Distribution of Matrix Elements of a Classically Chaotic System

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Distribution of Matrix Elements of a Classically Chaotic System.

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Abstract. – The statistics of matrix elements of a perturbation of a classically chaotic quartic oscillator system are investigated. Our numerical results confirm that the local variance of the matrix elements can be obtained from a classical correlation function. The probability distribution of the matrix elements (normalised using their local variance) was investigated. This is expected to be a Gaussian distribution in the semi-classical (high-energy) limit. The expected Gaussian form emerges slowly as the energy is increased. The form of the distribution at lower energies is identified.

In this letter we describe some results on the statistical properties of the matrix elements of an operator with a classical limit, in the basis formed by the eigenstates of a Hamiltonian with a chaotic classical limit. These matrix elements are important for problems in which the response of a classically chaotic system to a perturbation is required [1], and a theoretical understanding of these matrix elements is important for potential experimental investigations of «quantum chaos». It is natural to examine these matrix elements from a statistical viewpoint because the spectra and eigenfunctions of classically chaotic systems can only be described statistically: there are no methods available which provide explicit formulae for a given energy level or eigenfunction. Berry [2] has given an excellent review of the quantum mechanics of systems with a chaotic classical limit.

Berry [3] has argued that the eigenfunctions of systems with a chaotic classical limit resemble Gaussian random functions and gives a theory for the autocorrelation function. This model clearly predicts that the matrix elements of an operator should be Gaussian distributed. The Gaussian-random-function model for the wave functions does not predict the correct variance for the matrix elements, however (we discuss the correct formula later in this letter). This observation suggests that it would be prudent to check that the matrix elements really are Gaussian distributed.

We recently investigated the matrix elements of the operator corresponding to deforming the boundary of a quantum billiard [4], as part of an extensive study of statistics characterising the parameter dependence of energy levels of systems with a chaotic classical limit. This paper also contains references to important earlier work in related areas. Our results showed that the matrix elements are in fact Gaussian distributed in the semi-classical (high-energy) limit, but that the Gaussian distribution only emerges slowly as the semi-classical limit is approached. We found that at lower energies the matrix elements (normalised in a manner we will describe shortly) have the following probability distribution:

$$P_N(q) = \frac{\Gamma\left(\frac{N}{2}\right)}{\sqrt{\pi N}\,\Gamma\left(\frac{N-1}{2}\right)}\left(1 - \frac{q^2}{N}\right)^{(N-3)/2} \tag{1}$$

This is the distribution of the elements of an N-dimensional vector, distributed randomly over the surface of an N-dimensional sphere of radius $\sqrt{N}$ [5]. This function approaches a Gaussian as $N \to \infty$. The values of the parameter N fitted to the empirical matrix element distribution for the billiard were surprisingly small in view of the large number of matrix elements involved. A tentative explanation for this result was given, in terms of a semi-classical sum rule [6] which constrains the values of the matrix elements. The argument leading to (1) is general for systems possessing a chaotic classical limit, which suggests that the same distribution should be observed in other systems.

The purpose of the investigation reported here was twofold. Firstly we wanted to establish whether eq. (1) describes the distribution of matrix elements of other systems, or whether it is due to some special feature of quantum billiards. The results given below suggest that it is, in fact, universal. Secondly we wanted to verify that the semi-classical relation [6] between the variance of the matrix elements and the classical correlation function of the perturbation provides a useful means of calculating the former quantity. We were not able to investigate this latter question for the quantum billiard system because the derivation of the semi-classical formula for the variance depends on the classical limit of the operator being a smooth function, and this condition does not hold for deformations of a billiard.

Before considering our model system we discuss the theory for the variance of the matrix elements. The typical size of the matrix elements $A_{nm} = \langle \phi_n | \widehat{A} | \phi_m \rangle$, where $|\phi_n\rangle$ and $|\phi_m\rangle$ are eigenstates of $\widehat{H}$, will clearly depend on the energies E_n, E_m of these two states. It is therefore useful to define a local variance of the matrix elements as follows:

$$\sigma^2(E, \Delta E) = \frac{1}{n_0^2} \sum_{n \neq m} \sum_{m} |A_{nm}|^2 \delta_\varepsilon\left(E - \frac{1}{2}(E_n + E_m)\right) \delta_\varepsilon(\Delta E - (E_n - E_m)), \tag{2}$$

where n_0 is the smoothed density of states, and the $\delta_\varepsilon(x)$ are pseudo-δ-functions spread out over an energy range ε which is large compared to the mean level spacing, but small compared to the classical energy scales of the problem. When studying the statistics of the distribution of matrix elements, the matrix elements must be normalised by dividing each one by the local standard deviation $\sigma(E, \Delta E)$ before computing their distribution.

