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Statistical fluctuations of matrix elements in regular and chaotic systems

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A combination of semiclassical arguments and random-matrix theory is used to analyze transition strengths in quantum systems whose associated classical systems are chaotic. The mean behavior is found semiclassically while the local fluctuations are characterized by a Porter-Thomas distribution. The methods are tested numerically for a system with two degrees of freedom, the coupled-rotators model. The deviations of the strength distribution from a Porter-Thomas one when the system is nonchaotic are also investigated. It is found that the distribution gets gradually wider as the classical system becomes more regular.

The transition of a classical system from regular to chaotic behavior is fairly well understood.[1] The manifestations of this classical behavior in the associate quantum system has been the subject of many investigations in recent years with particular attention given to the chaotic regime.[2] The few quantitative results are based either on semiclassical arguments[3] or on random-matrix theory. For nonintegrable systems there is no working scheme for semiclassical quantization. The Einstein-Brillouin-Keller quantization breaks down in those regions of phase space where invariant tori do not exist. On the other hand, the extent to which random-matrix theory can be applied in chaotic regions is still not fully understood.[4]

In this paper we shall argue that a reasonable scheme for the analysis of a quantum system whose associate classical motion is chaotic involves a combination of semiclassical and random-matrix methods. In this scheme the mean behavior of the respective quantity is given semiclassically, while the local fluctuations are reproduced via random-matrix theory. Such a procedure had been invoked for the energy spectrum. The average level density is found semiclassically or by an empirical procedure and the spectrum is then renormalized by dividing out the mean spacing. The unfolded spectrum has then the statistical properties characterizing an ensemble of Gaussian orthogonal random matrices (GOE), as was found numerically for several chaotic systems.[5] In particular, a Wigner distribution is obtained for the level-spacing distribution.

A similar procedure emerges for the mean behavior[6] and fluctuation properties[7,8] of transition-matrix elements. In particular transition strength distributions seem to be characterized locally by Porter-Thomas distributions.[8] The purpose of this paper is to establish this procedure for the matrix elements and to study the deviations from a Porter-Thomas distribution as the classical system becomes more regular. The procedure consists of two steps. First, the average behavior of the transition strengths is found semiclassically or empirically. Second, the actual transition strengths are renormalized by dividing out their mean behavior and are then subjected to a statistical analysis. The statistical fluctuations of these renormalized strengths should be similar to the local fluctuations of transition strengths. We shall also explain how to determine the energy scale for local fluctuations. Our conclusions are supported by a numerical study of the coupled-rotators model.[9]

Transition-matrix elements offer a more sensitive probe of chaos than the spectrum alone. Given an operator T we construct its strength function

$$S(E,E')=\sum_{i,f}|\langle f|T|i\rangle|^2\delta(E-E_i)\delta(E'-E_f)\ , \quad (1)$$

where $|i\rangle$ and $|f\rangle$ are eigenstates of the Hamiltonian with eigenvalues E_i and E_f, respectively. One can easily show that S is the Fourier transform of the temporal autocorrelation function $C(t)$ of T

$$S(E,E')=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{i(E-E')t/\hbar}C(t)dt\ , \quad (2)$$

$$C(t)=\mathrm{Tr}[\delta(E-H)T(t)T(0)]\ , \quad (3)$$

where $T(t)$ is the Heisenberg representation of T at time t.

The first step in our approach involves the calculation of an average strength function. In practice, this can be done empirically as is explained below. However, for the method to have a predictive power and in analogy with the analysis of energy spectra we would like to establish a semiclassical (SC) estimate S_{SC} of the strength function. For that purpose we replace in (3) the autocorrelation function $C(t)$ by its classical analog $C_{cl}(t)$,

$$C_{cl}(t)=\int\frac{d\eta(0)}{(2\pi\hbar)^d}\delta[E-H(\eta(0))]T(\eta(t))T(\eta(0))\ . \quad (4)$$

Here d is the number of degrees of freedom and $\eta(t)$ is the classical trajectory evolving from a point $\eta(0)$ in phase space. In addition the infinite time interval in the Fourier transform (2) should be replaced by a finite time which is of the order of the shortest classical period of the system as is explained later.

