

## Test of a numerical approach to the quantization of billiards

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A method for computing large numbers of eigenvalues of self-adjoint elliptic operators [J. Comput. Phys. **184**, 321 (2003)] is tested in numerical studies of the spectral properties of quantum billiards. To this extent, we study a time-reversal invariant quantum billiard of threefold symmetry, that undergoes a transformation in its symmetry properties from  $C_{3v}$  to  $C_3$ . Thereby a transition from Gaussian orthogonal to Gaussian unitary ensemble statistics is observed, verifying earlier experimental indications and theoretical predictions. At the same time our numerical ansatz is shown to be applicable to arbitrary billiard shapes.

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### I. INTRODUCTION

The properties of quantum systems whose classical counterparts possess a chaotic dynamics have been studied extensively in billiards. These model systems [1] have been investigated numerically (see, e.g., the references listed under Ref. [2]) as well as experimentally, e.g., with microwave cavities [3–5]. In such analog experiments with superconducting microwave resonators complete sequences of typically about  $10^3$  eigenvalues are obtained [5]. Their analysis confirmed the conjecture [6] that chaos manifests itself in certain generic properties of the quantum spectral fluctuations, which can be modeled by random matrix theory [7]. While the spectral properties of time-reversal invariant systems without spin and Kramers degeneracies are well described by the random matrices of the Gaussian orthogonal ensemble (GOE), time-reversal violation requires a description by Gaussian unitary ensemble (GUE) matrices. Following the predictions by Leyvraz, Schmit, and Seligman [8] we study a transition from GOE to GUE statistics in a billiard that undergoes a transformation in its symmetry properties [9] from  $C_{3v}$  to  $C_3$ . The attempt of Ref. [10] to study this phenomenon experimentally with the help of a normal conducting microwave resonator posed problems, as it was not possible to assign the correct symmetries to the levels. In corresponding experiments with superconducting devices such assignments are possible [11], however, parametric deformations of the shape of a billiard boundary are difficult to realize experimentally. Hence a numerical study of the transition from GOE to GUE in such systems is of great interest. The billiard considered in this work is nonconvex and has a hole at its center, i.e., a second boundary. Thus its numerical treatment is nontrivial. We chose this problem as a test of a different numerical technique for computing large numbers of eigenvalues of self-adjoint elliptic operators [12]. The method is based on the finite element method and has almost no limitations with respect to the shape of a billiard and, e.g., allows the study of bounded domains with holes. Compared to other methods relying on the finite element method it can distin-

guish between true eigenvalues and the unavoidable spurious eigenvalues and discretization artefacts. Approximately one thousand levels were obtained for each symmetry class, thereby revealing a small deviation of the spectral statistics from the expected random matrix theory behavior, which can be understood in terms of classical periodic orbits. In Sec. II we will shortly review the theory and the results relevant for the underlying billiard problem. Then we will introduce the numerical method used for the quantization of the billiard in Sec. III and finally present the results of the statistical analysis of the calculated eigenvalues in Sec. IV.

### II. THEORY

An area  $A$  in which a pointlike particle moves frictionless along straight paths until it hits the boundary  $\partial A$ , where it is reflected according to the common law of reflection, is called a two-dimensional billiard. Whether its classical dynamics is regular, chaotic, or mixed only depends on the shape of the billiard. In quantum mechanics a billiard is described by the stationary Schrödinger equation for a free particle, that can be written in the form

$$(\Delta + k_i^2)\psi_i = 0 \quad (1)$$

with  $k_i^2 = 2mE_i/\hbar^2$ , where  $m$  is the mass of the particle and  $\psi_i$  and  $E_i$  denote eigenfunctions and eigenenergies, respectively. The eigenfunctions must satisfy the Dirichlet boundary condition, i.e.,  $\psi_i|_{\partial A} = 0$ , which together with Eq. (1) defines the problem to be solved. Equation (1) is also referred to as the scalar Helmholtz equation, as it describes the electromagnetic fields inside a flat microwave resonator that represents an analog system for a quantum billiard of corresponding shape [3]. For comparison with experimental results obtained in microwave resonators we express the numerical eigenvalues  $k_i$  as electromagnetic eigenfrequencies  $f_i = \omega_i/2\pi = ck_i/2\pi$ , where  $c$  is the speed of light.

