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Plane-wave quantization for polygonal billiards

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There is theoretical evidence indicating that generic polygons do not admit eigenfunctions that are superpositions of plane waves. However, we find that a plane-wave quantization for a family of polygonal billiards gives results in very good agreement with theoretical predictions. Indeed the fraction of missing states decreases as the number of sides is increased. We provide a resolution of this contradiction: While theory says that no plane-wave eigenfunctions are possible for polygonal boundaries, it is not applicable to the curvilinear boundaries approximating these polygons. This is analogous to the classical mechanics of polygonal billiards, where according to continuum mathematics there is no chaos, yet discrete mathematics finds it. In the quantum treatment considered here, according to continuum mathematics there can be no plane-wave eigenfunctions, yet discrete mathematics finds them.

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I. INTRODUCTION

Billiards are an excellent tool to study the general characteristics of dynamical systems since they exhibit a wide spectrum of behavior, ranging from complete integrability (circular billiard) to fully developed chaos (Bunimovich's stadium [1]). Indeed, starting with Birkhoff [2], physicists as well as mathematicians have resorted to the study of these simple systems as a tool to understand many global features of dynamical systems. In particular, billiards inside polygonal enclosures have proven to be particularly interesting for the almost contradictory behavior they show. Even though with few exceptions they are neither integrable nor strictly chaotic since they have null entropy, zero Lyapunov exponent [3], and zero algorithmic complexity [4], they also have been shown to mimic chaos when examined with finite precision [5].

In quantum mechanics, the billiard problem has proved to be an even more useful model because of its paradigmatic simplicity. By semiclassical arguments [6,7], it is always expected that the statistical properties of spectra should be related to the regularity or irregularity of the classical motion. In general for integrable systems one expects the nearest neighbor level spacings (NNLS) to obey a Poisson distribution, while for chaotic systems a distribution more along the lines of the Gaussian orthogonal ensemble of nuclear physics (Wigner surmise) [8] is more likely (though there are exceptions to both cases). From triangles to the stadium and from several different polygons to Sinai billiards, many calculations of the quantum spectra of billiards have been performed to check the validity of that assumption. Depending on the boundary under consideration, several methods are available to find the quantum spectrum of a billiard. If we know a basis that vanishes on the boundary, diagonalization methods are the standard procedure. This is the case for triangular billiards [9] but not for generic billiards.

This leaves one with several approximation schemes. One method, originally developed by Riddell [10] based on the Green's function for the problem, transforms the Schrödinger equation into an integral equation for a dipole distribution that "generates" the wave function and then discretizes this integral equation on the boundary. This well developed method (which is sometimes cumbersome to implement) has been used to compute eigenvalues of the stadium [11,12] and the spectra of several polygons [13–17]. Variations of Riddell's method have also been used by Berry [18] to find the spectra of triangles. Berry also used a variation of the Korringa-Kohn-Rostoker method of solid state theory to find eigenstates of the Sinai billiard [19] and also a polygonal version of it [20]. An alternative method based on expanding the eigenstates in a basis of adiabatic states has been successfully used to compute several low energy eigenstates of different billiards (stadium [21–23] and rhombi [13]), thus showing traces of separability in them.

Recently Heller [24,25] used an effective method to find eigenvalues and eigenfunctions of a billiard. The method assumes that the wave function can be expressed as a superposition of plane waves traveling along different directions but all having the same wave number k. The eigenvalues and eigenfunctions are obtained by minimizing a parameter called the tension [24,25]. The results agree very well with experiments [26–31]. There is just one difficulty: for boundaries with sharp corners, like polygons, it is conjectured that states could be missed, namely, those states with complex k_x and k_y (evanescent states); those states are not found because, simply, to keep the search one dimensional (a considerable numerical advantage), one usually chooses real values of k_x and k_y. Moreover, theoretical evidence seems to indicate [32] that no plane-wave superposition can be the solution to Schrödinger equation for a general polygonal boundary.

