Model of Quantum Chaotic Billiards: Spectral Statistics and Wave Functions in Two Dimensions

E. Cuevas,* E. Louis, and J. A. Vergés†
Departamento de Física Aplicada, Universidad de Alicante, Apartado 99, E-03080 Alicante, Spain
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Quantum chaotic dynamics is obtained for a tight-binding model in which the energies of the atomic levels at the boundary sites are chosen at random. Results for the square lattice indicate that the energy spectrum shows a complex behavior with regions that obey the Wigner-Dyson statistics and localized and quasi-ideal states distributed according to Poisson statistics. Although the averaged spatial extension of the eigenstates in the present model scales with the size of the system as in the Gaussian orthogonal ensemble, the fluctuations are much larger. [S0031-9007(96)01111-8]

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Recent advances in nanotechnology have made possible the fabrication of devices in which carriers are mainly scattered by the boundaries and not by impurities or defects located inside them [1–3]. As these devices, which are commonly referred to as quantum dots, resemble quantum billiards, the interest in the latter has increased considerably in the last few years. Although chaotic billiards have been intensively investigated in the last twenty years [4], the behavior of their quantum analogs has not yet been fully characterized. Some general characteristics of quantum chaotic systems have, however, a wide acceptance. It has been shown, for instance, that the quantum counterparts of billiards having chaotic trajectories have an energy spectrum which obeys Wigner-Dyson statistics [4–6]. This is the case of the stadium and Sinai's billiards [7–10]. On the other hand, it is commonly believed that there is a perfect mapping of quantum chaotic billiards into the more general and intensively investigated problem of random matrices [2,8,9,11].

The purpose of this Letter is to present a new model of a quantum chaotic billiard and investigate its spectral statistics and its relationship with random matrices of the Gaussian orthogonal ensemble (GOE). The model is a practical implementation of surface roughness and its main characteristics are the following. The quantum system is described by means of a tight-binding Hamiltonian with a single atomic level per lattice site in which the energies of the atomic levels at the surface sites S are chosen at random, namely,

$$H = \sum_{i \in S} \epsilon_i c_i^\dagger c_i + \sum_{\langle ij \rangle} V_{ij} c_i^\dagger c_j \,, \qquad (1)$$

where the operator c_i destroys an electron on site i, and V_{ij} is the hopping integral between sites i and j (the symbol $\langle ij \rangle$ denotes that the sum is restricted to nearest neighbor sites) [12]. We take $V_{ij} = V = -1$. The energies of the atomic levels at the boundary sites ϵ_i are randomly chosen between $-W/2$ and $W/2$. Calculations have been carried out on $L \times L$ clusters of the square lattice of sizes up to $L = 200$. Schwarz algorithm for symmetric band matrices [13] was used to compute the whole spectrum including eigenvectors for $L \leq 64$ and the complete set of eigenvalues for $L \leq 170$. Instead, for larger matrices individual eigenvalues and eigenfunctions were obtained by inverse iteration [14].

The basis for expecting chaotic behavior in this model lies in the fact that the shift of the eigenvalues promoted by the perturbation at the surface would be about $(W/\sqrt{3})L^{-3/2}$ if first-order perturbation theory were applicable, which is larger than the average level separation ($\sim 8L^{-2}$). This implies a mixture of $\sim W\sqrt{L}$ ideal eigenstates to form a given wave function of the perturbed system. A similar reasoning suggests quantum chaos for our model in any dimension greater than 2. Note also that, in contrast with standard chaotic billiards, our model has two length scales, namely, the size L and the lattice constant a. Thus even in the macroscopic limit ($L/a \to \infty$), microscopic roughness remains and is consequently felt by quantum particles, i.e., by particles of wavelengths of the order of a.

According to the theory of random matrices and the numerical results for the stadium and Sinai's billiards, a clear hallmark of chaotic behavior is a level separation statistics of the Wigner-Dyson type. Figure 1 shows the variance of the nearest-level spacings distribution for several cluster sizes of the billiard described by Hamiltonian (1) in the full energy spectrum. Away from the bottom of the band the levels are distributed according to Wigner-Dyson statistics (this is explicitly shown in the inset of the figure). The behavior is, nonetheless, somewhat different depending on the particular energy region. In fact, whereas for energies in the range $[-2, -0.5]$, the variance is close to that of the Wigner-Dyson distribution (0.286) even for small clusters, away from that region the variance tends to 0.286 as the size is increased. On the other hand, near the band edges the variance of the distribution clearly tends to 1 (uncorrelated levels) as the system size increases, while the distribution approaches Poisson distribution (see inset of Fig. 1). A similar behavior was obtained by Pavloff and Hansen in their study of the effects

