Quantum Eigenvalues from Classical Periodic Orbits

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We combine the cycle-expansion method with a functional equation to obtain highly excited semiclassical energy eigenvalues for chaotic Hamiltonian systems. Applications to the anisotropic Kepler problem and to a bounded billiard demonstrate the power of the method. The agreement with quantum results is surprisingly good even for highly excited states.

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There is growing theoretical and numerical evidence that the eigenvalues of a quantum Hamiltonian are intimately connected to the periodic orbits of the corresponding classical system. For geodesic flow on a surface of constant negative curvature one has an exact correspondence: The quantum eigenvalues are zeros of an infinite product over entries from classical cycles (Selberg trace formula) [1,2]. For general Hamiltonian systems, such a correspondence is suggested by a semiclassical expansion of the path-integral expression for the density of states around classical periodic orbits (Gutzwiller trace formula) [3,4]. As a consequence, one should be able to obtain classical periodic orbits from long-range correlations in the sequence of quantum eigenvalues, and this has in fact been demonstrated [5,6]. What has been missing is a demonstration of the validity and accuracy of the Gutzwiller theory for short-range correlations, i.e., individual eigenstates.

Attempts to obtain quantum eigenvalues for chaotic systems from classical periodic orbits face (at least) two serious problems: The Gutzwiller trace formula does not converge for real energies and the eigenvalues computed from it are not real. The first problem is caused by the exponential proliferation of periodic orbits for classically chaotic systems [7] and requires either smoothing of the density of states or analytic continuation of the theory. With the smoothing technique the lowest few eigenstates could be identified for chaotic billiards [8] and for hydrogen in a magnetic field [9]. Many scattering resonances were computed using the cycle expansion [10,11]. This method provides, at least for ideal hyperbolic systems, a rapidly converging continuation of the trace formula beyond its abscissa of absolute convergence [12].

The second problem may be overcome by appealing to the theory of the Riemann and Selberg zeta functions [13–15]. Both satisfy a functional relation from which one can derive that, formal appearance notwithstanding, a product of the zeta functions with an unimodular function is real along the axis containing the eigenvalues. Gutzwiller's theory suggests that the phase of the unimodular function is given by the smooth integrated density of states. Using this functional equation, one obtains a real function, the zeros of which should be the eigenvalues.

In this Letter we will combine the cycle-expansion method of Ref. [10] with a functional equation. Applications of this theory to two strongly chaotic models, the anisotropic Kepler problem and a bounded billiard, demonstrate that with moderate classical effort one can obtain accurate, high-lying semiclassical eigenvalues [16].

The starting point is the semiclassical expression for the response function $g(E)$ which splits into a smooth part $\tilde{g}_0(E)$ and modulations due to periodic orbits (po) of action $S_{\rm po}$ and weights $A_{\rm po}$ (see Refs. [3,4]),

$$g(E)=\sum_n \frac{1}{E-E_n}=\tilde{g}_0(E)+\sum_{\rm po} A_{\rm po}\exp[iS_{\rm po}(E)/\hbar]\,. \quad (1)$$

Integration and exponentiation of Eq. (1) yields the spectral Euler product as an infinite product of Selberg type (ignoring renormalizations of the left-hand side) [17],

$$\prod_n (E-E_n)\sim e^{-i\pi\bar{N}(E)}\prod_{\rm ppo}\prod_{k=0}^{\infty}(1-t_{\rm ppo}^{(k)}) = e^{-i\pi\bar{N}(E)}Z(E)\,, \quad (2)$$

where the last equality defines the Selberg zeta function as a product over periodic orbits. The mean spectral staircase function $\bar{N}(E)$ is given by the classical phase-space volume plus correction terms of lower order, which depend on the size and topology of the boundary of the classically allowed region. The weight $t_{\rm ppo}^{(k)}$ of each primitive (i.e., nonrepeated) periodic orbit (ppo) contains the action S and the stability exponent u of the orbit as well as phase factors depending on the topology of its stable and unstable manifolds (Morse index α, type of hyperbolicity) [18],

$$t_{\rm ppo}^{(k)}=(\pm 1)^k\exp[iS/\hbar-i\alpha\pi/2-(k+\tfrac{1}{2})u]\,. \quad (3)$$

The plus sign applies to hyperbolic orbits and the minus sign to hyperbolic periodic orbits with reflection.