In this paper we quantize a family of multisided polygons that mimic chaos in the classical case with as good a precision as one may wish [5]. We first find that the plane-wave method proposed by Heller agrees very well with theoretical predictions, despite the apparent contradiction, with the mathematical results indicating the contrary; indeed, the fraction of missing states decreases as the number of sides is increased. After resolving this contradiction, we show that the resulting spectra exhibit level repulsion corresponding to the classically chaotic dynamics. We restrict ourselves to the region of small energies because that region in quantum mechanics corresponds to the finite precision necessary to see the chaotic behavior in classical mechanics [5]. In Sec. II we describe the polygons we will be considering and state the problem. In Sec. III we summarize the quantization method. Section IV contains our results and their discussion. Conclusions are in Sec. V.

II. DEFINITION OF THE PROBLEM

Classically the dynamics of polygonal billiards may exhibit a wide range of behavior. Depending on the polygon of choice, one may have a completely integrable system (rectangle, right, and equilateral triangles) or a system believed to be ergodic (irradiational polygon) [27].

For rational polygons [i.e., those whose angles α_i obey $\alpha_i=(p_i/q_i)\pi$ with p_i, q_i integers], it has been proven that

$$F(\varphi)=|\varphi| \bmod \left[\frac{\pi}{M}\right] \tag{1}$$

(with M being the least common divisor of the q_i's) is a constant of motion [29]. In this expression φ is the initial angle between the velocity of the particle and some fixed direction in space. The existence of this constant of motion implies that the system will evolve in phase space on a invariant integral surface, the genus g given by [20]

$$g=1+\frac{M}{2}\sum_{i=1}^{N_S}\frac{p_i-1}{q_i} , \tag{2}$$

where N_S is the number of sides of the polygon. The mere existence of this constant of motion would seem to indicate that the motion of this billiard has nothing chaotic in it. However, in general this is not necessarily true [4,5].

The solution of the quantum billiard problem in a polygon P is then equivalent to the solution of Helmholtz's equation for the corresponding boundary; i.e., we want to solve the equation

$$\nabla^2\Psi+k^2\Psi=0 , \tag{3}$$

where

$$E=\frac{\hbar^2k^2}{2m} , \tag{4}$$

subject to the boundary condition

$$\Psi|_{\partial P}=0 . \tag{5}$$

From now on, we will consider the family of polygons P_n generated by circumscribing a rational polygon of n sides around a stadium. Since the Hamiltonian for all of these polygons is invariant under reflection both about the x axis and the y axis, we will analyze a desymmetrized version of the family of polygons, namely, $P_n^{(D)}$ to remove

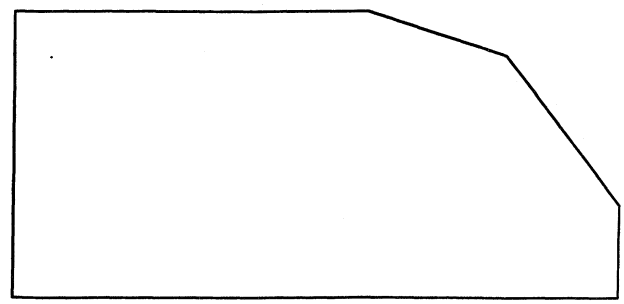

FIG. 1. An example of the class of polygons we consider. In the notation we use, this is P_{12}^D, i.e., a desymmetrized version of a polygon with 12 sides that approximates a stadium.

the degeneracies (see Fig. 1 for an example of the desymmetrized version of P_{12}). In this way we consider one class of eigenstates, namely, those with odd-odd symmetry. It is worth mentioning that from a classical point of view these billiards mimic chaos so well that they are in some aspects indistinguishable from a truly chaotic system [5].

III. NUMERICAL METHOD

We begin by summarizing Heller's method to find the eigenvalues and eigenfunctions of a billiard (the reader interested in learning more technical details should refer to the literature [24–26]). Since the Hamiltonian is invariant under time inversion, the wave function $\Psi(x,y)$ has to be real. Then, calling the eigenvalue k, we propose the solution

$$\Psi_k(x,y)=\sum_{l=1}^{M} a_l \sin(k_x^{(l)}x)\sin(k_y^{(l)}y) , \tag{6}$$

where for any value of l it is true that

$$k_x^{(l)2}+k_y^{(l)2}=k^2 . \tag{7}$$

This ansatz corresponds to a superposition of M plane waves, all with the same wave number but different directions of propagation. Obviously, this is a solution of Helmholtz's equation for the interior of the billiard for any selection of the coefficients a_l. The only errors will occur on the boundary. Our purpose is to find a solution that vanishes at every point on the boundary. In practice this is impossible; the best we can hope for is that our solution will vanish at M' points on the boundary instead. If these points are taken so that they are closer together than the wavelength by a factor of 3 or so, we can be confident that the quantum mechanics is actually "seeing" the boundary rather than the individual points [24,25]. We set the wave function to 1 at an arbitrary point inside the region. We then solve the resulting inhomogeneous system of equations for the a_l's by singular value decomposition.