If the classical system is *ergodic* the ensemble average in (4) can be replaced by a time average along a trajectory $\eta(t)$ and[6]

$$S_{SC}(E,E')=\left|\tilde{T}\left[\omega=\frac{E'-E}{\hbar}\right]\right|^2, \quad (5)$$

where $\tilde{T}(\omega)$ is the Fourier transform of $T(\eta(t))$.

S_{SC} describes the mean dependence of S on E and E'. The quantity

$$S_{SC}(E,E')/[\rho_{SC}(E)\rho_{SC}(E')] ,$$

with ρ_{SC} being the semiclassical level density, describes the mean transition strength per initial state at energy E and final state at energy E'. In practice[8] the semiclassical prediction can be reproduced by an empirically averaged strength function $S_\gamma(E,E')$ obtained by means of replacing the δ function in (1) by as Gaussian of width γ.

$$\frac{S_\gamma(E,E')}{\rho_\gamma(E)\rho_\gamma(E')} = \frac{\sum_{i,f} |\langle f|T|i\rangle|^2 e^{-(E-E_i)^2/2\gamma^2} e^{-(E'-E_f)^2/2\gamma^2}}{\sum_{i,f} e^{-(E-E_i)^2/2\gamma^2} e^{-(E'-E_f)^2/2\gamma^2}} . \quad (6)$$

The width γ has to be chosen properly. It should be large enough so that the finer structure of the strength S described by higher-order terms in a semiclassical expansion will not show up. Yet it should not be too large so as to wash the energy variations of S.

The proper width γ has a certain scaling with respect to $\hbar$. This can be derived from a semiclassical expansion of the level density in terms of closed trajectories.[10] Such a trajectory contributes a term proportional to $e^{iS/\hbar}$ where S is the action. This is an oscillatory term with period of $\Delta E \sim 2\pi\hbar/(\partial S/\partial E)$. The largest such ΔE is determined by the trajectory with the shortest period $\tau=\partial S/\partial E$. To wash that finer structure we need to choose $\gamma \geq 2\pi\hbar/\tau$. Thus γ scales linearly in $\hbar$ while in units of the mean level spacing D, $\gamma/D \geq O(\hbar^{1-d})$. This is verified later in our numerical model. In practical applications we use in (6) a constant (energy independent) γ. This is justified if before calculating (6) we unfold the spectrum with $E_i \to E_i\rho_{SC}(E_i)$ where $\rho_{SC}=1/D$.

In the semiclassical approach the smoothing of S is achieved by evaluating the Fourier transform in (2) over a finite time interval. Since the required energy resolution in S_{SC} should not be better than $2\pi\hbar/\tau$ we can use the time-energy uncertainty principle to infer that it is sufficient to compute the temporal correlation function over a time of order τ. We have checked that this S_{SC} compares reasonably well with S_γ for an integrable system, the two-dimensional rectangular billiard, and for an ergodic system.[6]

The second step in the analysis of transition-matrix elements involves their distribution over an energy band of order $\hbar$. In practice, for a given system, there are usually not enough levels in such an energy interval to produce good statistics. To compare transitions belonging to different regions of energy we define "normalized" intensities y_{fi} by

$$y_{fi}=\frac{|\langle f|T|i\rangle|^2}{S_\gamma(E=E_i,E'=E_f)/\rho_\gamma(E=E_i)\rho_\gamma(E'=E_f)} . \quad (7)$$

A strength distribution $P(y)$ of y is then constructed such that $P(y)dy$ is the probability to find the transition strength in an interval dy around y. In Refs. 8 and 11 it was argued that for a classically chaotic system that is time-reversal invariant this distribution should have the Porter-Thomas[12] form

$$P(y)=(2\pi\langle y\rangle)^{-1/2}y^{-1/2}\exp(-y/2\langle y\rangle) . \quad (8)$$

The distribution (8) characterizes a Gaussian orthogonal ensemble of random matrices.[13] An alternative derivation of (9) is based on the maximal entropy procedure.[8]

As the classical system becomes more regular, we expect to see deviations from the Porter-Thomas distribution. In Ref. 8 it was argued that a useful way to describe these deviations quantitatively is through a χ^2 distribution in ν degrees of freedom

$$P_\nu(y)=\left[\frac{\nu}{2\langle y\rangle}\right]^{\nu/2} y^{\nu/2-1}\exp(-\nu y/2\langle y\rangle)/\Gamma(\nu/2) . \quad (9)$$

For $\nu=1$ (9) reduces to a Porter-Thomas distribution (8) while for $\nu\neq 1$ it has a width which is $\nu^{-1/2}$ larger than that of Porter-Thomas with the same $\langle y\rangle$.

