Chaotic signatures in the spectrum of a quantum double well

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Abstract

The spectrum of a double well constructed of a square barrier embedded in an infinite well is analyzed. Level statistics for levels slightly above the barrier show signs of Wigner statistics usually associated with quantum chaos. The correspondence with Wigner statistics improves when an ensemble of systems with slightly different barrier heights is taken, possibly reflecting an adiabatic time-dependent modulation of the barrier.

One of the most celebrated definitions of classical chaos is the exponential divergence in time of neighboring points in phase space. In discussing the possible existence of quantum chaos, one would like to keep as close as possible to the above definition. Implicitly, one needs to construct a legitimate quantum mechanical paraphrase of the above definition. In fact, the wave function of a particle may be thought of as representing an ensemble of points in phase space while its spread as function of time is a measure of the divergence of those points. We have recently considered the time development of a wave packet, initially located on the left hand side of a square barrier embedded in an infinite well [1]. We found, in addition to the highly complex behavior of the wave packet, that the spread validity of the Ehrenfest approximation fails much more rapidly than for a wave packet in free space.

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Ballentine et al. [2] have argued that a quantum state may behave essentially classically, even when Ehrenfest's theorem does not apply. They conclude that Ehrenfest's theorem is neither necessary nor sufficient to identify the classical regime and that the classical limit of a quantum state is not a single classical trajectory but rather an ensemble of classical trajectories. However, Ehrenfest's theorem breaks down much sooner for a chaotic ensemble than for a regular one.

Pattanyak and Schieve [3] have studied a one-dimensional problem with a Duffing potential without external perturbation. Their results reflect the highly complex behavior of the quantum state even for a case in which the system is *not* chaotic in the classical limit.

Another indicator commonly used in the study of quantum chaos is the properties of the energy spectrum. It is well known [4–6] that the energy level statistics of quantum systems show different statistical characteristics corresponding to whether the system is chaotic or regular in the classical limit [7]. For systems which are regular in the classical limit, the energy level statistics correspond to Poisson statistics, while for systems which are chaotic in the classical limit, the statistics follow Gaussian ensemble statistics (also known as the Wigner statistics) according to the system's symmetry. Systems with time-reversal symmetry follow the Gaussian orthogonal ensemble, and systems without time-reversal symmetry follow the Gaussian Unitary ensemble.

A useful statistical measure of the energy level statistics is the level spacing distribution. The Poisson distribution is given by

$$P_P(s) = \exp(-s) \,, \tag{1}$$

where s is the level spacing in units of the averaged level spacing. For the Gaussian orthogonal ensemble

$$P_W(s) = \frac{\pi s}{2} \exp\left(\frac{-\pi s^2}{4}\right) \,. \tag{2}$$

One can also characterize the level statistics by the spectral rigidity $\Delta_3(L)$. The spectral rigidity is defined as the local average of the mean square deviation of the cumulative number of states $N(E)$ from the best fitting straight line over a range of energy corresponding to L mean level spacings

$$\Delta_3(L) = \left\langle \frac{1}{L} \int\limits_{\alpha}^{\alpha+L} dE[N(E) - AE - B]^2 \right\rangle \,. \tag{3}$$

For the Poisson statistics $\Delta_3(L) = L/15$ while for the Gaussian orthogonal ensemble $\Delta_3(L) = (1/\pi^2)(\ln(L) - 0.0687)$. The spectral rigidity is often a stronger tool than the level spacing distribution in the analysis of complex systems, since it takes into account the correlations between levels on large energy scales while the spacing distribution takes into account only nearest neighbor correlations.