We study a billiard of the shape shown in Fig. 1. Its classical dynamics has turned out to be chaotic, except for a few periodic orbits that will be discussed below. The billiard has an outer and an inner boundary which both possess threefold symmetry. The two boundaries are rotated against each other by an angle  $\alpha$ . For  $\alpha \neq 0$  the only symmetry is  $C_3$ , i.e.,

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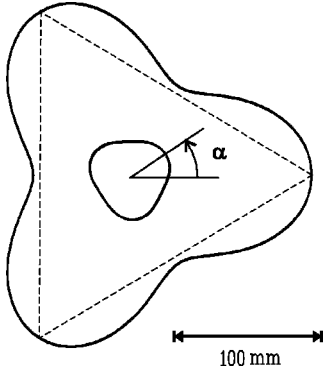


FIG. 1. Shape of the billiard. When rotating the inner boundary from  $\alpha=0$  to  $\alpha \neq 0$ , a transition of the symmetry properties from  $C_{3v}$  to  $C_3$  is induced. The dashed line shows a periodic classical orbit that is nonchaotic and that influences the spectral properties of the quantum system.

”pure” threefold symmetry. If  $\alpha$  is set to zero, there are mirror symmetries and one speaks of  $C_{3v}$  symmetry. The two boundaries can be parametrized in polar coordinates  $(r, \phi)$  by

$$r_{\text{outer}}(\phi) = r_{\text{outer}}^0 [1 + 0.3 \cos(3\phi)] \quad (2)$$

and

$$r_{\text{inner}}(\phi) = r_{\text{inner}}^0 \{1 + 0.1 \cos[3(\phi + \alpha)]\} \quad (3)$$

with  $r_{\text{outer}}^0 = 100.00$  mm and  $r_{\text{inner}}^0 = 27.27$  mm. By tuning the value of the angle  $\alpha$  one can study the effect of the transition from  $C_{3v}$  to  $C_3$  on the properties of the spectra. According to the predictions by Ref. [8] these properties should show a transition from GOE to GUE statistics. While in similar studies of GOE-GUE transitions [13] time-reversal invariance was broken by magnetic fields, in our case a change of the shape of the billiard boundary induces the GOE-GUE transition, as already suggested in Ref. [8]. The authors of Ref. [8] showed that a chaotic quantum billiard with  $C_3$  symmetry has a spectrum consisting of single (nondegenerate) and double (degenerate) eigenvalues. The degeneracies are due to time-reversal invariance and these so-called Kramers doublets are known to show GUE-like statistical fluctuations, while the single eigenvalues possess the common GOE properties [8,11,14]. However, in the presence of additional symmetry axes ( $C_{3v}$ ), one also expects GOE statistics for the degenerate modes [8]. As the nondegenerate modes of a  $C_{3v}$  billiard may have odd or even parity with respect to *all* of the three mirror axes, the spectral properties of the single eigenvalues should rather coincide with those of a superposition of two independent GOE spectra (see also Refs. [15,31]) than with those of a single GOE spectrum [10].

### III. NUMERICAL SIMULATION

The numerical eigenvalues were obtained with the help of a method that is described in Ref. [12] in detail and that is *applied* here. Many other methods have been developed in this context. The most common approaches are based on the scattering approach, the finite element method, the boundary

integral method, and their variants [16]. The main drawback of these approaches is the difficulty, if possible at all, to treat general domains, especially domains with re-entrant corners or with holes. We tested a numerical method [12] that can give complete sequences of large numbers of eigenvalues for an arbitrarily shaped billiard beginning from the ground state with a high numerical precision.