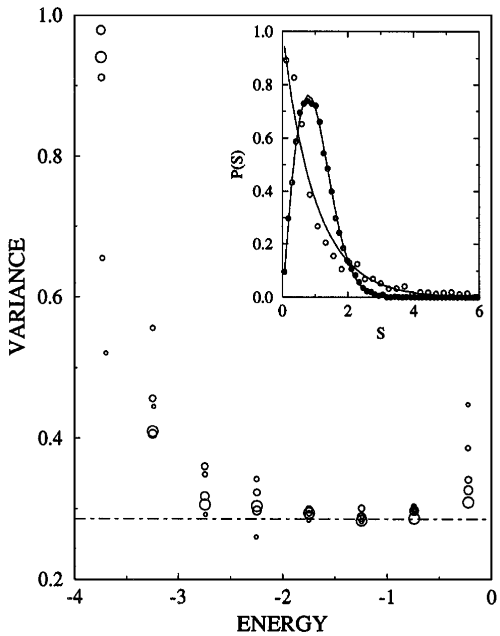

FIG. 1. Variance of nearest-level spacings in the whole energy spectrum. The circle size is proportional to the actual size of the system ($L = 15$, 30, 60, 110, and 150). The horizontal chain line indicates the value of the variance corresponding to the Wigner-Dyson distribution (0.286). Inset: Distribution of nearest-level spacings in a 170×170 cluster for energy levels between -4 and -3.7 (empty circles) and -1.2 and -0.9 (filled circles); for the sake of comparison, the Wigner-Dyson and the Poisson distributions (continuous lines) are also shown. The disorder parameter is $W = 2$.

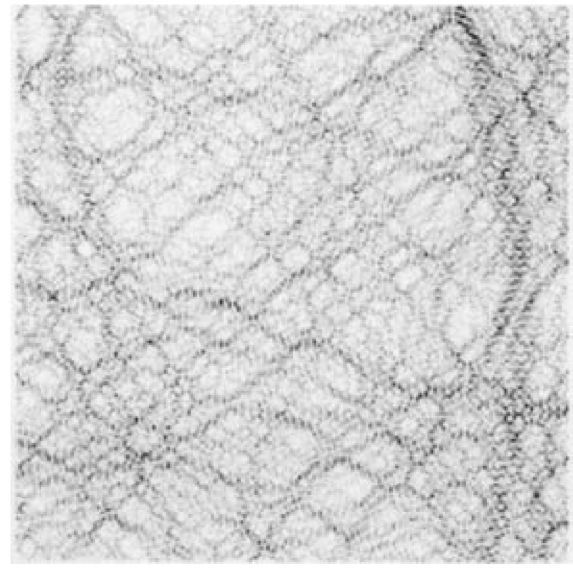

FIG. 2. Probability amplitude of the eigenstate at $E \approx -3.3$ of a 200×200 cluster of the square lattice with the energies of the atomic levels at the boundary sites randomly chosen between -1 and 1. The probability amplitude is roughly proportional to the darkness.

of surface roughness on metallic clusters [15]: in the bottom of the spectrum the de Broglie wavelength is large, only the averaged disorder is felt, and the perturbation is accordingly small. These features differ from those of random matrices which show a spectrum characterized by the Wigner-Dyson statistics throughout the whole energy range, suggesting that, at least at a mesoscopic level, random matrices and chaotic billiards are not equivalent.

The spatial dependence of the probability density of an eigenfunction in the energy range where chaotic behavior is expected is illustrated in Fig. 2. The pattern shows speckles with valleys in between, reminiscent of the patterns found in billiards showing quantum chaotic behavior [4] and in prelocalized states in 2D [16]. In comparing our results with those for prelocalized states it should be noted that in the latter case disorder is present at all lattice sites of the system, whereas in our model disorder is restricted to the surface (it is in this sense that our model can be called a billiard). Another important difference, which is a consequence of the previous one, is the fact that in the present case Anderson localization should not be expected.