In this paper we calculate the spectrum of a double well constructed of a square barrier embedded in an infinite well. We have calculated the level spacing distribution
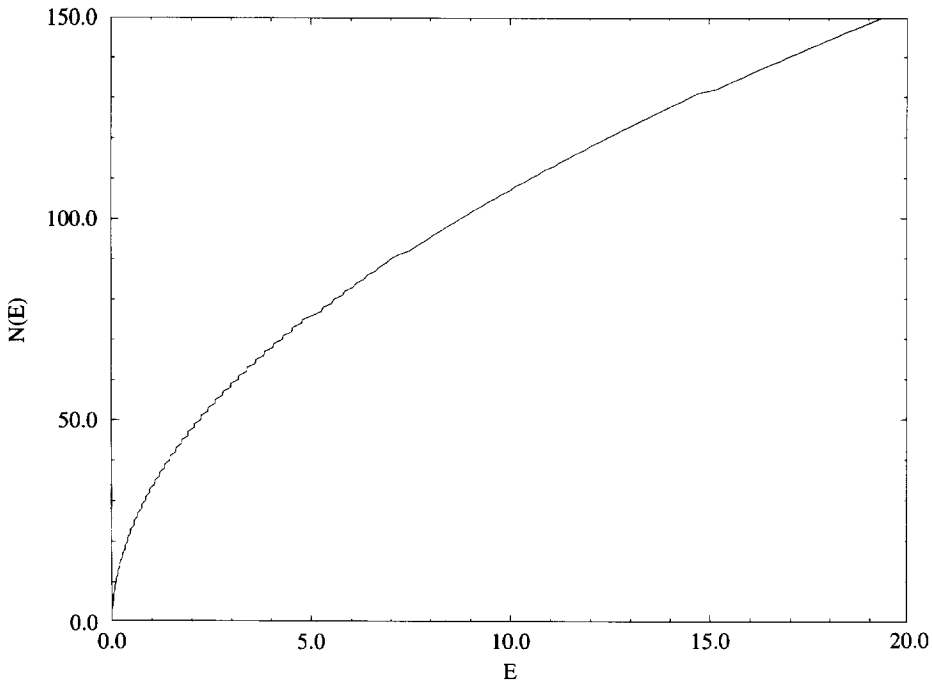
Fig. 1. The cumulative number of levels $N(E)$ as function of energy.

and the spectral rigidity for different regions of the spectrum. For energies significantly below or above the barrier level we find the behavior consistent with the simple square well level statistics. In the neighborhood of the barrier edge we find statistics which are closer to the Wigner statistics. When the spectral rigidity is averaged over several different barrier heights (different from the original height by no more than a level spacing), which has the effect of increasing the sample population, the correspondence with the Wigner prediction is very good. Thus, for energies in that region the spectrum exhibits a signature of chaos. We emphasize however that the use of the energy level statistics as an indication of chaos must be taken with a grain of salt, since for the system we are studying there is no classical limit [7].