#### A. Numerical method and its properties

The considered method relies on a basis diagonalization. Localized basis functions (piecewise polynomial functions) are used, thereby yielding sparse matrices. Taking advantage of that sparsity pattern as well as of the elliptic properties of the Laplace operator, we solve the resulting generalized eigenvalue problem by means of a highly efficient multigrid method.

The starting point for the numerical calculations is the discretization of Eq. (1) by means of the finite element method. This leads to a self-adjoint generalized eigenvalue problem of the form

$$\mathbf{A}^h \psi_i^h = \lambda_i^h \mathbf{M}^h \psi_i^h, \quad i = 1, \dots, n, \quad (4)$$

where  $h \in R_+$  is the discretization parameter,  $\mathbf{A}^h \in R^{n \times n}$  (respectively  $\mathbf{M}^h \in R^{n \times n}$ ) represents the *stiffness* (respectively *mass*) matrix, and  $\lambda_i^h$  is the approximation of the eigenvalue  $\lambda_i = k_i^2$  (see, e.g., Ref. [17]). The sparsity pattern of  $\mathbf{A}^h$  and  $\mathbf{M}^h$  leads to memory requirements which behave like  $O(n)$ . Under usual assumptions on the finite element discretization (see Ref. [18]), the discretization error satisfies

$$\lambda_i^h - \lambda_i \leq C \lambda_i^l h^{2(l-1)}, \quad (5)$$

where  $(l-1)$  is the polynomial degree of the finite element shape functions. This error bound indicates that for a given triangulation the accuracy of the higher eigenvalues deteriorates with the coefficient  $\lambda_i^l$ . The accurate determination of a large number of eigenvalues relies therefore on much finer discretization of Eq. (1) than for the computation of a few eigenvalues.

The considered method which is described in Ref. [12] allows to compute the  $m$  smallest eigenvalues in Eq. (4) with the optimal complexity of  $O(mn)$  arithmetic operations and  $O(n)$  memory requirements. Notice that in practice  $m \ll n$  due to the *a priori* error estimation (Eq. (5)). Our approach is based on the symmetric Lanczos method [19]. The Lanczos recursion leads to a tridiagonal matrix for which all eigenvalues can be computed by means of a bisection method with  $O(m)$  arithmetic operations (see, e.g., Ref. [19]). The relevant eigenvalues of the problem given by Eq. (4) are in the lower part of the spectrum. In order to obtain the convergence towards these eigenvalues we therefore consider the following spectral transformation:

$$[(\mathbf{A}_h - \sigma \mathbf{M}_h)^{-1} \mathbf{M}_h] \psi_i^h = \frac{1}{\lambda_i^h - \sigma} \psi_i^h. \quad (6)$$

The operator  $(\mathbf{A}_h - \sigma \mathbf{M}_h)^{-1} \mathbf{M}_h$  is nonsymmetric but self-adjoint with regard to the inner product  $\langle \cdot, \cdot \rangle_{\mathbf{M}_h}$ . Therefore the Lanczos method remains valid provided it relies on this scalar product.

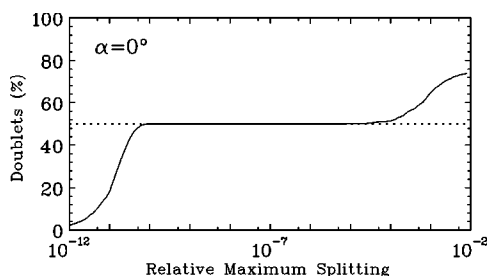


FIG. 2. Percentage of doublets as a function of the assumed maximum doublet splitting, shown for the  $\alpha=0$  case. As one can see it is possible to vary the parameter taken for the maximum splitting from  $10^{-10}$  up to  $10^{-5}$ , i.e., by five orders of magnitude, without changing the singlet and doublet subspectra. This indicates that the numerical lifting of the degeneracies is extremely small compared to the smallest eigenvalue spacings.

