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Gaussian-orthogonal-ensemble level statistics in a one-dimensional system

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Energy-level statistics are studied for a one-dimensional integrable system. Direct evidence is found that "chaotic," i.e., Gaussian-orthogonal-ensemble, level statistics can occur in such an integrable system.

I. INTRODUCTION

One of the most intensely pursued questions of "quantum chaos" is the existence of generic properties of quantum systems that would reflect the integrability (or nonintegrability) of their classical analogs. One route of such investigation is via level statistics.[1-20] Berry and Tabor[1] first pointed out that the spectrum of a system quantized from a classical integrable system should in general obey uncorrelated Poisson level statistics, and that level repulsion in the quantal spectrum might indicate the presence of chaos in the classical limit. Discussing the relationship between classical chaos and quantum level statistics, Bohigas, Giannoni, and Schmit conjectured[6] that "*Spectra of time-reversal-invariant systems whose classical analogs are K systems show the same fluctuation properties as predicted by the Gaussian orthogonal ensemble.*" Most examples supporting this conjecture concern simple low-dimensional systems, such as the billiard problems,[2,3,5,6] and two particles with nonlinear interaction moving in a one-dimensional space,[11-13] which have been studied extensively and yielded celebrated results. Others, like the three-level Lipkin-Meshkov-Glick model,[18] also lend support to this conjecture. Because of this, one sometimes calls levels of Gaussian-orthogonal ensemble (GOE)-type "chaotic" levels.

Still, the deep connection between GOE level statistics and classical chaos is far from being understood and is in fact the center of a currently active debate.[14,15,17,20] Besides providing positive examples relating classical chaos to quantum GOE level statistics, it is also interesting to ask the following two questions.

(i) Can we find classical chaotic systems whose quantum analogs obey non-GOE level statistics?

(ii) Can we find classical integrable systems whose quantum analogs obey GOE level statistics?

The first question concerns the existence of direct counterexamples to the conjecture, and thus may help to reveal any restrictions on it. The answer to this question is yes, and Refs. 14–16 represent examples of such systems. Although the validity of the conjecture does not imply that the answer to the second question is yes, it is nevertheless interesting to see if GOE behavior in a quantum spectrum implies chaos in its classical analog. This is because most positive examples supporting the conjecture can also be used to support the reversed form of the conjecture (GOE→*chaos*). Most recently, Cheon and Cohen[20] have concocted a two-dimensional rectangular variant of the generalized Richens-Berry billiard[4] problem. The system being studied is pseudointegrable and yet could have GOE level statistics, thus partially answering the second question.

To fully answer the second question, one ought to provide a truly integrable system whose level statistics are GOE. In this paper we do this for a pointlike particle in a one-dimensional (1D) local potential. The reason for such a choice is obvious: this system has energy as a constant of motion, it possesses only one degree of freedom and is therefore (by definition) integrable. Thus our goal here is to find such a potential that will generate GOE level statistics. Success in doing this provides an unambiguous and straightforward counterexample for the conjecture! The theme of this paper is to show that such a potential does indeed exist.

II. PROCEDURE TO FIND THE POTENTIAL

Consider a pointlike particle of unit mass in a one-dimensional space moving under the influence of a potential $V(x)$. In quantum mechanics, eigenvalues and eigenvectors are to be found by solving the Schrödinger equation ($\hbar=m=1$)

$$H\phi_i(x)=\left[-\frac{1}{2}\frac{d^2}{dx^2}+V(x)\right]\phi_i(x)=E_i\phi_i(x) . \qquad (1)$$

In our case, we would like to know whether a potential $V(x)$ exists whose spectrum will obey GOE statistics. The standard way to numerically study energy-level statistics and chaos is to set up a model which includes a few parameters, then vary these parameters in some domain to see how the level statistics change. However, this method is bound to fail in our case. It is difficult to get GOE statistics from such a trial form of potential. The reason for this is perhaps due to the nature of our problem, no matter how we change the form of the potential and adjust parameters, we still deal with an integrable system. Owing to this difficulty, we are forced to set up a systematic procedure to obtain $V(x)$, instead of intuitively guessing it.