We still need to check that our solution is appropriate, i.e., that the boundary conditions are approximately satisfied at other points of the boundary. To this end we first normalize the wave function and then compute the "tension" [24–26], namely,

$$\sigma^2(k)=\sum_{i=1}^{8M}[\Psi_k(x_i,y_i)]^2 , \tag{8}$$

where the points (x_i,y_i) are on the boundary. This function is found to have deep minima as a function of k. The values of k corresponding to those minima are the eigenvalues of the corresponding billiard. Moreover, since the trial function of Eq. (6) is by definition zero on the two axes, we only need to analyze the tension on the upper boundary.

IV. RESULTS AND DISCUSSION

A. Calculations

We have used Heller's method to find the spectra of different polygons. To check how many eigenstates we are missing, we compared the integrated density of states $N(E)$ computed numerically,

$$N(E)=\sum_{E_i<E}\Theta(E_i-E) , \tag{9}$$

with the average integrated density of states $\overline{N}(E)$, given by Weyl's law,

$$\overline{N}(E)=\frac{A}{4\pi}E-\frac{P}{4\pi}\sqrt{E}+K , \tag{10}$$

where A is the area of the billiard, P is its perimeter, and K is a constant that depends on the curvature and the angles of the corners [33]. We also define the fraction of missing states as $F(E)$,

$$F(E)=\frac{N(E)-\overline{N}(E)}{\overline{N}(E)} , \tag{11}$$

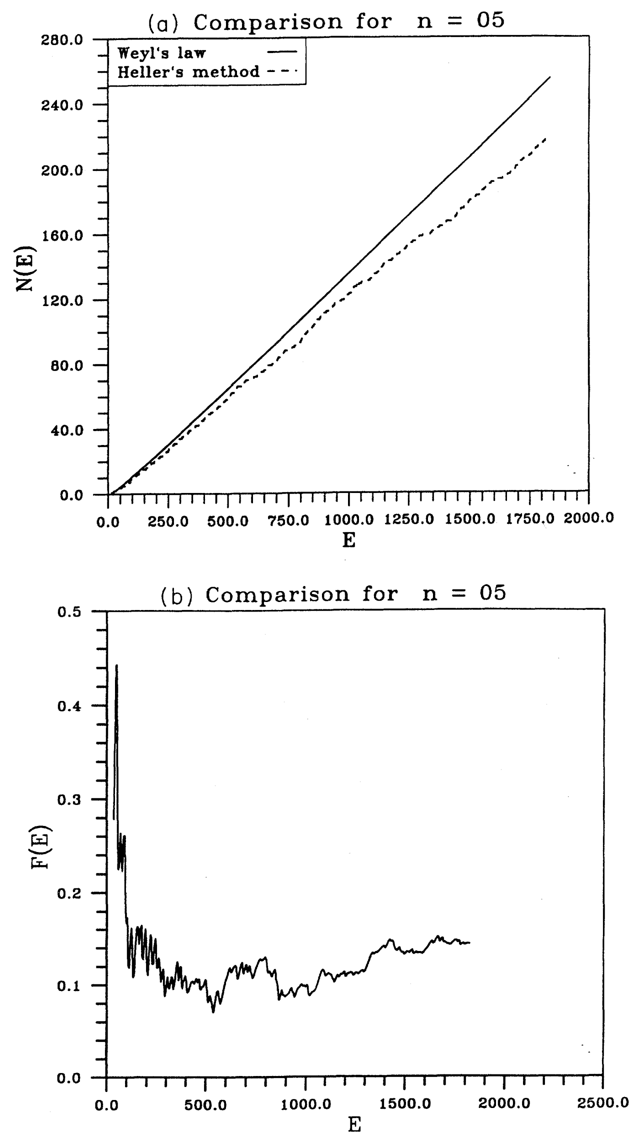

FIG. 2. Comparison of our numerical results for $n=5$ with Weyl's law for $P_{12}^{(D)}$: (a) comparison of the integrated density of states; (b) fraction of missing states $F(E)$.