The most time consuming part of the proposed method is the resolution at each step of the Lanczos iteration of the linear system involved in Eq. (6). Due to the elliptic character of the considered operator we apply multigrid methods for the step which allows to solve such linear systems with CPU and memory costs which behave like  $O(n)$  (see, e.g., Refs. [20,21]). For increasing  $m$ , due to rounding errors, a loss of global orthogonality leads to so-called *spurious* eigenvalues (see, e.g., Ref. [19]). Beside the multigrid method, one of the cornerstones of the method is the ability to control a posteriori the validity of the computed eigenvalues and to distinguish the true approximated eigenvalues from the discretization artefacts and the spurious eigenvalues. The treatment of this issue is based on extrapolation techniques which are described in more detail in Refs. [12,22].

### B. Performed calculations

Our calculations were performed on 64 nodes of the Heidelberg Linux Cluster System (HELICS). Each node consists of two AMD Athlon 1.4-GHz processors which share 2 gigabytes memory. The size of the eigenvalue problem Eq. (4) had been set to  $n=1.5$  Mi. for all considered configurations. This allowed to compute accurately  $m=3000$  eigenvalues with regard to the discretization error. The needed CPU time for each configuration was approximately 6 h.

We have computed spectra of approximately 3000 eigenvalues  $\{f_i\}$  for three different configurations of our billiard ( $\alpha=0^\circ$ ,  $\alpha=1.7^\circ$ ,  $\alpha=10^\circ$ ). For the given dimensions of the billiard, these spectra correspond to the frequency range from 0 GHz to approximately 54 GHz. Our numerically obtained spectra are indeed composed of singlets (nondegenerate eigenvalues) and doublets (twofold eigenvalues). The relative splitting of the degenerate eigenvalues  $\Delta f/f$  lies between  $10^{-5}$  and  $10^{-9}$ . For the topmost levels the numerical splittings are larger, accordingly we omit the last 300 levels. Moreover, we skipped the first 600 levels in each spectrum, since we are interested in semiclassical properties. We utilized the (extremely small) numerical doublet splitting as a tool for separating the remaining 2100 levels into subspectra of singlets and doublets (similar to Ref. [14]). To this end we studied the percentage of doublets as a function of the as-

sumed maximum splitting of the doublets (Fig. 2). The result is convincing as we can vary the value taken for the maximum splitting by several orders of magnitude without changing the relative fraction of one half for singlets and doublets. Thus we can separate the eigenvalues in subspectra of the same size.

## IV. STATISTICAL ANALYSIS AND TRANSITION FROM $C_{3v}$ TO $C_3$

Before analyzing the statistical properties of the eigenvalue sequences we have to unfold the spectra, i.e., to extract the mean level density and to appropriately rescale the level spacings. By fitting the Weyl formula [25],

$$N_{\text{Weyl}}(f) = \frac{A\pi}{c^2}f^2 - \frac{U}{2c}f + K, \quad (7)$$

to the "staircase" function

$$N(f) = \sum_i \Theta(f - f_i) \quad (8)$$

the coefficients  $A$ ,  $U$ , and  $K$  can be determined ( $c$  denotes the speed of light). We perform this procedure for the subspectra of singlets and doublets, respectively, thus  $A$  and  $U$  are not the area and the perimeter of the billiard, respectively, but related to them. With the transformation

$$f_i \rightarrow \epsilon_i = N_{\text{Weyl}}(f_i) \quad (9)$$

we obtain unfolded spectra  $\{\epsilon_i\}$ , that possess a constant mean eigenvalue spacing rescaled to unity, but still contain the information on the spectral fluctuation properties.

These spectral fluctuation properties are evaluated on short scales as well as on long scales. On short scales the nearest-neighbor-spacings distribution (NNSD), i.e., the statistical distribution  $P(s)$  of the spacings  $s_i = \epsilon_{i+1} - \epsilon_i$ , is utilized to measure the spectral properties of the unfolded eigenvalue sequences. On larger scales we analyze the data with the help of the Dyson-Mehta ( $\Delta_3$ ) statistics [7,23,24], which gives a measure for the spectral correlations in intervals of length  $L$ . In order to compute the  $\Delta_3$  statistics for the large sets of eigenvalues we use the method given in Ref. [24].

