three- and four-disk scatterers. Phys. Rev. **A 45**, 8383–8397

Gaspard P., Rice S.A. (1989a): Scattering from a classically chaotic repellor. J. Chem. Phys. **90**, 2225–2241

Gaspard P., Rice S.A. (1989b): Semiclassical quantization of the scattering from a classically chaotic repellor. J. Chem. Phys. **90**, 2242–2254

Gaspard P., Rice S.A. (1989c) Exact quantization of the scattering from a classically chaotic repellor. J. Chem. Phys. **90**, 2255–2262

Gutzwiller M.C. (1971): Periodic Orbits and Classical Quantization Conditions. J. Math. Phys. **12**, 343–358

Gutzwiller M.C. (1988): J. Phys. Chem. **92**, 3154

Gutzwiller M.C. (1990): *Chaos in Classical and Quantum Mechanics* (Springer, New York)

Heller E. J. (1975): Time-dependent approach to semiclassical dynamics. J. Chem. Phys. **62**, 1544–1555

Heller E. J., Tomsovic S., Sepúlveda A. (1992): Time domain approach to semiclassical dynamics: Breaking the log time barrier. CHAOS **2**, 105–116

Holland P. R. (1993): *The quantum theory of motion, - An account of the de Broglie-Bohm casual interpretation of quantum mechanics* (Cambridge Univ. Press, Cambridge)

Kohn W., Rostoker N. (1954): Solution of the Schrödinger equation in periodic lattices with an application to methalic lithium. Phys. Rev. **94**, 1111–1120

Lloyd P., Smith P.V. (1972): Multiple-scattering theory in condensed materials. Adv. Phys. **21**, 69–142

Madelung E. (1926): Z. f. Physik **40**, 332

Nelson E (1985): *Quantum Fluctuations* (Princeton Univ. Press, Princeton)

Mayer D. H. (1990): On the Thermodynamic Formalism for the Gauss Map. Comm. Math. Phys. **130**, 311–333; Mayer D. H. (1992): in *From Phase Transitions to Chaos*, Györgyi G., et al., eds., 521–529

Pollner P., Vattay G. (1996): New Method for Computing Topological Pressure. Phys. Rev. Lett. **76**, 4155–4158

Rosenqvist P. E., Vattay G., Wirzba A. (1996): Application of the Diffraction Trace Formula to the Three Disk Scattering System. J. Stat. Phys. **83**, 243–257.

Ruelle D. (1987): *Statistical Mechanics, Thermodynamical Formalism* (Addison-Wesley, Reading Mass.)

Rugh H. H. (1992): The Correlation Spectrum for Hyperbolic Analytic Maps. Nonlinearity **5**, 1237–1263; see also ref. Cvitanović et al. (1993) for a discussion of the applicability of the theorem

Schrödinger E. (1926): Annalen der Physik **79**, 361, 489, **80**, 437, **81**, 109

Selberg A. (1956): J. Ind. Math. Soc.**20**, 47

Spiegel E.A. (1995): private communication

Tanner G. (1995): private communication

Vattay G. (1994): Differential equations to compute $\hbar$ corrections of the trace formula. chao-dyn/9406005, unpublished

Vattay G. (1996): Bohr-Sommerfeld Quantization of Periodic Orbits. Phys. Rev. Lett. **76**, 1059–1062

Vattay G, Rosenqvist P. E. (1996): Periodic Orbit Quantization beyond Semiclassical Approximation. Phys. Rev. Lett. **76**, 335–339

Vattay G., Wirzba A., Rosenqvist P. E. (1994): Periodic Orbit Theory of Diffraction. Phys. Rev. Lett. **73**, 2304–2307

Vattay G., Wirzba A., Rosenqvist P. E. (1995): Inclusion of Diffraction Effects in the Gutzwiller Trace Formula. Proc. Int. Conf. *Dynamical Systems and Chaos*, Tokyo, May 1994, chao-dyn/9408005, (World Scientific, Singapore) Vol. **2**, 463–466

Voros A. (1988): Unstable periodic orbits and semiclassical quantisation. J. Phys. **A**: Math. Gen. **21**, 685–692

Wirzba A. (1992): Validity of the semiclassical periodic orbit approximation in the 2-and 3-disk problems. CHAOS **2**, 77–83

Wirzba A. (1993): Test of the Periodic Orbit Approximation in n-Disk Systems. Nucl. Phys. **A 560**, 136–150

Wirzba A. (1995): Zeta functions in scattering problems evaluated on the real wave number axis. http://crunch.ikp.physik.th-darmstadt.de/~wirzba/, unpublished

Wirzba A. (1996): Comparison of the quantum mechanical cumulant and the semi-classical curvature expansion for classically chaotic scattering systems. http://crunch.ikp.physik.th-darmstadt.de/~wirzba/, unpublished

Wirzba A., Henseler M. (1995): The missing-link between the quantum mechanical and semi-classical determination of scattering resonance poles. http://crunch.ikp.physik.th-darmstadt.de/~wirzba/, unpublished