The quantity $\sigma^2(E, \Delta E)$ can be related to the correlation function of the classical function $A(\boldsymbol{q}, \boldsymbol{p})$ corresponding to $\widehat{A}$ under the motion generated by the classical Hamiltonian [6]:

$$\sigma^2(E, \Delta E) = \frac{1}{2\pi\hbar\rho\Omega} \int_{-\infty}^{\infty} \mathrm{d}t\, C(E, t) \exp[i\,\Delta E t/\hbar], \tag{3}$$

where the correlation function $C(E, t)$ is

$$C(E, t) = \int \mathrm{d}\boldsymbol{q} \int \mathrm{d}\boldsymbol{p}\, A(\boldsymbol{q}, \boldsymbol{p}) A(\boldsymbol{q}'(\boldsymbol{q}, \boldsymbol{p}, t), \boldsymbol{p}'(\boldsymbol{q}, \boldsymbol{p}, t))\, \delta(E - H(\boldsymbol{q}, \boldsymbol{p})). \tag{4}$$

Here $(\boldsymbol{q}', \boldsymbol{p}')$ is the phase space point that the point $(\boldsymbol{q}, \boldsymbol{p})$ evolves into after time t under the classical equations of motion, and the weight of the energy shell $\Omega(E)$ is

$$\Omega(E) = \int \mathrm{d}\boldsymbol{q} \int \mathrm{d}\boldsymbol{p}\, \delta(E - H(\boldsymbol{q}, \boldsymbol{p})). \tag{5}$$

The derivation of the relationship (3) for a system with a semi-classical limit also generates a series of correction terms related to periodic orbits of the classical Hamiltonian [6], and it is not clear how to sum their contributions. This makes it desirable to check that the leading-order term (3) provides a useful approximation.

Our numerical experiments used a quartic oscillator

$$\hat{H} = \frac{p_x^2}{2} + \frac{p_y^2}{2} + \frac{x^4}{\gamma} + \gamma y^4 + 2\lambda x^2 y^2, \tag{6}$$

with $\lambda < 0$ and $\gamma \neq 1$, as an example of a classically chaotic quantum system. For this Hamiltonian the classical motion becomes unbounded when $\lambda = -1$. As λ approaches -1 from above, the classical dynamics are known to be chaotic [7]. The eigenvalues and eigenvectors of the totally symmetric states of $\hat{H}$ were obtained for $\hbar = 1$, $\gamma = 1.2$ and several values of λ by diagonalising (6) in a basis formed from one-dimensional quartic oscillator states. The matrix elements of the operator $\hat{x}^2$ were calculated in the basis of the eigenstates of $\hat{H}$.

Some scaling properties of the quartic Hamiltonian (6) which arise because the potential is a homogeneous polynomial can be used to simplify the analysis of the statistics of the matrix elements. The coordinates and momenta can be seen to obey the scaling relations

$$\boldsymbol{p} = E^{1/2}\boldsymbol{p}_0(E^{1/4}t), \qquad \boldsymbol{x} = E^{1/4}\boldsymbol{x}_0(E^{1/4}t). \tag{7}$$

Substituting into (3), (4) and (5) and taking $A = x^2$, the scaling relation

$$\sigma^2(E, \Delta E) = E^{1/4} g\left(\frac{\Delta E}{E^{1/4}}\right) \tag{8}$$

can be obtained, where $\sigma^2(E, \Delta E)$ is the variance of the off-diagonal elements of $\hat{x}^2$ and the function g is related to the Fourier transform of the classical correlation function of x^2 at $E = 1$. For this system the smoothed density of states is $n_0 = \alpha E^{1/2}$; the numerical value of α can be obtained either directly from the eigenvalue spectrum or by performing the corresponding classical phase space integral of Ω with respect to energy numerically using the Monte Carlo method. For the case illustrated in fig. 1 the value $\alpha = 0.24$ was found. The function $g(y)$ can be obtained as

$$g(y) = \frac{1}{(2\pi\hbar\alpha)^2} \int_{-\infty}^{\infty} \mathrm{d}t\, c(t) \exp[iyt/\hbar], \tag{9}$$

with $y = \Delta E/E^{1/4}$ and $c(t) = C(1, t)$. By dividing each matrix element by the local standard deviation obtained from (8), we obtained the scaled matrix elements, $q = A_{nm}/\sigma(E, \Delta E)$. For a system with GOE behaviour, the result of scaling the matrix elements in this manner will be a Gaussian of unit variance.

Figure 1 shows a plot of the function $g(y)$ obtained numerically from the quantum-mechanical matrix elements (displayed as a histogram) with the Fourier transform of the classical correlation function (continuous curve) superimposed. The correlation function was obtained by integrating the classical equations of motion and calculating the average value of

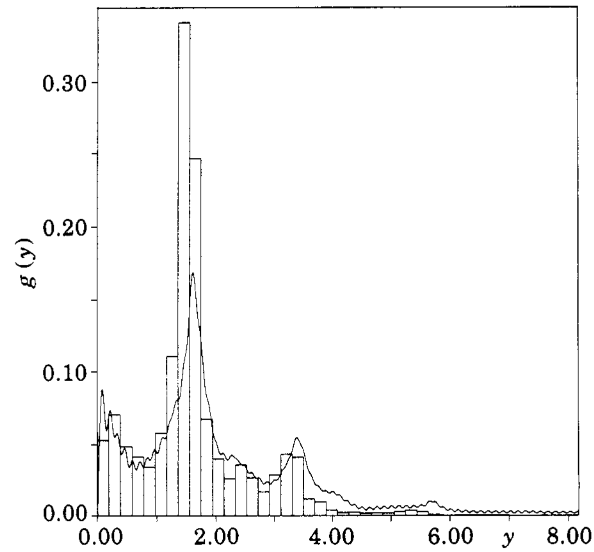

Fig. 1. – Scaling function $g(y)$ for the variance of the matrix elements of $\widehat{x}^2$ (histogram), compared with the Fourier transform of the classical correlation function of x^2 for the quartic oscillator at energy $E = 1$.