Following the standard random matrix theory,[21] a GOE-type spectrum can be easily obtained by diagonalizing an $N\times N$ real symmetric random matrix. Generally speaking, $N=500$ is sufficient to ensure confidence in the statistics.[6] Since we are interested in fluctuations of the local energy-level spacing, the spectrum resulting from diagonalizing a random matrix should be unfolded. This is done with Dyson's standard unfolding procedure, i.e.,

$$e_{i+1}-e_i=(E_{i+1}-E_i)\rho_s(E_i) , \qquad (2)$$

where $\{E_i\},\{e_i\}$ are levels before and after unfolding, and $\rho_s(E_i)$ is the smooth level density of spectrum. The unfolding process gives a spectrum with unit density of states on average. In practice, the unfolding is carried out by fitting the local average level density with cubic splines.

Now we are facing the core problem of all: how to find a potential which reproduces a given spectrum. In fact, this is a fundamental quantum-mechanical problem: instead of solving for energy levels from a Hamiltonian, we want to construct a Hamiltonian from given energy levels. In one sense, this is the analog to finding a scattering potential from known phase shifts. Our scheme is to construct the potential iteratively, starting from a trial potential, but allowing its value at any point x to be an adjustable parameter. The new potential is obtained by minimizing the difference between the predicted and given spectra.

Let us denote the unfolded spectrum as $e_i(i=1,\ldots,n)$. Also, denote the eigenvalues found by solving the Schrödinger equation by $e_i^s(i=1,\ldots,n)$; $V(x)$ will then be selected to minimize

$$F=\sum_i(e_i^s-e_i)^2 . \qquad (3)$$

We will need the functional derivative of F with respect to $V(x)$. Since

$$\frac{\delta e_i^s}{\delta V(x)}=\frac{\delta}{\delta V(x)}\langle i|H|i\rangle=\phi_i^2(x) , \qquad (4)$$

where $\phi_i(x)$ is the normalized eigenfunction for the ith state,

$$\frac{\delta F}{\delta V(x)}=2\sum_i(e_i^s-e_i)\phi_i^2(x) . \qquad (5)$$

The potential is then found iteratively according to the standard gradient search method:

$$V_{\text{new}}(x)=V_{\text{old}}(x)-\left[2\sum_i(e_i^s-e_i)\phi_i^2(x)\right]\epsilon , \qquad (6)$$

where ϵ is an appropriate small number which makes $F[V_{\text{new}}(x)]<F[V_{\text{old}}]$. In practice, we specify the potential on a numerical lattice and solve the Schrödinger equation using Numerov's method.[22] The iterative formula then reads

$$V_{\text{new}}(L)=V_{\text{old}}(L)-\left[2\sum_i(e_i^s-e_i)\phi_i^2(L)\right]\epsilon ,$$
$$1\le L\le M , \qquad (7)$$

where L labels the lattice points. This procedure defines a minimization problem in an M-dimensional space with M the number of points used to define the potential. The potential at each point is considered to be an independent variable.

The unfolding procedure yields a spectrum with average energy spacing of 1 unit, therefore $V(x)$ is expected to be a harmonic oscillator (HO) potential ($V=\frac{1}{2}x^2$) on average. This provides us with a good initial guess for the potential. The search procedure preserves the evenness of the potential; thus an even potential, i.e., $V(x)=V(-x)$, will be generated from the initial HO potential and only $(M+1)/2$ points need to be treated as independent variational parameters. From equation (6), we know that the search method also preserves the continuity and differentiability of the potential.

It should be noticed that although we have provided a practical method to find the potential fitting a given spectrum, the conditions for the existence of the potential still need to be proven mathematically. Also, if the solution exists, it may not be unique. This can be easily understood by the following argument: In principle, we are using an infinite number of parameters to satisfy a finite number of conditions, thus if one solution exists, there might be infinite number of others. In our method, the multiple solutions can be found by taking different initial potentials and/or different values of ϵ. Our conjecture on this general problem is that, given a finite number of nondegenerate energy levels, one could always find an infinite number of potentials in one-dimensional space to reproduce them. The lack of uniqueness in the solution to the potential does not affect the discussion of this paper, as any solution is equally good for our purpose.

