Novel Rule for Quantizing Chaos

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Numerical tests of a novel semiclassical quantization rule are carried out for three strongly chaotic systems: the hyperbolic billiard, Artin's billiard, and the Hadamard-Gutzwiller model. The results demonstrate that this novel rule is very effective and capable to generate sensible approximations to the quantal energy levels.

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One main goal in the study of quantum chaos during the last few years has been to find an effective quantization rule for strongly chaotic systems as a substitute for the well-known WKB method for integrable systems and its multidimensional generalization, the Einstein-Brillouin-Keller (EBK) quantization rules. (For a comprehensive review, see the recent textbook by Gutzwiller [1].) Nearly all semiclassical approximations which have been applied to classically chaotic systems have started from Gutzwiller's periodic-orbit theory [1,2]. Recently, there have been several exciting developments. Among them are the derivation and application of a smoothed version of the Gutzwiller theory [3-6], the proposal of a Riemann-Siegel look-alike formula [7], a rule for quantizing chaos based on dynamical zeta functions and their associated functional equations [6,8-10], and a quantization condition derived from a quantum version of a classical Poincaré map [11].

In this Letter we study a novel semiclassical quantization condition [12] that is based on a semiclassical representation of the spectral staircase $\mathcal{N}(E) = \sum_{n=1}^{\infty} \Theta(E - E_n)$. [The systems to be discussed possess only a discrete energy spectrum $\{E_n\}$, and $\mathcal{N}(E)$ counts the number of energy levels below E. $\Theta(E)$ is the Heaviside step function.] The quantization condition reads

$$\cos\{\pi \mathcal{N}_{\rm sc}(E)\} = 0, \qquad (1)$$

where $\mathcal{N}_{sc}(E)$ denotes a semiclassical approximation to $\mathcal{N}(E)$. Equation (1) is equivalent to the condition $\mathcal{N}_{\rm sc}(E) = n - \frac{1}{2}, n = 1, 2, \dots$ In comparison with the recent developments mentioned above, the quantization rule (1) has the advantage that it is much simpler. For example, no pseudo-orbits [6-9] have to be calculated and no functional equation is required. Moreover, it is very closely related to the original formulation of the periodic-orbit theory. Most importantly, it yields surprisingly good results as our numerical applications shall show. The reason for the success is that it is not necessary that the whole staircase be approximated well by its semiclassical approximation. If only the semiclassical curve goes through the middle of the steps of the staircase function, the quantum condition (1) already yields the correct energies.

In order to formulate the quantization condition in a convergent form, one has to start with a smoothed trace formula [3,4]. We are thus led to consider a smoothed version [12] of the spectral staircase which is given here for billiard systems ($\varepsilon > 0$):

$$\mathcal{N}_{\varepsilon}(E) = \frac{1}{2} \sum_{n=1}^{\infty} \left[\operatorname{erf}\left(\frac{p-p_{n}}{\varepsilon}\right) + \operatorname{erf}\left(\frac{p+p_{n}}{\varepsilon}\right) \right] \approx \int_{0}^{\infty} dp' \,\overline{\mathcal{N}}(E(p')) \frac{1}{\varepsilon\sqrt{\pi}} \left[\exp\left\{-\frac{(p-p')^{2}}{\varepsilon^{2}}\right\} - \exp\left\{-\frac{(p+p')^{2}}{\varepsilon^{2}}\right\} \right] + \frac{1}{\pi} \sum_{\gamma} \sum_{k=1}^{\infty} \frac{\exp\left\{-i\pi k v_{\gamma}/2\right\}}{k|2 - \operatorname{Tr}M_{\gamma}^{k}|^{1/2}} \sin\left\{\frac{pkl_{\gamma}}{\hbar}\right\} \exp\left\{-\frac{\varepsilon^{2}k^{2}l_{\gamma}^{2}}{4\hbar^{2}}\right\}.$$
(2)

(This formula can be considered as an integrated version of the Gaussian-smoothed level density [3,4].) Here $E(p) = p^2/2m$, and $p_n = (2mE_n)^{1/2}$ denote the momenta corresponding to the energy eigenvalues E_n of the Schrödinger equation. $\overline{\mathcal{N}}(E)$ is the mean spectral staircase. In the limit $\varepsilon \to 0$, $\mathcal{N}_{\varepsilon}(E)$ approaches the spectral staircase $\mathcal{N}(E)$. The double sum on the right-hand side runs over all primitive periodic orbits, which are denoted by γ , and their multiple repetitions k. I_{γ} is the length of a primitive periodic orbit, and M_{γ} is its monodromy matrix. v_{γ} is the maximal number of conjugate points along a periodic orbit plus twice the number of reflections on those parts of the boundary, where Dirichlet boundary

conditions are required. In formula (2) it is assumed that v_{γ} is an even number. If there exist periodic orbits along the boundary, Eq. (2) has to be slightly modified in order to take into account also contributions of these orbits (see [13]).