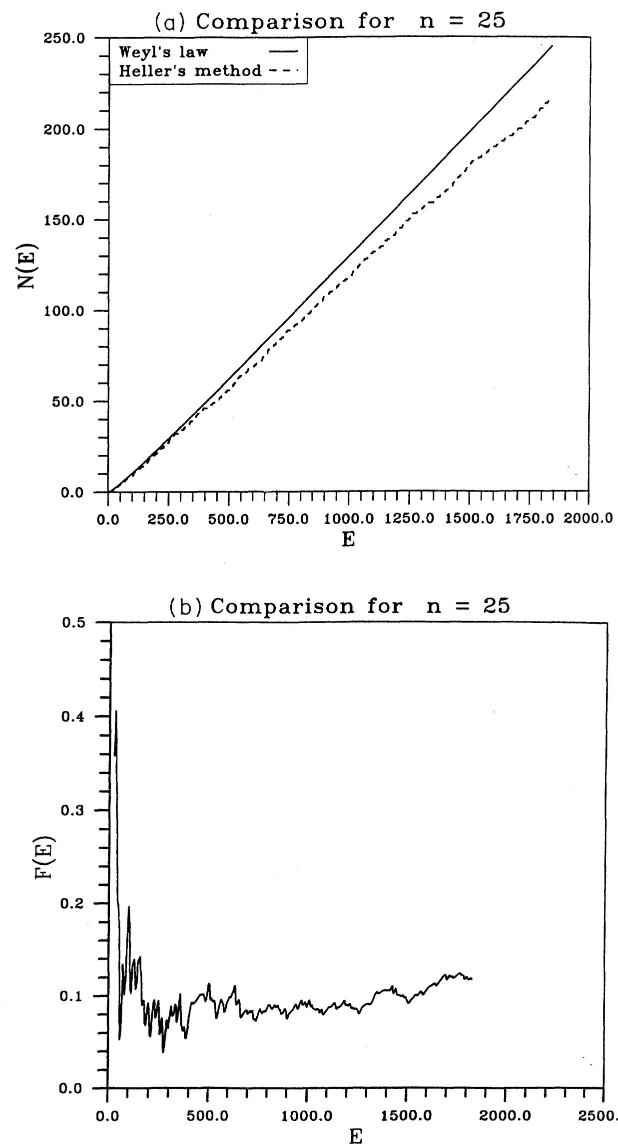

FIG. 3. Same as Fig. 2, except for $P_{52}^{(D)}$ and for $n=25$.

and study its convergence as we increase the energy.

In Figs. 2–4 we compare our numerical calculation for $N(E)$ with $\bar{N}(E)$ from Weyl's law for three polygons, namely, $P_{12}^{(D)}$, $P_{52}^{(D)}$, and $P_{152}^{(D)}$. Figure 2(b) shows that the fraction of missed eigenstates for $P_{12}^{(D)}$ oscillates around 12% of the average total given by Weyl's law without really stabilizing. In fact, one can see a trend toward more and more missed states. In Fig. 3(b) we can see that for $P_{52}^{(D)}$ the integrated density of states stays very close to Weyl's law for very low energies (up to about 600). The fraction of missing states starts also to oscillate without stabilizing around 9%, i.e., a behavior somewhat similar to $P_{12}^{(D)}$ but with smaller fractions. One can see that the fraction tends to increase, but the rate is somewhat less steep than in the case of $P_{12}^{(D)}$. In contrast, Fig. 4(b) shows that for $P_{152}^{(D)}$ the fraction of missing states finally stabilizes at around 2% of the total average number of states. One can compare this result with the 2%