Suppose the periodic orbits could be labeled with a binary code (as in our examples below). The idea of the cycle expansion [10,12] is to expand the infinite product (2) and to group the resulting terms in ascending order of the symbol length. For $k=0$ this reads

$$\prod_j (1-t_j) = 1 - t_0 - t_1 - (t_{01} - t_0 t_1) - (t_{001} - t_0 t_{01}) - (t_{011} - t_{01} t_1) - \cdots . \quad (4)$$

Except for the *fundamental orbits* 0 and 1, each orbit contribution is accompanied by a compensating term pieced together from shorter orbits. Thus, terminating the expansion at a given symbol length effectively means a resummation of *all* orbits with the approximation that the longer orbits are exactly shadowed by the shorter ones. The scattering system discussed in Ref. [10] is hyperbolic, all Lyapunov exponents (stability exponent per period of an orbit) are strictly bounded away from zero, the compensation is exponential, and the eigenvalues E_n [i.e., the zeros of the infinite product (4)] converge rapidly. For bounded systems, this ideal behavior is typically spoiled by marginally stable orbits, pruning of the symbolic tree, and accumulating orbits. However, good behavior can be recovered, if a functional equation is built in.

In general, the cycle-expanded product $Z(E)$ in Eq. (2) is complex valued, even for real energies. However, the functional determinant (2) should be real, indicating that the integrated mean density of states cancels the phase accumulated by $Z(E)$, so that the right-hand side of (2) is again real. From this there follows a relationship for complex energies between $Z(E)$ and its complex conjugate,

$$Z(E) = e^{2\pi i \bar{N}} Z^*(E) . \quad (5)$$

Such relations are known to hold true for Selberg zeta functions and for the Riemann zeta function and the present generalization to more general systems suggests itself. It has also been related to a bootstrapping of long orbits [14] and to unitarity of the quantum evolution [15]. Taking this relation for granted, one concludes that the zeros of the real expression

$$D(E) = e^{-i\pi\bar{N}} Z(E) + e^{i\pi\bar{N}} Z^*(E) \quad (6)$$

should be semiclassical approximations to the eigenvalues. As this function is almost the functional determinant [19], we will henceforth refer to it under this name.

As a first example of the utility of the above method, consider the anisotropic Kepler problem (AKP), described by the Hamiltonian

$$H = \frac{p_x^2 + p_y^2}{2} + \gamma \frac{p_z^2}{2} - \frac{1}{r} . \quad (7)$$

Its classical properties have been studied thoroughly by Gutzwiller [4] and an efficient method to obtain quantum eigenenergies is available [20]. The azimuthal quantum number m and parity π are the only conserved quantities, thus reducing the Schrödinger equation to two degrees of freedom. There is strong evidence that for a mass anisotropy of $\gamma=0.2$ the classical dynamics is completely hyperbolic [4]. After desymmetrization, the periodic orbits of the systems can be labeled with a binary code with only one restriction: The orbit 0 is not realized in the system [21]. We computed actions and stability exponents of all primitive periodic orbits up to symbol length 8 (71 orbits). The discrete properties of the periodic orbits (Morse index, type of hyperbolicity) are available through the coding [21].

The absence of the period-one orbit 0 is a typical example of pruning. As a consequence, an infinite number of terms in the expanded product remain uncompensated. However, the long orbits shadow a fictitious orbit 0 and their dynamics suggest to attribute an action $S=0$, instability $u=0$, and index $\alpha=2$ to this orbit. Formally, adding this fictitious orbit to the infinite product corresponds to a multiplication by 2, but such tricks can be used to speed up convergence [22]. With the action of the orbit being zero, one also finds a strong tendency for orbits to accumulate; i.e., there are families of infinitely many orbits whose actions converge to finite values.

Calculations using just the expansion (4) without functional equation (see also Ref. [23]) yield results comparable to the transfer matrix calculations of Gutzwiller [4]. The zeros do not converge to the real axis when including more and more orbits and an exceedingly large number of orbits is needed to reproduce the correct mean density of states. This behavior is perhaps special to the AKP and connected to the peculiar properties of orbits accumulating to the 0 orbit.

Nevertheless, the situation improves dramatically if the functional equation (5) is used, as shown in Fig. 1 for the $m^\pi = 0^+$ subspace. The effective quantum number $z = \sqrt{-1/2E}$ defines the natural energy scale in Coulombic systems. We included all orbits up to symbol lengths 4 [Fig. 1(a)] and 8 [Fig. 1(b)], respectively, and consistently expanded the product over k in (2). Increasing the number of orbits improves the resolution of the higher-lying states without destroying the resolution of the lower-lying ones.