Inserting Eq. (2) into Eq. (1) leads to a quantization condition which contains absolutely convergent terms only. Although, in general, only an evaluation of the *smoothed* staircase is well defined, practical applications show that it is often possible to apply the quantization condition for $\varepsilon = 0$. One possible explanation for this might be that the periodic-orbit sum is conditionally convergent, because the orbits contribute with different phase factors $\exp\{-i\pi k v_{\gamma}/2\}$ to the sum over orbits. (For a discussion of the convergence properties, see [4,6,8,9,12, 13].) In the case that the periodic-orbit sum is divergent, good results are often obtained as a consequence of the fact that not too many orbits are included in the sum and that indications of the divergence show up late. In general, however, the divergent sum has to be regularized [6] as, e.g., in Eq. (5) below.

An evaluation of the semiclassical formula (2) for $\varepsilon = 0$ is shown in Fig. 1 for the hyperbolic billiard [5] (desymmetrized, even symmetry), which is described in more detail below. The discontinuous curve represents the staircase as obtained from a numerical solution [14] of the Schrödinger equation, while the smooth curve has been computed from the right-hand side of Eq. (2). As can be seen, the steps of the discontinuous function $\mathcal{N}(E)$ are well approximated by the continuous curve at low energies. At higher energies the approximation slowly gets worse due to the limited number of periodic orbits which are included in the sum, but the semiclassical approximation still describes very well the mean behavior of the staircase function.

In the following we shall present a test of the quantization condition (1) by evaluating it for three strongly chaotic systems: the hyperbolic billiard [5,13], Artin's billiard [9], and the Hadamard-Gutzwiller model [3,15]. All three systems are billiards, but with very different properties. The first system is a plane billiard, while the other two can be considered as billiards on a surface of constant negative curvature. For billiard systems, it is convenient to use a scaled topological entropy τ which is energy independent. The number of periodic orbits γ with a length l_{γ} below a value l is given by $N(l) \sim \exp{\{\tau l\}/\tau l, l \rightarrow \infty}$. In the following, dimensionless units are used with $\hbar = 2m = 1$.

The first system to be discussed is the hyperbolic bil-



FIG. 1. The spectral staircase $\mathcal{N}^+(E)$ and its semiclassical approximation $\mathcal{N}_{sc}^+(E)$ for the hyperbolic billiard. $\mathcal{N}_{sc}^+(E)$ was evaluated by Eq. (2) with $\varepsilon = 0$ using all periodic orbits with length $l_{\chi} \leq 25$.

liard [5,13] whose boundaries are the x axis, the y axis, and the hyperbola y = 1/x. The mean spectral staircase has the following asymptotic expansion [16,17]:

$$\overline{\mathcal{N}}^+(E) = \frac{1}{8\pi} E \ln E + \frac{a}{8\pi} E + \frac{b^+}{8\pi} \sqrt{E} + c^+, \quad E \to \infty.$$
(3)

Here $a = 2(\gamma - \ln 2\pi)$ and $b^+ = 2\sqrt{2} + 4\pi^{3/2}/\Gamma^2(\frac{1}{4})$ (γ denotes Euler's constant). The last term in Eq. (3) has been estimated numerically [13]: $c^+ = -0.173$. The + sign refers to the partial spectrum corresponding to wave functions which are even with respect to reflection on the straight line $\gamma = x$. Numerically, this system has a topological entropy of $\tau = 0.593$.

The quantization condition (1) has been evaluated using (2) for $\varepsilon = 0$ and taking into account all orbits with length $l_{\gamma} \leq 25$, which amounts to a total number of 101265 orbits with different lengths. Figure 2 shows the result of an evaluation of condition (1) in the energy range 200 < E < 400. As can be seen, there is good agreement between the zeros of the function $\cos{\{\pi N_{sc}^+(E)\}}$ and the "true" quantum energies [14], which are marked by triangles.