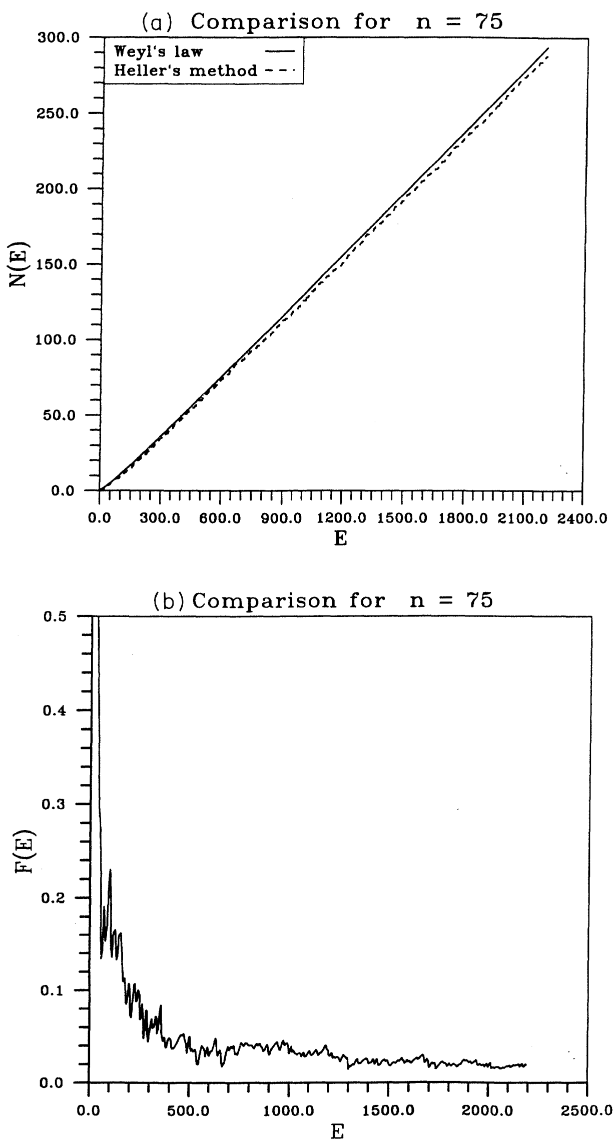

FIG. 4. Same as Fig. 2, except for $P_{152}^{(D)}$ and for $n = 75$.

difference obtained in Ref. [17] using the Green's function method for several nonintegrable polygons: there is actually not much of a difference in precision. Apart from some remaining evanescent states, accidental degeneracies [18] account for our missing some eigenstates; one notices, however, that none of the aforementioned methods would be able to resolve this kind of degeneracy.

In Fig. 5 we show a typical nodal line distribution for $P_{12}^{(D)}$. One can see that the nodal line structure looks erratic, resembling that of a fully chaotic system [11,12]. Moreover, the boundary is very well reproduced by the approximated solution.

Theoretical evidence has been given [32] indicating that, with the exception of the rectangle and a few triangles, no polygonal billiard has a solution expressible as a sum of plane waves (finite or otherwise). It is usually stated in the following way: for a superposition of plane waves to be nonzero at a vertex, the vertex has to have an angle of π/n. This can also be understood in terms of a theorem in analysis [34,35], which states that any solution of the Helmholtz equation with the appropriate boundary conditions can be represented as an integral over the angular spectrum of plane waves, i.e., an integral over the angle of the direction of propagation of plane waves along some path in the complex plane. If we allow the angle to take complex values, we obtain the evanescent state contributions to the spectrum (see, for example, Refs. [35,36]). These evanescent contributions constitute the difference between the true eigenfunction and a sum of plane waves. Since we do not include evanescent waves in our basis (both k_x and k_y are taken as real), we could miss states [25,26] or miss contributions to the eigenfunctions. The question is this: How many of those states do our polygons hold? Or phrased differently, how important is the contribution of these evanescent waves to the spectrum of our polygons?

As has been argued before [25,26], these evanescent waves will be more significant near the corners. However, the evanescent contribution will depend on the angle of the corner in such a way that the closer it is to π, the smaller the evanescent contribution will be. Then in such a limit one expects the eigenstates to look increasingly like a superposition of plane waves. In that case the plane-wave method should work better, as it indeed does,

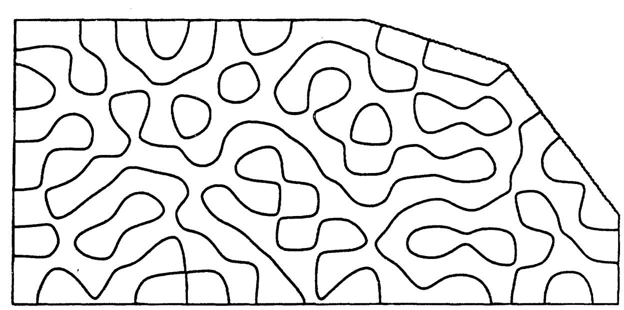

FIG. 5. Nodal line obtained from the plane-wave quantization of $P_{12}^{(D)}$ (the polygon in Fig. 1). One can see that the boundary is well reproduced by the wave function. The nodal lines look as erratic as those for a truly chaotic system.

as we increase the number of sides. To check that this approximation yields the correct results, one can solve the Helmhotz equation by the plane-wave method for different wedges (with angle $n\pi/m$) and compare the approximated solution with the exact solution.