$x^2(t)\,x^2(t+\tau)$ over a range of τ from 0 to 50. The convergence of this function was checked both by increasing the averaging time and by doubling the range of τ. The small-amplitude, high-frequency oscillations in the Fourier transform are an artefact of the numerical method employed and have no physical significance. The agreement between the approximate semi-classical formula (3) and the numerical data is very good except for the height of the

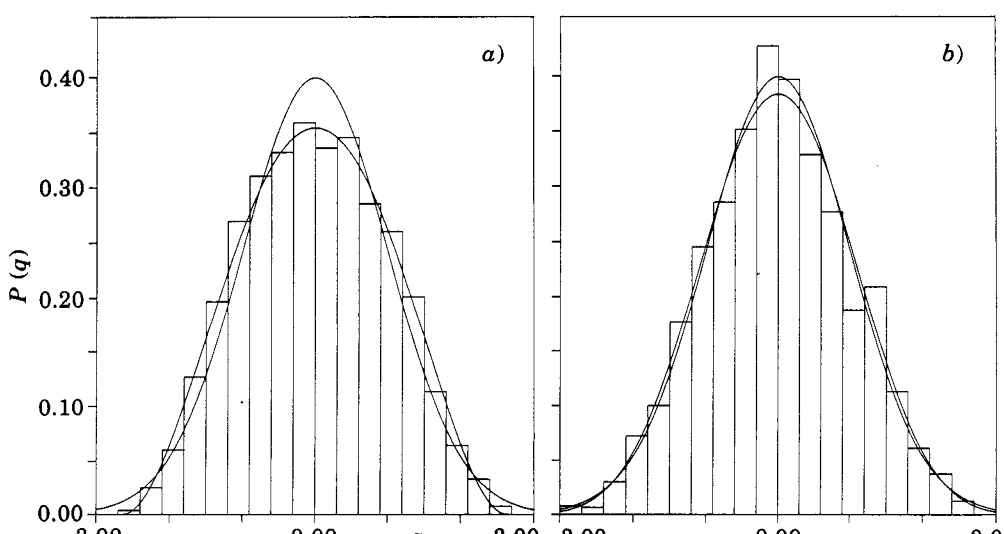

Fig. 2. – Histogram of the probability distribution function of the scaled matrix elements q of the operator $\widehat{x}^2$ for the quartic oscillator with $\gamma = 1.2$, $\lambda = -0.7$, *a*) $E < 60$, *b*) $100 < E < 120$. The smooth curves are a Gaussian of unit variance, and a fit to the distribution (1) with $N = 6.96$, 19.65, respectively. In each case the Gaussian is the curve with the larger maximum at $q = 0$.

principal peak at $y = 1.6$. Since the classical correlation function was checked for convergence, the principal peak of the function $g(y)$ obtained numerically must include a contribution from the periodic-orbit corrections to (3). By integrating the classical equations of motion, it was possible to verify that the principal peak corresponds to a periodic orbit along the x-axis.

Figure 2 shows histograms of the distribution of the scaled matrix elements q for *a*) $E < 60$ and *b*) $100 < E < 120$. The best fit to eq. (1) and a Gaussian curve are also shown. As was found previously for the quantum billiard, the value of N increases with increasing energy, so the Gaussian behaviour expected for a system with a chaotic classical limit emerges gradually as E increases. The mean-square deviations of the fit of (1) and a Gaussian to the data are $6 \cdot 10^{-4}$ and $1.2 \cdot 10^{-3}$, respectively. For fig. 2*b*) the corresponding figures are $1.05 \cdot 10^{-3}$ and $1.1 \cdot 10^{-3}$, indicating that in this case the data is much closer to the limiting Gaussian form. When the distribution approaches a Gaussian, the value of the fitting parameter N becomes very sensitive to small changes in the data, and we were not able to identify unambiguously how N diverges as $E \to \infty$.

The results presented above provide evidence that the semi-classical relation (3) is a useful method for estimating the variance of matrix elements in systems with a chaotic classical limit. The underlying Gaussian statistics of the system at high energy are also confirmed, thus providing additional strong evidence for the applicability of parametrised GOE models [1] to Hamiltonians with a chaotic classical limit. The deviation from Gaussian behaviour at low energy confirms the form of the distribution (1) previously observed [4] for a quantum billiard, and provides evidence that this distribution is universal.

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