Figure 3 shows the NNSDs for the singlet and doublet spectra of the three billiard configurations studied numerically. For  $\alpha=0^\circ$  the NNSDs show agreement with GOE behavior for singlets and doublets. However, in the case of the singlets the distribution is close to the behavior expected for a superposition of two independent GOE sequences, which reflects that the singlets possess odd or even parity. Thus for  $\alpha=0^\circ$  the statistical properties coincide with the predictions for the  $C_{3v}$  case. For  $\alpha=10^\circ$  the NNSD is compatible with GOE statistics in the case of the singlets and with GUE statistics in the case of the doublets, as expected. The  $\alpha=1.7^\circ$  configuration shows a similar behavior, thus we resolve the slight breaking of the mirror symmetries within our numerical accuracy.

For the Dyson-Mehta statistics (Fig. 4) there is agreement with the expected behavior for  $\alpha=0^\circ$  ( $C_{3v}$ ), whereas for  $\alpha$

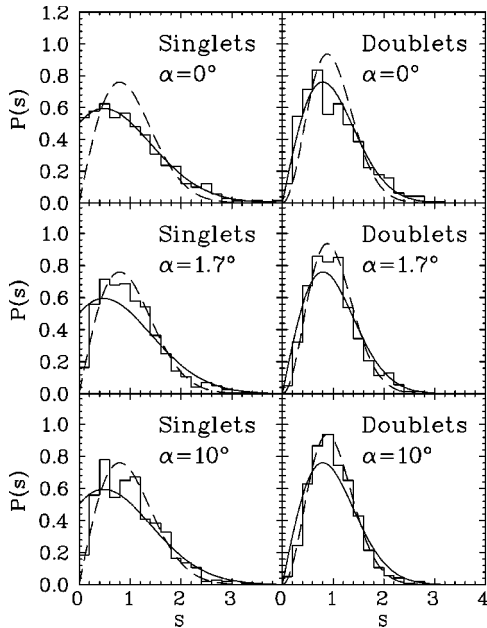


FIG. 3. Nearest-neighbor-spacings distributions (NNSDs) of the spectra *calculated* for the three different configurations of the billiard (histograms). The full lines and the dashed lines mark the theoretical predictions for  $C_{3v}$  and  $C_3$  symmetry, respectively. For all cases the results coincide with the predictions: for  $\alpha=0^\circ$  one has two superimposed GOE spectra for the singlets and a GOE spectrum for the doublets. The other configurations show GOE statistics for the singlets and GUE behavior for the doublets.

$=1.7^\circ$  and for  $\alpha=10^\circ$  the results are intermediate in between the limiting cases expected for  $C_{3v}$  and  $C_3$  symmetry. However, these deviations observed for the long-range correlations (which are often more sensitive with respect to certain subtle effects than the NNSD) can be understood in terms of classical periodic orbits [26,27]. The Fourier transform of the level density  $\rho(f)=dN/df$  gives the length spectrum [27–29], i.e.,

$$l(x) = \left| \int_{f_{\min}}^{f_{\max}} \rho(f) \exp\left(i \frac{2\pi x}{c} f\right) df \right|^2. \quad (10)$$

Analyzing our calculated eigenvalue spectra (see, e.g., Fig. 5) yields below  $x=2$  m prominent peaks for orbits with lengths  $x \approx 0.59, 0.92, 1.18, 1.92$  m. For all three billiard shapes these peaks appear in the length spectra and are surely due to nonchaotic periodic orbits, which do not hit the inner boundary. The orbit with length 0.59 m is indicated in Fig. 1. There are certainly more complicated (but less prominent) orbits of that kind. For a comparison of the spectral properties with the random matrix theory predictions the contribution of the nonchaotic periodic orbits to the spectrum has to be removed. Usually, this is done by searching the classical orbits corresponding to such “bouncing ball orbits” and proceeding as, e.g., in Refs. [27,30] in order to reconstruct their contribution to the level density. We, instead, identify peaks in the length spectrum corresponding to the orbits which never hit the inner boundary by a mere comparison of the length spectra obtained for the three values of  $\alpha$ , remove