The energy levels were calculated for a square barrier of height $V = 5$ and width $2a = 2$ ($\hbar \equiv 1, 2m \equiv 1$) embedded in an infinite well of width $2b = 110$. The cumulative number of levels is presented in Fig. 1. As can be expected the low eigenvalues ($E < V$) appear as almost degenerate pairs around $E_{2n} \sim E_{2n+1} \sim \hbar^2 (\pi n)^2 / 2m(b - a)^2$, which is the energy level for an infinite square well of width $b - a$. This can be clearly seen in $N(E)$ which has a step-like shape where each step is equal to two. The spacings between the high eigenvalues ($E \gg V$) correspond to the spacings expected from an infinite well of width $2b$, i.e., the barrier has little influence on those levels. For energies just above the barrier height $V < E < 2V$, the behavior of $N(E)$ is more complex and cannot be described by any simple formula. Therefore, this region is a natural candidate for a more sophisticated analysis of its statistical properties.
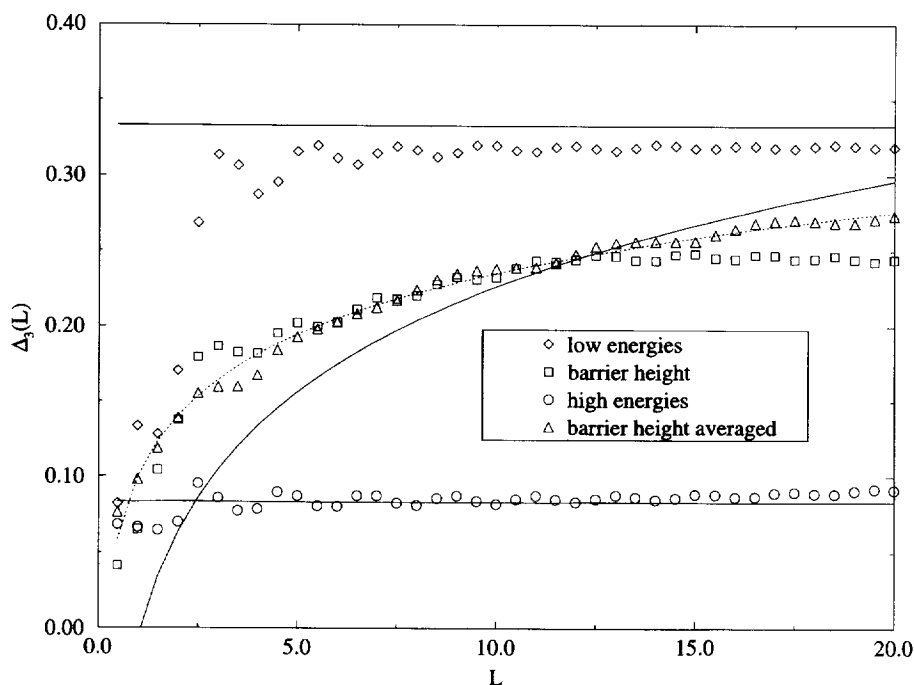
Fig. 2. The spectral rigidity $\Delta_3(L)$ as a function of the energy interval L for different regions of the spectrum. The full curve corresponds to the Wigner predictions $\Delta_3(L) = (\ln(L) - 0.0687)/\pi^2$, while the dotted curve corresponds to $\Delta_3(L) = 0.58(\ln(L) - 0.0687)/\pi^2 + 0.1$.

After performing the standard unfolding procedure of the spectrum [4–6], the spectral rigidity $\Delta_3(L)$ for different regions of the spectrum is calculated. The results are plotted in Fig. 2. For the high-energy levels $\Delta_3(L) = \frac{1}{12}$ which is the rigidity of equally spaced levels known as a "picket fence". This is expected since the levels in this region have almost no local fluctuations, and the global increase of $N(E) \sim \sqrt{E}$ is removed by the unfolding. A similar situation is seen for the low-lying levels with a small difference which stems from the fact that those levels are composed of sets of two degenerate levels equally spaced, i.e., a double picket fence, resulting in $\Delta_3(L) = \frac{1}{3}$. For energies just above the barrier height ($V < E < 2V$, or $70 < N(E) < 110$) the situation is quite different. The rigidity seems closer to the Wigner rigidity although no clear fit can be seen.

One can also consider an average of the rigidity over an ensemble of systems with slightly different barrier heights. There are two main reasons for considering an ensemble. First, since the region just above the barrier contains only about 40 levels which is relatively a small number of levels, statistics over a larger number of levels are most desirable. Another reason is that the averaging over different barrier heights may be thought of as a time average over the energy levels of a system in which the barrier height oscillates with a low frequency [8]. It is well known in classical chaos that such a time-dependent potential is necessary for the development of chaos in one-
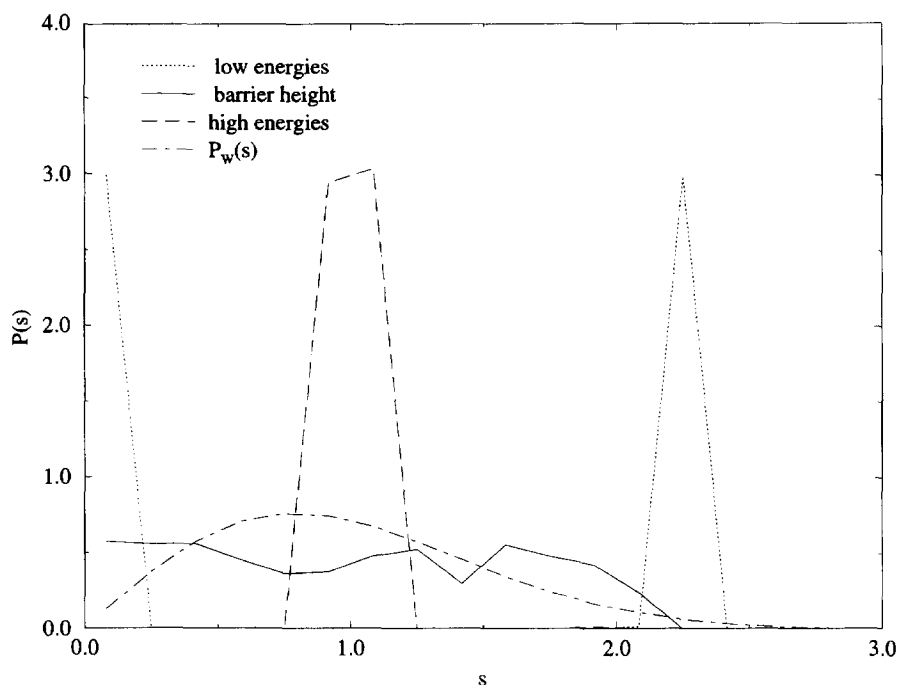
Fig. 3. The level spacing distribution for different regions of the spectrum.