The second system is Artin's billiard [9]. It describes the free motion of a point particle on a noncompact Riemann surface with constant negative curvature. On the Poincaré upper half plane $\mathcal{H} = \{z = x + iy, y > 0\}$ endowed with the measure $dx dy/y^2$, the billiard region is identical to the domain $D = \{|z| > 1$ for $-\frac{1}{2} < x < 0$ and $|z| \ge 1$ for $0 \le x \le \frac{1}{2}$ with periodic boundary conditions. For this system the Gutzwiller trace formula is an *exact* relation between the quantum-mechanical energies and the classical orbits, since it is identical to the Selberg trace formula [18,19]. Here we consider a desymmetrization of the system, which is obtained by introducing additional Dirichlet boundary conditions along the line x=0. Relation (2) is valid with an equality sign with



FIG. 2. The function $\cos{\{\pi N_{sc}^{+}(E)\}}$ for the hyperbolic billiard. $\mathcal{N}_{sc}^{+}(E)$ was evaluated as in Fig. 1. The triangles mark the positions of the "true" quantum-mechanical energies.



FIG. 3. The function $\cos{\{\pi N_{sc}^{-}(E)\}}$ for Artin's billiard. $N_{sc}^{-}(E)$ was evaluated using Eq. (2) with $\varepsilon = 0$ and taking into account all periodic orbits with length $l_{\gamma} \le 19.360...$ The triangles mark the positions of the "true" quantum-mechanical energies.

 $E(p) = p^2 + \frac{1}{4}$. The mean spectral staircase has the following asymptotic expansion [20]:

$$\overline{\mathcal{N}}^{-}(E) = \frac{1}{24}E - \frac{1}{4\pi}\sqrt{E}\ln E - \frac{3\ln 2 - 2}{4\pi}\sqrt{E} + \frac{23}{144} + \frac{1}{32\pi}\frac{\ln E}{\sqrt{E}} + O(E^{-1/2}).$$
(4)

The scaled topological entropy of this system (and of the Hadamard-Gutzwiller model) is exactly known to be $\tau = 1$.

An evaluation of the quantization condition (1) for Artin's billiard is shown in Fig. 3 in the energy range 1500 < E < 2500. Again there is very good agreement between the zeros of the function $\cos{\{\pi N_{sc}^-(E)\}}$ and the true quantum energies which have been computed by Hejhal [21].

The third system to be discussed is an example of the *Hadamard-Gutzwiller model* [3,6,12,15]. It describes the free motion of a point particle on a compact Riemann surface with constant negative curvature and genus $g \ge 2$. Again Gutzwiller's trace formula is exact since it is identical to the Selberg trace formula [18]. Here we consider a generic Riemann surface with genus g=2 which can be represented by an asymmetric hyperbolic octagon in the Poincaré disk.

The Hadamard-Gutzwiller model differs from the previous two systems in that all numbers v_{γ} are equal to zero. For that reason all periodic orbits contribute to the sum over orbits with the same sign, and the region of conditional convergence in the complex energy plane is identical to the region of absolute convergence. As a result, the periodic-orbit sum (2) diverges for $\varepsilon=0$. However, it is possible to use Eq. (2) for $\varepsilon=0$, if one regularizes the sum by introducing a cutoff L and adding a regularized remainder term (for details see [12]). One then obtains the following semiclassical approximation to the staircase



FIG. 4. The function $\cos{\{\pi N_{sc}(E)\}}$ for the Hadamard-Gutzwiller model. $N_{sc}(E)$ was evaluated using Eq. (5) and taking into account all periodic orbits with length $l_y \le 11.962...$ The triangles mark the positions of the "true" quantum-mechanical energies.

function:

$$\mathcal{N}_{\rm sc}(E) = \overline{\mathcal{N}}(E) + \frac{1}{2\pi} \sum_{\gamma} \sum_{k=1}^{\lfloor L/l_{\gamma} \rfloor} \frac{\sin(pkl_{\gamma})}{k \sinh(kl_{\gamma}/2)} + \frac{1}{\pi} \operatorname{Im} E_{1}[-(\frac{1}{2} + ip)L], \qquad (5)$$

where $E = p^2 + \frac{1}{4}$ and $E_1(z) = \int_z^{\infty} dt \, e^{-t}/t$. In this formula the smoothing is a consequence of the fact that only a finite number of periodic orbits with length $kl_{\gamma} \le L$ is included in the sum. The mean spectral staircase is given asymptotically by [12] $\overline{\mathcal{N}}(E) = E - \frac{1}{3} + O(\sqrt{E} \times \exp\{-2\pi\sqrt{E}\})$.