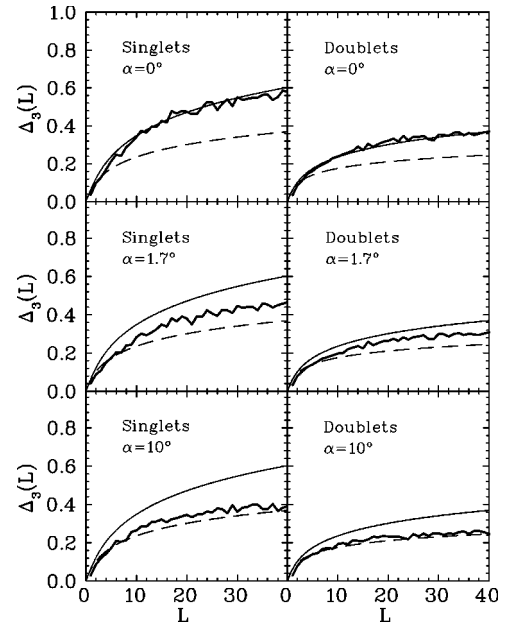


FIG. 4. Long-range correlations of the *calculated* spectra for three different configurations of the billiard (thick lines). The thin, full, and dashed lines mark the theoretical predictions for  $C_{3v}$  and  $C_3$  symmetry, respectively. For the limiting cases of  $\alpha=0^\circ$  the  $\Delta_3$  statistics coincides with the predictions for the  $C_{3v}$  case. In the  $\alpha=1.7^\circ$  case and also for  $\alpha=10^\circ$  the statistics deviates from the theoretical predictions for  $C_3$  symmetry.

these peaks from the length spectrum, and then obtain the fluctuating part of the level density with the bouncing ball orbits extracted by an inverse Fourier transformation [see Eq. (10)]. The resulting statistical properties are—all in all—closer to the theoretical predictions (Fig. 6). However, the agreement is slightly worse for  $\alpha=0^\circ$ .

We thus see a transition of the statistical properties due to symmetry breaking: from GOE to GUE in the case of the doublets and from the two superimposed GOE to a pure GOE in the case of the singlets. The latter kind of transition is trivial when destroying a twofold symmetry as, e.g., in Refs. [15,31]. Gaussian unitary ensemble statistics, however, is characteristic of broken time-reversal symmetry in chaotic systems [13,32] and—although predicted before in Ref.

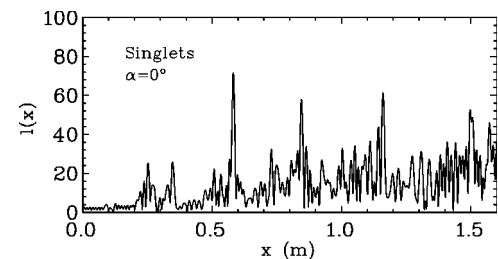


FIG. 5. Length spectrum, i.e., the Fourier transform of the eigenvalue spectrum according to Eq. (10), for the singlet spectrum of the  $\alpha=0^\circ$  configuration. The prominent peaks at  $x \approx 0.59$  m and at  $x \approx 1.18$  m are due to the orbit shown in Fig. 1 and have been extracted from the data discussed in Fig. 6. Note that we do not simply remove the strongest peaks, but those peaks that appear in *all* spectra and that show at least one or two repetitions.