To further investigate the nature of the states in the different energy ranges we have calculated the participation ratio, which is a good measure of the spatial extension of a given eigenstate. Inverse participation numbers are defined as the moments of the distribution function of the local weights of the eigenstates, namely,

$$t_{q\alpha} = \sum_{i=1}^{L\times L} |a_{\alpha i}|^{2q}, \tag{2}$$

where $a_{\alpha i}$ is the amplitude of the αth eigenstate at site i, i.e., $|\phi_\alpha\rangle = \sum_i a_{\alpha i}|i\rangle$. Then the participation ratio P_α is given by the inverse of the second moment defined by (2):

$$P_\alpha = t_{2\alpha}^{-1}. \tag{3}$$

P_α is interpreted as the number of lattice sites covered by the eigenstate α. Figure 3 shows P_α in the whole energy spectrum for two values of the disorder parameter W. For low disorder ($W = 2$) the energy levels close to the band edges and part of the states close to the band center are quasi-ideal. The probability amplitude of eigenstates in that energy region is much like that of eigenfunctions in the fully ordered system [17]. These states appear in energy regions in which the wave functions of the ordered cluster have small weight on the surface layer (at band edges *all* states have a small surface sensibility whereas close to the band center *some* of the states show small amplitudes at the surface) whenever the value of W is small enough to allow them to keep their unperturbed characteristics. In any case, what matters in the present analysis is that the size of the regions of appearance of quasi-ideal states diminishes both with the increase of L and the strength W of surface disorder. Results of Fig. 1 are consistent with this qualitative analysis. The behavior is even more complex for large W (see

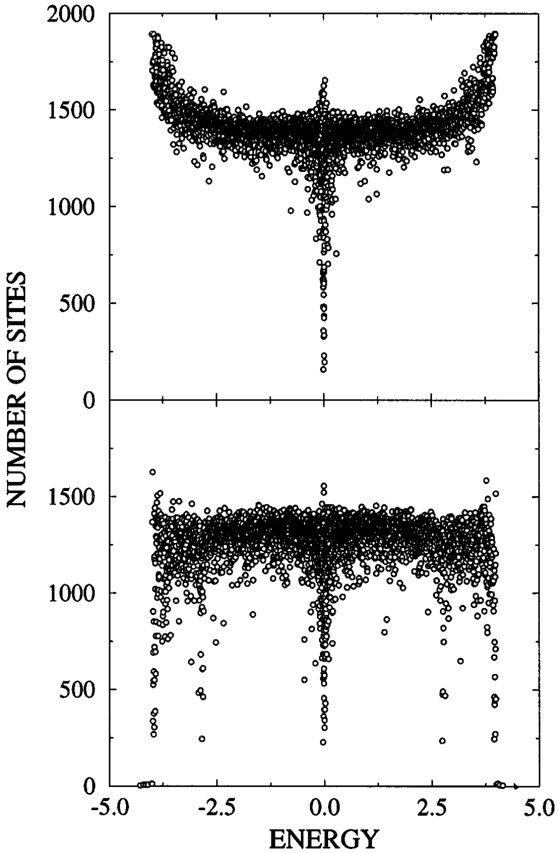

FIG. 3. Spatial extension of all eigenstates corresponding to a realization of Hamiltonian (1) for a 64×64 cluster and two values of the disorder parameter, namely, $W = 2$ (top) and $W = 5$ (bottom).

bottom of Fig. 3). *Bona fide* exponentially localized states appear outside the band (see circles close to the x axis in Fig. 3). Quasi-ideal states still appear at band edges and at the band center but in a reduced amount. Other states show now a small spatial extent due to their character of bulk states resonating with a particular surface impurity. Actually, we have collected a large sample of states showing different characteristics and allowing therefore for different names. To the best of our knowledge this complex behavior has not been pointed out in previous discussions of quantum chaotic billiards. In the limit of infinite disorder we expect a rather simple scenario in which bulk and surface are decoupled and, consequently, ordered states would lie on bulk sites whereas localized states would be located at surface sites. This is a trivial limit and the most interesting situations are of course expected for finite W values.