The quantization condition (1) has been evaluated for the Hadamard-Gutzwiller model in the energy range 1 < E < 14 using (5) with L = 11.96242... As is seen in Fig. 4, the zeros of $\cos{\{\pi N_{sc}(E)\}}$ yield reasonable approximations to the true eigenvalues, but the agreement is much worse than in the two previous cases. In fact, a better resolution of even the lowest energy levels would require a much larger number of periodic orbits. To demonstrate this point, we show in Fig. 5 for the three systems an estimate of the number N(l) of periodic orbits which is required to get a good approximation to the first \mathcal{N} energy levels. The results depend very sensitively on the various values of the topological entropy and the mean level spacing $\overline{\Delta E} = [d\overline{\mathcal{N}}(E)/dE]^{-1}$. While Artin's billiard (dotted line) constitutes the most favored case, it is seen from Fig. 5 that the number of relevant periodic orbits grows extremely fast in the case of the Hadamard-Gutzwiller model (solid line). The hyperbolic billiard (dashed line) lies between these two extremes, but the situation is by far better than for the Hadamard-Gutzwiller model.

In this Letter we have studied the semiclassical quantization condition (1), which is based on the continuous ap-



FIG. 5. Estimate of the number N(l) required to determine semiclassically the first \mathcal{N} energy levels of Artin's billiard (dotted line), the hyperbolic billiard (dashed line), and the Hadamard-Gutzwiller model (solid line).

proximations (2) and (5), respectively, to the discontinuous spectral staircase $\mathcal{N}(E)$, and have applied it to three strongly chaotic systems. As illustrated in Fig. 5, the systems cover a wide range of different behavior, and thus provide a nontrivial test of the quantization condition (1). Even in the case of the Hadamard-Gutzwiller model, where some of the earlier quantization rules did not provide satisfactory results [6], we have obtained useful approximations to the energy levels. Altogether, the numerical results presented in Figs. 2 to 4 give strong support to this novel quantization condition.

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[2] M. C. Gutzwiller, J. Math. Phys. 12, 343 (1971).

- [3] R. Aurich, M. Sieber, and F. Steiner, Phys. Rev. Lett. 61, 483 (1988); R. Aurich and F. Steiner, Physica (Amsterdam) 39D, 169 (1989).
- [4] M. Sieber and F. Steiner, Phys. Lett. A 144, 159 (1990).
- [5] M. Sieber and F. Steiner, Physica (Amsterdam) 44D, 248 (1990).
- [6] R. Aurich and F. Steiner, DESY Report No. DESY 91-044, 1991 (to be published); Proc. R. Soc. London A (to be published).
- [7] M. V. Berry and J. P. Keating, J. Phys. A 23, 4839 (1990); J. P. Keating, Proc. R. Soc. London A (to be published).
- [8] M. Sieber and F. Steiner, Phys. Rev. Lett. 67, 1941 (1991).
- [9] C. Matthies and F. Steiner, Phys. Rev. A 44, R7877 (1991).
- [10] G. Tanner, P. Scherer, E. B. Bogomolny, B. Eckhardt, and D. Wintgen, Phys. Rev. Lett. 67, 2410 (1991).
- [11] E. B. Bogomolny, Comments At. Mol. Phys. 25, 67 (1990); Orsay Report No. IPNO/TH91 (to be published); E. Doron and U. Smilansky, Phys. Rev. Lett. 68, 1255 (1992).
- [12] R. Aurich and F. Steiner, DESY Report No. DESY 91-082, 1991 (to be published); Phys. Rev. A 45, 583 (1992).
- [13] M. Sieber, Ph.D. thesis, University of Hamburg, 1991 (unpublished).
- [14] M. Sieber and F. Steiner, Phys. Lett. A 148, 415 (1990).
- [15] R. Aurich and F. Steiner, Physica (Amsterdam) 43D, 155 (1990); 48D, 445 (1991).
- [16] B. Simon, Ann. Phys. (N.Y.) 146, 209 (1983); J. Funct. Anal. 53, 84 (1983).
- [17] F. Steiner and P. Trillenberg, J. Math. Phys. 31, 1670 (1990).
- [18] A. Selberg, J. Indian Math. Soc. 20, 47 (1956).
- [19] A. B. Venkov, Math. U.S.S.R. Izv. 12, 448 (1978).
- [20] C. Matthies and F. Steiner, DESY report (unpublished).
- [21] D. A. Hejhal, in International Symposium in Memory of Hua Loo-Keng, edited by S. Gong, Q. Lu, Y. Wang, and L. Yang (Science Press and Springer-Verlag, Berlin, 1991), Vol. 1, p. 59.

^[1] M. C. Gutzwiller, Chaos in Classical and Quantum Mechanics (Springer, New York, 1990).