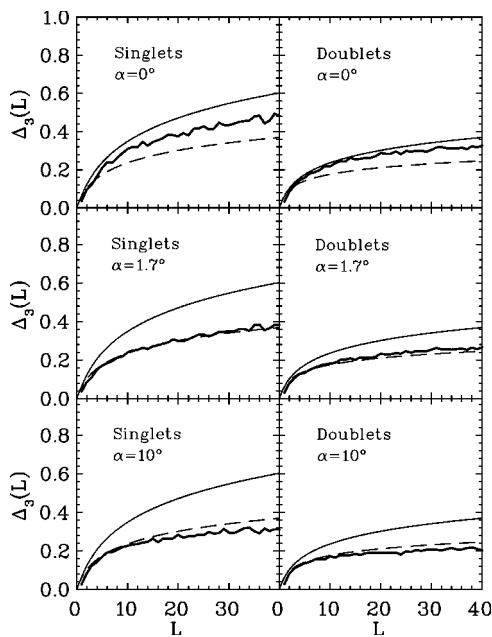


FIG. 6. Long-range correlations of the *calculated* spectra after extraction of the influence of nonchaotic periodic orbits (Fig. 1). The resulting long-range correlations are closer to the theoretical predictions as in Fig. 4, except for the case  $\alpha=0^\circ$ . Most importantly, the doublets show GOE statistics for  $\alpha=0^\circ$ , while different angles  $\alpha$  lead to GUE-like spectral correlations.

[8]—at first not expected in such a situation, where only *spatial* symmetry properties are changed and time-reversal invariance is preserved.

Finally, we compare our numerical with experimental results for  $\alpha=0^\circ$ , stemming from a superconducting microwave cavity, where spectra in the frequency range from 0 to 20 GHz were measured with a spectral resolution of 10 kHz (cf. final remark in Ref. [14]). It has been possible to separate the experimental spectrum of 389 eigenfrequencies into singlets and doublets with the help of the doublet splittings as in Ref. [14]. The nearest-neighbor-spacings distributions (see Fig. 7) show a behavior that is consistent with the theoretical expectations and with our numerical studies. Thus our new numerical results agree well with the ones found experimentally.

## V. CONCLUSION

We applied a recently proposed numerical method to compute spectra of a special chaotic two-dimensional quantum billiard of threefold symmetry. With the help of these numerical results we observed a transition from GOE to GUE statistics of the spectral fluctuations when changing the spatial symmetry of the billiard properties from  $C_{3v}$  to  $C_3$ .

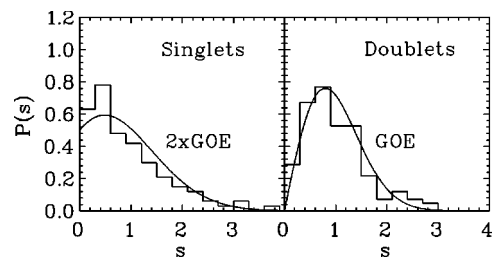


FIG. 7. Nearest-neighbor-spacings distributions for the *experimental* single and double eigenfrequencies of the  $C_{3v}$  billiard (histograms), to be compared with the uppermost part of Fig. 3. Degenerate modes (doublets) and nondegenerate modes (singlets) both obey GOE statistics. However, the singlet modes have odd or even parity with respect to the symmetry axes and thus one sees a superposition of two statistically independent GOEs.

This confirms theoretical predictions [8] and verifies early numerically [8] as well as experimentally observed indications [10] for this phenomenon.

*The aim of the present work was, however, not only to study the GOE-GUE transition but also to present an application of a different numerical approach in billiard systems.* For a prototypical billiard the method described in Ref. [12] provides an accurate computation of several thousands of eigenvalues starting from an eigenvalue problem with several millions of unknowns in less than half a day of CPU time on a standard PC cluster. The main advantages of the proposed approach are that there are no restrictions with regard to the geometry of the billiard. Moreover, the method allows the derivation of a robust *a posteriori* error estimator for the control of the accuracy of the computed eigenvalues with regard to the discretization error. The shape of the investigated billiard is complicated (curved nonconvex boundary, a hole). Several thousands of eigenvalues were computed with a precision sufficient for the statistical analyses of spectral fluctuation properties. From this one can directly conclude that the numerical approach is quite general and not limited to certain types of billiards. We are planning to extend our simulations towards larger numbers of eigenvalues and to apply it to different physical problems, such as those discussed in Ref. [33].

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