To verify our predictions and to study systematically the deviations from (9) we have used a numerical model, the coupled-rotators model.[9] It describes two angular momenta, **L** and **M**, coupled to an external field and among themselves according to $H=L_z+M_z+L_xM_x$. This model has the advantage that for any given values of $\mathbf{L}^2$ and $\mathbf{M}^2$ the space of quantum states is finite and no truncation is needed for its numerical solution. The model has been studied extensively both classically and quantum mechanically.[6] In particular, the regular, chaotic, and mixed domains of the classical Hamiltonian were determined as a function of energy for $L=M$. The numerical calculations presented here were done at $L=M=3.5$, for which the system is chaotic for $|E|<6.6$, regular for $|E|>9.1$, and mixed in between. In the quantum calculations we used $l=m=20$ so that $\hbar=0.17$. As a transition operator we chose $T=L_z+M_z$.

For S_{SC} we have used the empirical smoothing (6). The behavior of $S_\gamma(E,E')/\rho_\gamma(E)\rho_\gamma(E')$ shows an exponential decay versus $|E-E'|$. The smoothing width γ is determined as the minimum one needed to make this decay smooth and monotonic. The distribution of the normalized strength (7) was then calculated for initial and final states in a "block" $E_1<E_i; E_f<E_2$. The calculations were repeated for several values of E_1 and E_2, moving the block gradually from a completely chaotic region (top left of Fig. 1) to the completely regular region (top right of Fig. 1). To each distribution we have fitted a χ^2 distribution (9) by optimizing ν. The fits are shown by the solid lines in Fig. 1. Notice that we are using a logarithmic scale for y due to the large number of small transition strengths. The results show that in the chaotic region the distribution is very nearly Porter-Thomas ($\nu=1$). As the system becomes classically more regular the deviations from Porter-Thomas (dashed lines) are

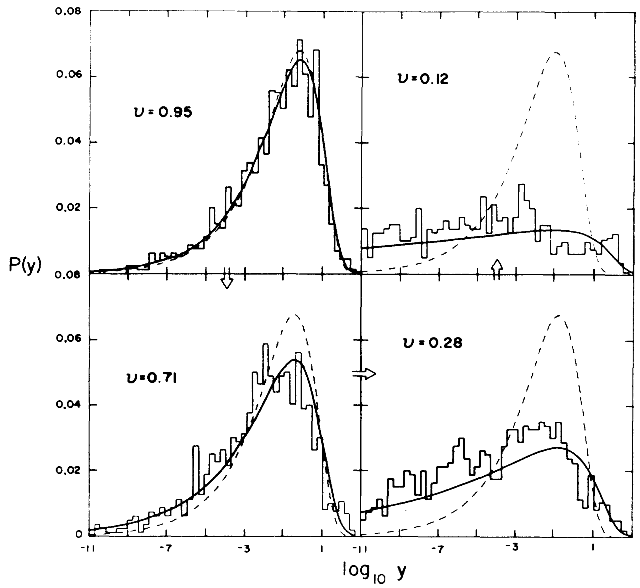

FIG. 1. Four histograms of calculated transition strength distribution for the coupled rotators model with $l=m=20$. The transition strengths were normalized according to (7) with $\gamma\approx 3$. The top left histogram corresponds to a completely chaotic "block" $1.25\leq E_i$, $E_f\leq 2.56$ while the top right is the one obtained from the mostly regular region $6.97\leq E_i$, $E_f\leq 12.11$. The bottom left and bottom right describe intermediate regions $4.05\leq E_i$, $E_f\leq 5.82$ and $5.90\leq E_i$, $E_f\leq 8.62$, respectively. The solid curves show the best fit (9) with the optimal ν. The dashed lines are Porter-Thomas distributions. Note that ν is gradually decreasing from 1 as the system becomes more regular. Each block is 40×40, so that each histogram samples 1600 strengths.