III. RESULTS AND DISCUSSION

Since the $\{e_i\}$ follow GOE statistics, the individual energies exhibit local fluctuations away from the average HO spectrum. This should produce deviations in $V(x)$ away from the HO average. Figure (1a) shows the result of the fit for $V(x)$; Fig. 1(b) shows some details concerning the fluctuations in $V(x)$. We find that there are enough points to well define the potential. To show the goodness of our fit, we plot the error of the fitted levels against the given energies in Fig. 2. It is found that even at energy as high as 500, $e^s - e$ is less than 0.06. The average of $e^s - e$ is 0.0019, giving a slight upward bias to the figure. The standard deviation of $e^s - e$ (average error of the fitting) is 0.0060. Since $0.0019 \ll 0.0060$ the asymmetry of Fig. 2 with respect to $y = 0$ is within statistical error. Figures 3(a) and 3(b) show the nearest-level statistic $P(x)$ and the Δ_3 statistic, respectively, calculated from the original set of energies generated by using a random matrix, and the fitted energies; this figure shows how well the fitted levels reproduce the fluctuation properties of the original set. Notice that the quality of the fit depends on the computer time we spend. We believe that the fit can be made arbitrarily accurate given enough computer time. The spectrum fitted here reproduces GOE statistics very well and this procedure can be applied to any given spectrum resulting from diagonalizing a random matrix; thus we have found a set of potentials which generate a GOE-type quantum solution.

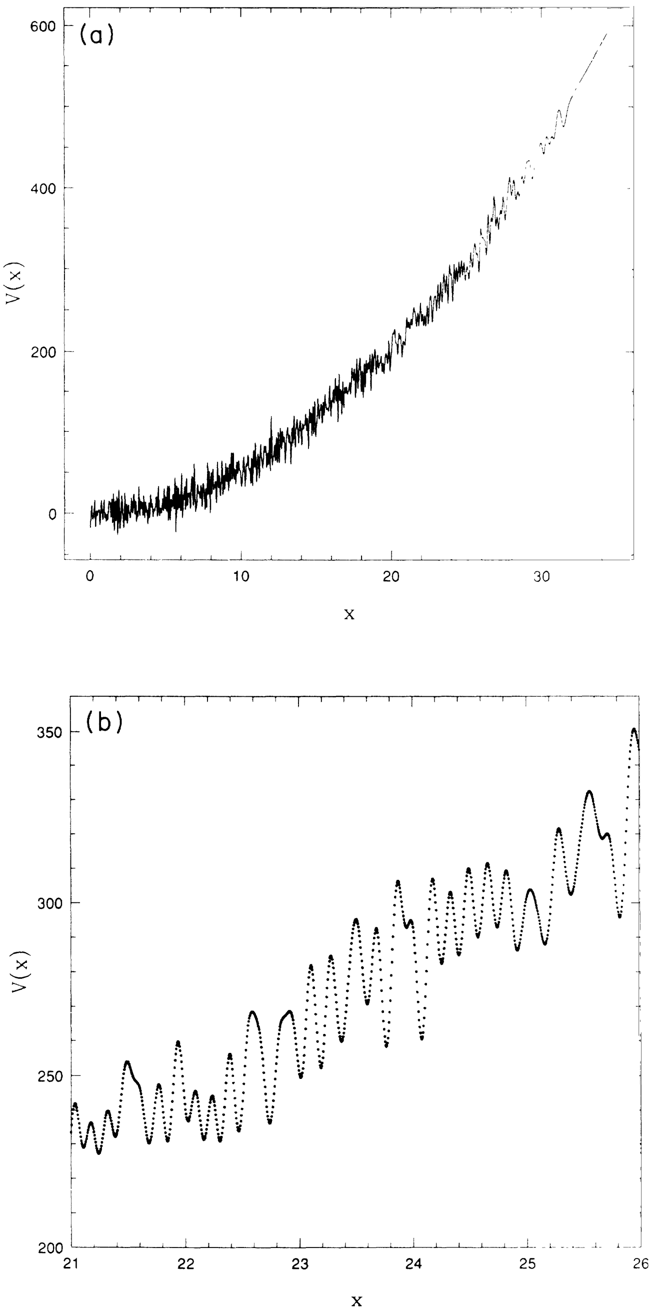

FIG. 1. (a) The fitted potential $V(x)$ to 500 energy levels which follow GOE statistics. Since $V(x) = V(-x)$, only $x \geq 0$ is plotted. (b) $V(x)$ between $x = 21$ and 26 to show some of the details of the potential. The potential is plotted with the actual fitted points to illustrate that a large number of points is used to describe each oscillation.