dimensional systems. Therefore, one might expect the ensemble-averaged rigidity to approach more closely the Wigner form. The rigidity after an ensemble average over 20 different barrier heights equally spaced between $V = 4.8$ and $V = 5.2$ is indicated by the $\triangle$ symbols in Fig. 2. It can be seen that the resulting rigidity is closer to the Wigner rigidity. Since one may expect that some remnant of the picket fence statistics will linger in the region just above the barrier height, it makes sense to try a fit to the rigidity as a function of the form $\varDelta_3(L) = c_1(\ln(L) - 0.0687)/\pi^2 + c_2$. As can be seen in the figure, for $c_1 = 0.58$ and $c_2 = 0.1$, a perfect fit is obtained.

In Fig. 3 the level spacing distributions for the ensemble-averaged case is presented. The high energies retain the picket fence distribution while the low energies retain the double-picket fence distribution. The intermediate regime shows a distribution which is more akin to the Wigner one. Nevertheless, this distribution is too messy for a more precise statement, since the level spacing distribution is a less precise tool than the spectral rigidity.

It is interesting that the Wigner-type distribution is found for energies just above the barrier height, while the most complex behavior of the wave function is observed for much lower energies [1]. We therefore conjecture that the usual energy level statistics criteria correspond to a signature of chaotic behavior in energy regions for which the classical behavior of the system is similar to its quantum behavior. For energies deep in the well, where the classical behavior is totally different than the quantum one,

the level statistics do not show a strong evident signature of chaos from the point of view of the usual criteria. However, other, and perhaps more delicate tests should be investigated. For example, the double-picket structure of the low-lying spectrum is only approximate. Our results [1] in the study of the wave function with support in the neighborhood of $\sim \frac{1}{10}$ of the barrier height showed very complex behavior. Lewenkopf [7] has found that significant deviations occur for a δ-function barrier.

We have, furthermore, investigated the case in which the barrier is shifted slightly off-center (the size of the regions outside the barrier was chosen to be incommensurate so that there exist no symmetry classes). We find that the results are essentially identical, and therefore do not depend qualitatively on the symmetry of the example that we have given.

One may also note that classical Hamiltonian chaos usually occurs in the neighborhood of a separatrix, which in our case corresponds to energies in the neighborhood of the barrier height. This is also in agreement with the study of Pattanyak and Schieve [3], who have shown that, for a double-well potential, squeezed coherent states show the most complex behavior for energies close to the separatrix. They argue [9] that the interplay between the classically unstable orbits and the quantum tunneling effects is the origin of this complex behavior. This is in agreement with our observations on the behavior of the energy level statistics in that regime.

In conclusion, we have calculated the energy level statistics of a square barrier embedded in an infinite well. For energies just above the barrier level, we find statistics which are closer to the Wigner statistics than in other regions of the spectrum. When the spectral rigidity is averaged over several different barrier heights the correspondence with the Wigner prediction is very good. Thus a double-well system exhibits signs of chaos for energies close to the separatrix.

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