It is interesting to note that a calculation for random matrices similar to that shown in Fig. 3 gives an almost energy independent distribution with a finite width. An interesting question is how this width (or, more precisely, this standard deviation) evolves with the size of the system for both random matrices and the present billiard. In the case of random matrices of dimension $N = L^2$ the results for the participation ratio averaged over the whole energy range ($P = \langle P_\alpha \rangle$) in clusters of sizes $L = 4, 8, \ldots, 44, 48$, can be accurately fitted by $P = 2.2 + 0.33L^2$, and those for the relative standard deviation of the distribution by $\sigma/P = 1.64/L - 3.05/L^2$ (see Fig. 4). Thus in the asymptotic limit the ratio σ/P behaves as $1/L$. On the other hand results for the present model of quantum billiard obtained for $L = 4, 8, \ldots, 60, 64$ and $W = 2$ lead to the following fittings: $P = 0.71L + 0.33L^2$ and $\sigma/P = 0.074 + 1.98/L - 11.8/L^2 + 24.5/L^3$ (see Fig. 4). Averaging sets always include more than 8000 eigenstates. These results indicate that in the macroscopic limit σ/P is a constant, suggesting that fluctuations of the spatial extension of wave functions are much larger than for random matrices. The reason for this significant difference should be the surface resonances and quasi-ideal states found in the present chaotic billiard which seem to determine the asymptotic behavior of fluctuations in this system. On the other hand, we note that the fittings of the numerical results for P show that the asymptotic behaviors of this magnitude for random matrices and for the present billiard are the same, and that significant differences between the two models are only found for small L. These results would suggest that, for $L \rightarrow \infty$, *whereas averaged properties of quantum chaotic billiards approach those of random matrices, fluctuations are much larger in the former*.

The results for P allow us to connect with a question of much recent interest. We refer to the eventual multifractality [18,19] of the wave functions predicted [20,21] and numerically calculated [16] for prelocalized states in disordered two dimensional systems. The point is whether this exotic behavior of the eigenstates could also be a characteristic of chaotic wave functions. Multifractality occurs whenever $t_{q\alpha} \propto L^{-\tau(q)}$, $\tau(q)$ being a noninteger; in particular $\tau(q) = (q - 1)D(q)$, where the $D(q)$ are the generalized fractal dimensions. Our results for P_α (or

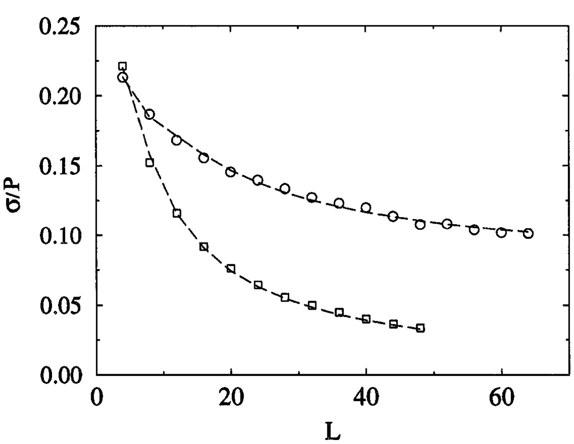

FIG. 4. Scaling behavior of the relative fluctuation of the participation ratio for random matrices of the GOE (squares) and for our quantum billiard (circles). Fits are shown as dashed lines.

$t_{2\alpha}$) averaged over the whole energy range indicate that this behavior is not expected in the present case, as from the above fittings it is concluded that $D(2) = 2$. In order to ensure this conclusion we have carried out several analyses in selected energy ranges by means of the above method and by the standard box-counting method [19] for clusters of a fixed size. If size effects are properly accounted for, all results point to the same conclusion: The wave functions of the billiard herewith investigated do not show multifractal behavior. In fact all results for $t_{q\alpha}L^{2q}$ can be most accurately fitted by parabolic functions.

Summarizing, we have presented a new model of quantum chaotic billiards which is an efficient implementation of surface roughness. The essential feature of the model is the inclusion of diagonal disorder at the surface of the system. The spectral statistics of this billiard changes through the band in a manner not previously reported in other models of chaotic billiards. In particular, exponentially localized, quasi-ideal surface resonances and chaotic states are found to exist within the band. The probability amplitude of chaotic eigenstates is reminiscent of that found in more standard chaotic billiards and for prelocalized states in two dimensions. We have also shown that whereas the asymptotic behavior of the participation ratio in the present billiard is almost identical to that found in random matrices, the standard deviation (fluctuations) of that magnitude is much larger in the former. This result suggests that mapping between chaotic billiards and the random matrix problem should be expected only for averaged properties and not for their fluctuations. It is very likely that these features are not exclusive of the present billiard and that the behavior of quantum chaotic billiards cannot be fully described, at least at a mesoscopic level, by random matrices. Finally, we note that the simplicity of our model allows the study of several situations of physical interest including the case of 3D billiards.

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*Permanent address: Departamento de Física, Universidad de Murcia, E-30071 Murcia, Spain.

†Permanent address: Instituto de Ciencia de Materiales de Madrid, Consejo Superior de Investigaciones Científicas, Cantoblanco, E-28049 Madrid, Spain.

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