Note that $V(x)$ shown in Fig. 1(a) is a HO potential on the average with small fluctuations dictated by the fit. Asymptotically, when $x \gg x_{\mathrm{ct}}$, with x_{ct} the classical turning point of the Nth, i.e., the 500th state, $V(x)$ is strictly a HO potential. One difficulty of the procedure is that the fluctuations in $V(x)$ have relatively small wavelength; however, this can be accommodated easily by using a fine mesh. In practice a mesh of 6500 points (for $x \geq 0$) was used; it resulted in each oscillation being described by at least 20 mesh points which is more than adequate. On the other hand, the amount of computer time required for the fit was large. Notice that since the number of lattice points is much larger than the number of states to fit, the fitted potential is by no means unique as we have stated earlier.

Another difficulty for the fit is that some states have small energy separations according to the GOE $P(x)$ statistics, even though there is strictly no degeneracy in the spectrum. This constitutes a large deviation from the equally spaced HO spectrum (the starting point for the fit) and requires many iterations to achieve good convergence. Note that the same argument points to the fact that it is theoretically impossible to fit, in 1D, a spectrum obeying a Poisson distribution, since the latter requires a large number of degeneracies. Berry and Tabor[1] pointed out this fact as early as 1977; they remarked that when relating Poisson level statistics to an integrable classical analog, a one-dimensional system should be regarded as an exception.

Since we are dealing with a relatively complicated potential and a large number of eigenvalues and eigenvectors are needed to high accuracy, it is very important to ensure that the solutions of the Schrödinger equation are sufficiently accurate. To do so, we checked e_i against $\langle i|H|i\rangle$. It is found that the largest difference between them is less than 10^{-2} which for $e \sim 500$ means five digits of accuracy in energy. This results in two digits of accuracy for any level spacing, which makes the $P(x)$ statistic reliable. Of course, the computation was done in double precision. Note that the fitted potential exhibits many local maxima and minima. The structure of the resulting classical orbits is very complicated. The maxima are homoclinic points, in the neighborhood of which the classical motion exhibits critical slowing down. Nevertheless, this system is strictly integrable.

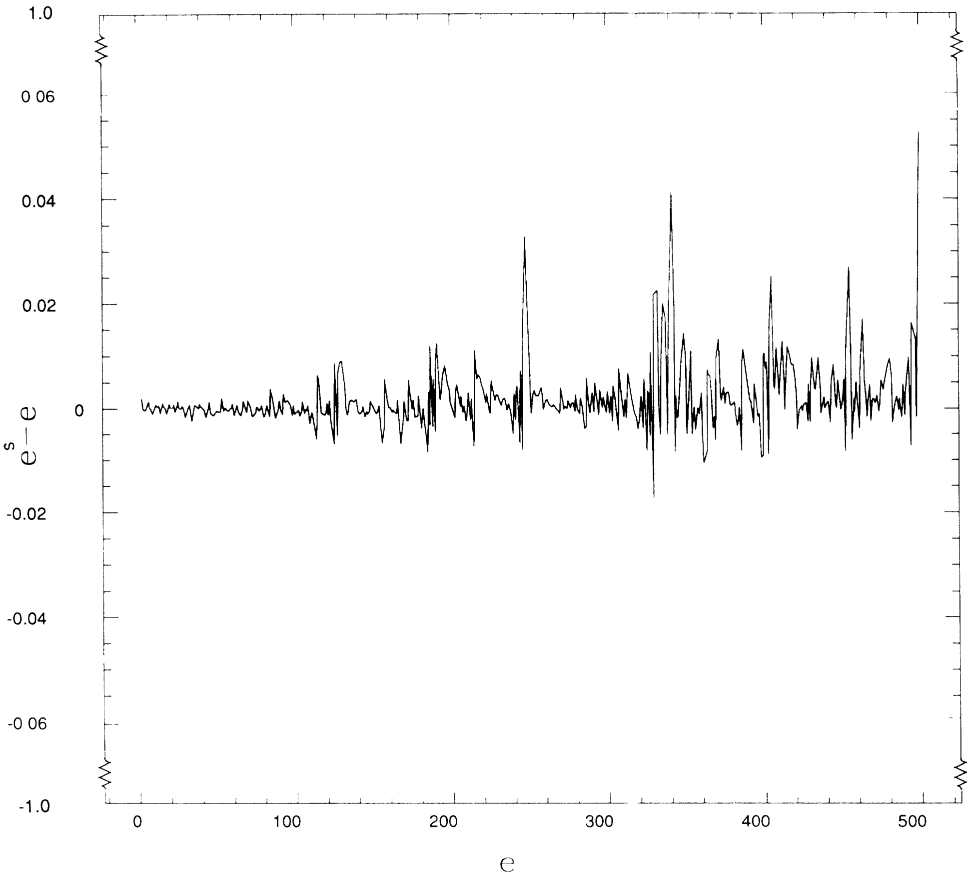

FIG. 2. Errors of fitted energies $e^s - e$ plotted against e.