Similar results have been obtained for the billiard bounded by three touching disks (the bounded limit of the system studied previously [10,24]). After desymmetrization a binary coding is possible; the orbit 0 is absent as well as some orbits of length ≥ 6 (details will be given elsewhere). The scaling behavior of families of orbits asymptotic to the 0 orbit is different from the AKP (no accumulation of infinitely many orbits of finite length). Convergence of the cycle expansion is found to deteriorate when going from the open system to the closed billiard. Nevertheless, the zeros of the full product over the classical orbits move towards the real axis (when including longer and longer orbits) and end up close to

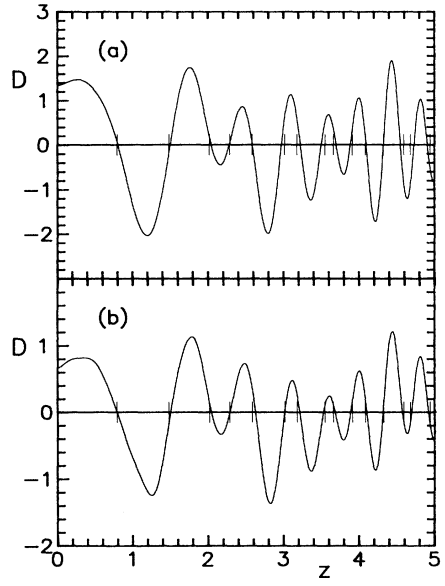

FIG. 1. The cycle-expanded functional determinant for the $m^{\pi}=0^{+}$ subspace. The quantum eigenvalues are marked with vertical bars on the real axis. (a) All orbits up to length 4 (8 in number) included. (b) All orbits up to length 8 (71) included.

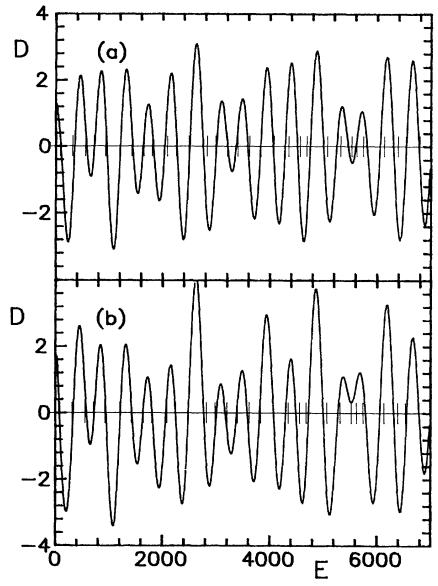

FIG. 2. The cycle-expanded functional determinant for the closed three-disk billiard (radius of a disk is unity). The vertical bars mark the exact quantum eigenvalues. (a) All orbits up to length 2 (3 in number) included. (b) All orbits up to length 3 (5) included.

the true eigenvalues. Including the functional equation, however, again improves the representation of the eigenvalues. Figure 2 shows the real functional determinant including orbits up to length 3 and including the extrapolation for the missing 0 orbit (bouncing back and forth between two disks). Note that the lowest 30 eigenvalues are represented very accurately down to a fraction of the mean density of states. Adding more orbits changes predominantly the amplitude of the oscillations. Thus in regions with large amplitude, the positions of the zeros are very stable with the addition of more orbits, but in other regions there can be rather significant changes.

These results suggest that the cycle expansion combined with a functional equation can be used to calculate accurate semiclassical eigenvalues for bounded chaotic Hamiltonian systems. Using only 8 orbits for the AKP the lowest five states could be reproduced to within $\sim 1\%$ of the mean level spacing. For the billiard the situation was less uniform, there being rather large deviations for the low-lying states (where the semiclassical approximation is poor) and an intermediate regime with deviations less than 2%; eventually the number of orbits included did not suffice to represent the eigenvalues to better than a mean spacing. A second advantage of the method used here is that it does not produce spurious oscillations as does the direct summation [9] and that it gives the correct mean density of states (we checked this for the AKP for the first 2500 states). The method is straightforward to use and requires only moderate effort to obtain good results. At least in practical applications convergence properties and possible truncation requirements for long orbits do not cause any trouble (in contradistinction to the Riemann zeta function, where truncation is of crucial importance [13,14]). Although we cannot rigorously prove that the functional determinant converges with the cycle length, the results shown indicate such a behavior.

For general hyperbolic systems, where no symbolic coding is known, we suggest to order periodic orbits by their Maslov indices and expand group cycles by their (total) phases. Applied to the present examples this would reproduce the cycle expansion in terms of symbolic length (this is in line with previous suggestions [18,25] to base the symbolic coding on the Maslov phases).

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