In Figs. 6 and 7 we show this comparison for two different wedges. In these figures we have plotted both solutions (the exact and the approximated) as functions of the radial coordinate only, taking a fixed value for the angular coordinate; the actual value of the angular coordinate does not appreciably change the relationship between the two functions. One can see that the approximated solution and the exact solution (Bessel function) behave exactly the same. The nodal lines manifest some difference close to the vertex, but this difference decreases as the angle approaches π; indeed, for the wedge in Fig. 6 the difference between the two functions may increase up to 60%, while for the wedge in Fig. 7 the maximum difference between the two is of the order of 7.5%. Still it may be argued that the boundary one quantizing with this method is not exactly the polygon of interest but a nearby continuous curve. At this point one can use a theorem that states that for a Dirichlet problem, such as the one we are considering, the eigenvalues vary continuously with the boundary under very broad conditions [37]. Thus the eigenvalues computed by this method will converge to the actual eigenvalues if we take enough points, namely, if we take enough plane waves. The curvilinear character of the boundary on which the wave function vanishes is the real reason there is no conflict between our results and those of Ref. [32]. If one looks back at Fig. 5 one can see that the actual boundary of the polygon is very well reproduced by the approximated solution.

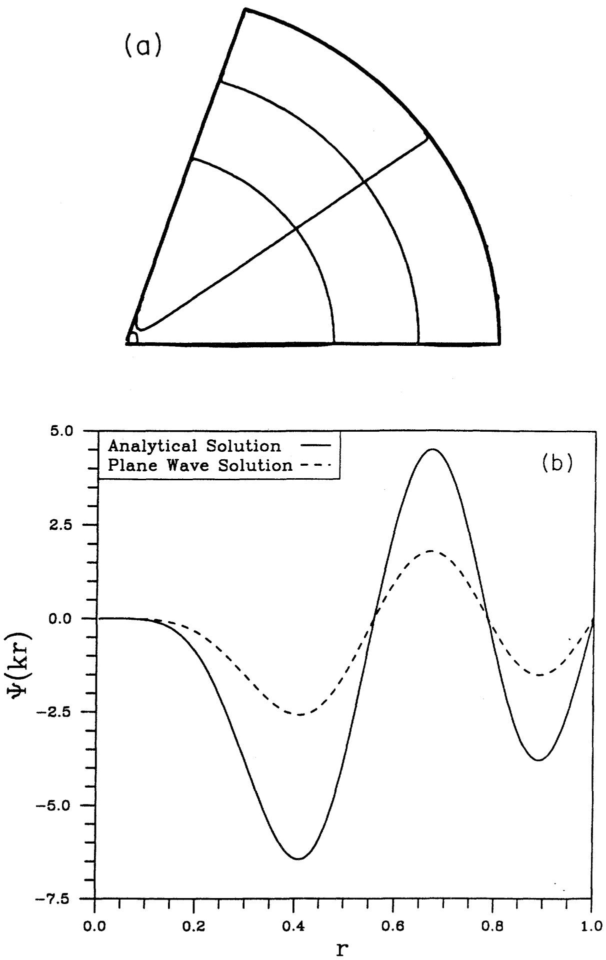

FIG. 6. Comparison of plane-wave solutions with analytic solutions for two wedges with different angles $\alpha = m\pi/n$. (a) Nodal line of the plane-wave solution for $\alpha = 2\pi/5$. One can see that the only appreciable differences occur near the corner. (b) Comparison of the true eigenfunction and the corresponding plane-wave solution for the eigenfunction plotted in (a). One can see that even though the qualitative behavior is quite similar, the two functions are very different quantitatively. In both functions we have considered the variation with the radial coordinate only, taking the angular coordinate as a constant.