As we can see from equation (6), the fluctuations in the potential are related to the oscillations in the wave function squared $\phi_i(x)^2$. As we move up to higher and higher energy, wave functions have smaller and smaller wavelengths and thus we introduce more fine structure into the potential. However, as long as we fit a finite number of energy levels, these wavelengths are not infinitely small, and thus the resulting potential is a regular function. If one insists on fitting an infinite number of states, it is obvious that we will need an infinitely long time to achieve the result, and thus the present procedure would lose its utility.

The potential $V(x)$ is an harmonic oscillator with some small fluctuations imposed on it. These fluctuations are responsible for the fluctuations in the spectrum. Thus changing the fluctuations in the potential will result directly in changes in spectral fluctuation properties. It is interesting to see how sensitively these changes depend on the local potential oscillations. Of course, the general situation is complicated. Here we only discuss two simple cases. In the first case, we keep all oscillations but change only one by a small amount; it is easy to see that the change only affects a few levels close to the change point in the potential plot diagram. Since only a small portion of levels is involved in such changes, the global picture of level statistics will not change. In the second case, we perform a global magnification or reduction on the potential fluctuations $V - x^2/2$. After the global

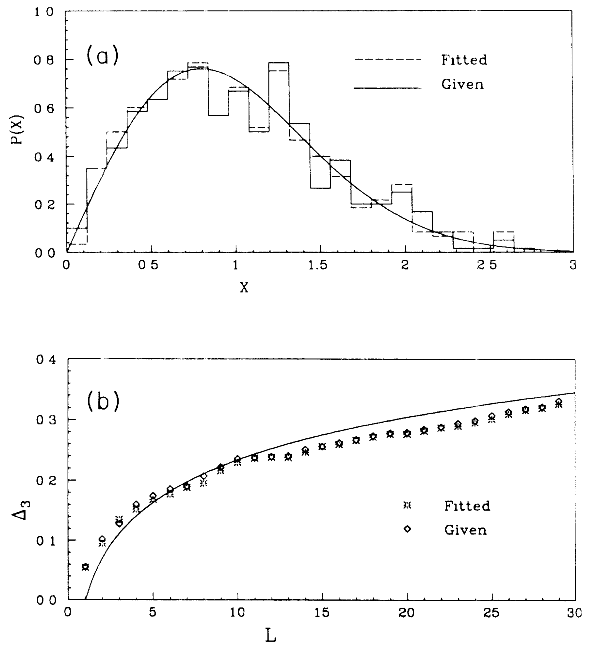

FIG. 3. (a) $P(x)$ for the original set of unfolded energies (solid line histogram) and for the fitted energies (dotted line histogram) as compared to the GOE $P(x)$ function (smooth solid line). (B) Δ_3 for the original set of unfolded energies (diamond) and for the fitted energies (star) as compared to the GOE Δ_3 function (solid line).