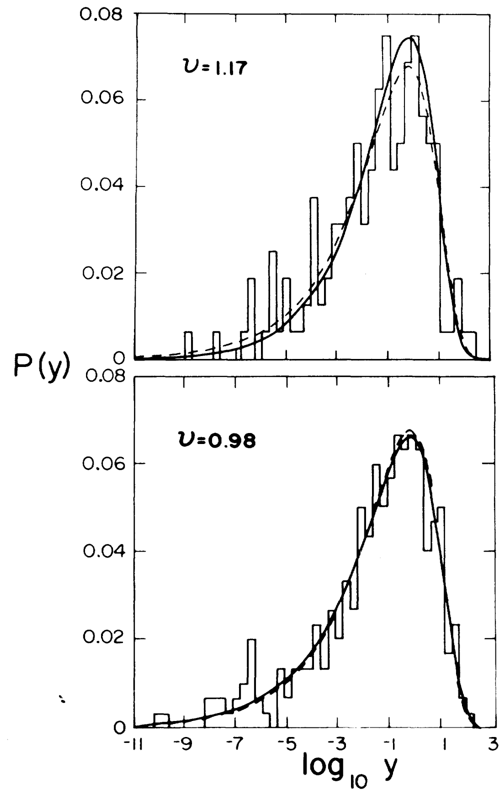

FIG. 2. Top: histogram for transition strengths in a mixed block $0.024\leq E_i\leq 1.21$ (chaotic); $6.97\leq E_f\leq 12.1$ (regular). Bottom: strength histogram for a fixed initial state $E_i=0.34$ and final states in the interval $0\leq E_f\leq 5.3$ (chaotic). Solid and dashed lines are as in Fig. 1.

greater. The general trend is that ν decreases towards zero and that the distribution becomes wider. Indeed, when the system becomes more regular, there is a larger number of small matrix elements and few large ones (due to selection rules) so that the fluctuations around the average are larger.

If either the initial or final states are in the chaotic regime we find that the strength distribution is also a Porter-Thomas distribution. Figure 2 (top) demonstrates that for a strength distribution with E_i in the chaotic region and E_f in the regular region. This implies that the chaotic states are dominant. Moreover, in the analysis of strengths we can take a fixed initial state and sample only over the final states. For final chaotic states the distribution is very nearly Porter-Thomas (see bottom of Fig. 2). Similar results are obtained for the transition operator $T=(L_z+M_z)^2$.

TABLE I. Comparison between numerically determined values of γ and the values γ_s determined from the scaling $\gamma_s\propto\hbar^{-1}$ (for $d=2$, see text). Various values of l correspond to different values of $\hbar$ ($\hbar=L/[l(l+1)]^{1/2}$ with $L=3.5$). We have assumed $\gamma_s=\gamma$ at $l=20$.

	$l=15$	$l=20$	$l=26$	$l=32$
γ	1.7–2	2.5	~ 3	3–4
γ_s	1.9	2.5	3.2	4

To check the scaling of the smoothing width γ with $\hbar$ we have considered other values of $\hbar$ by changing the values of $l=m$ [such that $L^2=\hbar^2 l(l+1)$ remains constant]. The results are summarized in Table I which shows general agreement with $\gamma/D=O(\hbar^{-1})$.

In conclusion, we have observed that signatures of the classical chaos in the associate quantum system can be seen not only in the spectral fluctuations but also in the strength distribution of a generic observable. The "local" fluctuations are well described by a universal distribution, that of Porter and Thomas and the mean behavior is found semiclassically using Eqs. (2)–(5).

It is not clear whether there is a universal distribution also in the regular limit (the analog of the Poisson distribution for the spectral fluctuations). What does seem to be universal is the monotonic decrease of ν from the Porter-Thomas value 1 as the system becomes more regular.

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