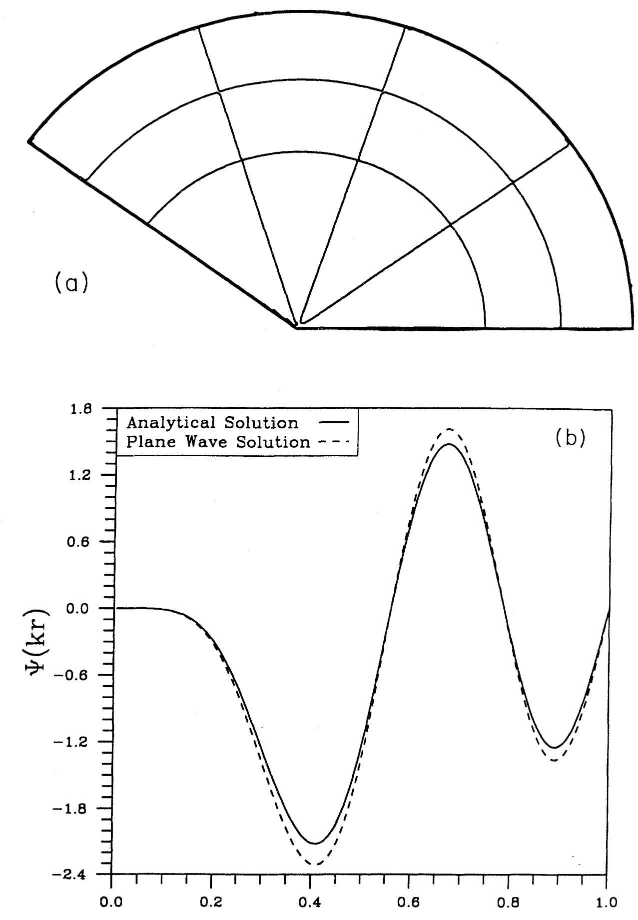

FIG. 7. (a) Same as Fig. 6(a) for $\alpha = 4\pi/5$. In this case the region in which the nodal lines show differences is a little smaller than in the case of $\alpha = 2\pi/5$. (b) Same as Fig. 6(b) for the eigenfunction plotted in (a). In this case the true eigenfunction and the plane-wave approximation coincide both qualitatively and quantitatively. In both functions we have considered the variation with the radial coordinate only, taking the angular coordinate as a constant.

B. Statistics

We now proceed to the statistical properties of the eigenvalues. For this purpose we need to "unfold" the spectrum to be sure that the average spacing is 1 for all the polygons and thus compare the behavior of the different spectra. We first compute the unfolded, spectrum ϵ_i by

$$\epsilon_i = \bar{N}(E_i) , \tag{12}$$

where $\bar{N}(E)$ is given by Weyl's law. We then define the spacings s_i as

$$s_i = \epsilon_{i+1} - \epsilon_i \tag{13}$$

and find $P(s)$, the distribution function for the spacings s.

Since the calculations for $P_{12}^{(D)}$ and P_{52}^{D} show a large number of missing stages, we will analyze only the nearest-neighbor level spacing distribution (NNLSD) for the other polygon. In Fig. 8 we show the level statistics (histogram) obtained for $P_{152}^{(D)}$. As one can see, the statistics show strong level repulsion. This result, which is in agreement with the underlying chaotic dynamics, has also been observed for different kinds of nonintegrable polygons like triangles [9] or rhombi (see, for example, [13,14,17,16]). In the case of the rational rhombus [13,14], for example, the statistics look similar to ours, with the difference being that the level repulsion is not so strong. The fitting to Wigner's surmise is not so close either. It is worth noticing also that we are far from the semiclassical limit; in fact, we are only considering levels in the "deep quantum region." This is somewhat similar to the case of the generalized Sinai billiard studied by Cheon and Cohen [34]. The difference is that, in our case, both the genus and the number of singular points of the boundary are much higher. We find similar results when analyzing similar polygons with an even larger number of sides.