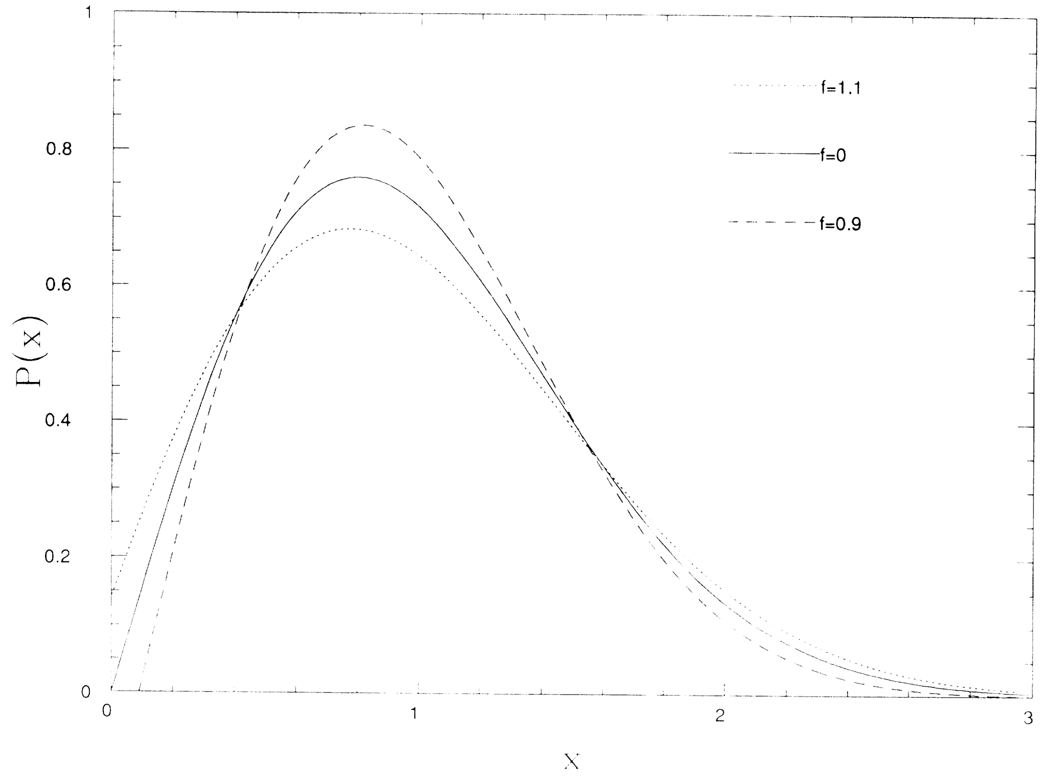

FIG. 4. Nearest-level spacing Wigner distribution and those resulting from enhanced and reduced potential fluctuations.

change, we have a potential

$$V' = \left[V - \frac{x^2}{2} \right] f + \frac{x^2}{2} . \tag{8}$$

In the first-order approximation,

$$e_n' = \langle e_n' | \tfrac{1}{2} P^2 + V' | e_n' \rangle \tag{9}$$

and

$$\frac{de_n'}{df} = e_n - \langle e_n' | \tfrac{1}{2} P^2 + \tfrac{1}{2} x^2 | e_n' \rangle . \tag{10}$$

Considering $V - \frac{1}{2}x^2$ as a perturbation to the harmonic-oscillator potential, the difference between the wave function $|e_n'\rangle$ and corresponding harmonic oscillator wave function is small to second order, thus $\langle e_n' | \frac{1}{2}P^2 + \frac{1}{2}x^2 | e_n' \rangle \approx n + \frac{1}{2}$, and $de_n'/df = e_n' - (n + \frac{1}{2})$. Let x' be the nearest level spacing,

$$\frac{dx'}{df} = x - 1 . \tag{11}$$

The solution of this differential equation is just

$$x' = 1 + (x - 1)(1 + \delta), \quad \delta = f - 1 , \tag{12}$$

where x denotes the nearest-level spacing when $f = 1$. In this calculation, we have not included a possible level reordering effect. Owing to this level spacing shift, the nearest-level spacing statistic $P(x)$ now becomes

$$P(x) = \left[P_0(x) + \frac{dP_0(x)}{dx} (1 - x)\delta \right] (1 - \delta) , \tag{13}$$

where $P_0(x) = P(x)|_{f=1}$. If we choose $P_0(x)$ as a Wigner distribution, then

$$P(x) = \frac{\pi}{2} \left[x + \left[1 - \frac{\pi}{2} x^2 \right] (1 - x)\delta \right] \times \exp\left[-\frac{\pi}{4} x^2 \right] (1 - \delta) \tag{14}$$

Since $P(x)$ should always be greater than zero, equation (14) should not be used when it predicts negative values; then zero could be used. As we can see from this expression, the characteristics of the $P(x)$ statistic will be preserved as long as δ is small. Since $P(x)$ includes a Gaussian decay factor, the change to the tail of the curve is small whereas the most sensitive place is located at $x = 0$. In Fig. 4 we have plotted the Wigner distribution ($\delta = 0$) and distorted curve when ($\delta = 0.1$) and ($\delta = -0.1$). The actual solutions from solving the differential equation yield qualitatively the similar results.

IV. CONCLUSION

In summary, we have used a one-dimensional model to demonstrate that the GOE type of quantum spectrum can indeed occur in a system whose classical analog is *strictly* integrable. Our concept is simple, our approach is straightforward. Since most current research which aims at revealing quantum manifestations of classical chaos uses low-dimensional problems, it is clearly interesting to understand the one-dimensional problem. In attempting to establish a universal relationship between classical chaos and quantum level statistics, it is important to know of any constraint which might apply. Our result is a step towards this final goal.

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