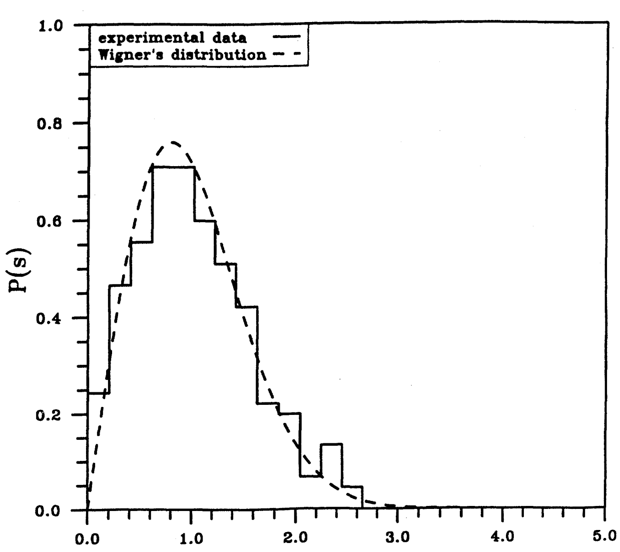

FIG. 8. NNLSD for the lowest first 210 eigenstates of $P_{152}^{(D)}$. We have discarded the first 50 states to ensure the constancy of the level spacing. The dashed line is the prediction of the Gaussian orthogonal ensemble (Wigner surmise).

V. CONCLUSIONS

Our results show that plane-wave quantization is applicable for polygons, provided that the angles at the vertices are not too far from π. In fact, as previously mentioned, the actual curvilinear boundary on which the eigenfunction vanishes will be increasingly similar to the polygon as we increase the number of points on the boundary (and consequently the number of plane waves in the expansion). Consequently, the difference between the actual eigenvalues and the ones obtained from plane-wave quantization will be negligible if one takes enough points [37]. It is worth mentioning that we are not in the semiclassical limit but rather in the limit of "poor resolution of the boundary by the wave function." In a nutshell, one could say that even though the theoretical results seem to be quite restrictive, for any practical purpose one can use a plane-wave quantization for polygonal boundaries without any severe loss of information. This is analogous to the classical treatment of polygonal billiards, in which according to continuum mathematics there is no chaos, yet discrete mathematics finds it [5]. In the quantum case treated here, according to continuum mathematics there can be no plane-wave eigenfunctions, yet discrete mathematics finds them. The theory is not applicable to the continuous boundary on which the approximating wave function vanishes, so our findings do not contradict it.

Regarding the level statistics, one can see that for our polygons it shows level repulsion. This is consistent with the mimicking of chaos observed in the classical case. These results are consistent with others in the literature (see, for example, [13,14,16,17,34]) and confirm that systems containing invariant integral surfaces with genus larger than 1 show level repulsion in quantum mechanics. However, this rule is still qualitative. We still do not have a way of associating a definite law of repulsion with a definite genus. A question that one could ask is this: Does the number of singular points in the boundary matter?

Shudo and Shimizu [16] showed that for the case of the rhombus, rational or otherwise, the level statistics, even though it shows a strong level repulsion, as mentioned before, deviates appreciably from Wigner's surmise. Our results, together with those of Cheon and Cohen [34] for the generalized Sinai billiard, suggest that the existence of more singular points will somehow enhance the level repulsion. In fact, if one compares these two cases with the rhombi, for example, the level repulsion is stronger in the systems with more singular points. This is analogous to the classical case: there the existence of singular points causes the mimicking of chaos (they are responsible for the divergence of the trajectories); genus alone is not enough. It has been suggested [17] that the results obtained by Cheon and Cohen [34] are related to the existence in their case of convex corners that split the banded trajectories that will, otherwise, move in a rectangular (integrable) billiard. Our results show that one can obtain the same kind of statistics in polygonal billiards without any convex corner if the number of singular points is high enough.

However, there is still much to be done. A more detailed analysis of the rigidity as well as the NNLSD up to energies in the semiclassical region should provide more information on where, if anywhere, this classical mimicking of chaos starts to be relevant in quantum mechanics. Furthermore, an analysis of the statistical properties of systems with the same genus but different number of singular points should shed more light on the issue of which one is the classical feature (if any) that defines the statistical properties of almost integrable systems.

Note added. After this work was finished we discovered Ref. [38], in which it is shown that the solutions of Helmholtz's equation inside polygonal regions can always be expanded in plane waves if one allows for a somewhat singular expansion. This then indicates that the differences between the exact and the approximated solutions in Figs. 6 and 7 are just a measure of this singularity.

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