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LETTER TO THE EDITOR

Distribution and fluctuation properties of transition probabilities in a system between integrability and chaos

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Abstract. We study the statistical properties of transition probabilities (or generalized intensities, equal to the squared matrix elements of operators having a classical limit). We first generalize the Shnirelman theorem to include semiclassically integrable states and use this to generalize the Feingold–Peres formula for the average value of generalized intensities. We perform an unfolding procedure to separate the smooth mean part of the intensities (as a function of frequency) from its fluctuating part by applying the generalized Feingold–Peres formula. (This formula relates the mean value of squared matrix elements to the power spectrum of the given observable over classical trajectories.) Our approach is illustrated numerically by analysing the dipole transition probabilities in a family of billiards between integrability and chaos as introduced by Robnik. The average values of the intensities as a function of frequency are excellently described by the generalized Feingold–Peres formula, especially in the classically ergodic case where the agreement is excellent. In the ergodic case the fluctuations of intensities are perfectly well described by the Porter–Thomas distribution, whilst in the predominantly regular regime (almost integrable KAM) we find a great abundance of approximate selection rules, some apparent systematics of line series and some strongly enhanced transition probabilities which we believe is typical for such a regime. Our approach is expected to be very useful and practical in the context of nuclear, atomic and molecular physics.

In the development of quantum chaos the major emphasis in the research of stationary problems so far has been in analysing the statistical properties of energy spectra and of eigenfunctions (Berry 1983, Bohigas and Giannoni 1984, Robnik 1985, Eckhardt 1988, Bohigas and Weidenmüller 1988, Gutzwiller 1990, Heller 1991). One of the main results in this field was the discovery that the predictions of random matrix theories (Brody *et al* 1981) also apply to dynamical Hamiltonian systems of few freedoms if the classical dynamics is ergodic (Bohigas *et al* 1984, Berry and Robnik 1986, Robnik and Berry 1986, Robnik 1992, 1993b). In the mixed-type systems with dynamics in the transition region between integrability and chaos the approach of nonlinear dynamics has also been fruitful (Berry and Robnik 1984, Seligman *et al* 1984, Prosen and Robnik 1992, 1993b). However, the expectation values and generally the matrix elements of other reasonable observables (Hermitian operators having a classical limit) have been little studied (Feingold and Peres 1986, Alhassid and Levine 1986, Wilkinson 1987, 1988). One well known result concerns the fluctuation properties of

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generalized intensities (squares of matrix elements) within the framework of random matrix theories, namely the Porter–Thomas distribution (Brody *et al* 1981), which has been experimentally observed and suggested by Porter and Thomas (1956) in the context of nuclear physics. We expect that this fluctuation law also applies in classically ergodic systems with few freedoms. The main motivation of the present work is to explain this and to find the appropriate generalization for Hamiltonian systems in the transition region of mixed dynamics. We will illustrate this numerically for a family of billiards which we have extensively studied recently (Prosen and Robnik 1992, 1993b).

In order to study the fluctuation properties of generalized intensities one must be able to clearly separate the smooth mean part of the intensities as the function of frequency (equal to the energy difference between the final and initial state divided by $\hbar$) from its fluctuating part. So, given the frequency of the intensity we ask what is its mean value and which is the distribution of its fluctuating part in units of the mean value. In the classically ergodic case Feingold and Peres (1986) propose a formula expressing the mean intensities in terms of the power spectrum of the given observable taken over a dense chaotic classical orbit. In deriving this result they rely on the Shnirelman theorem (Shnirelman 1979) expressing the quantum expectation value of a reasonable operator as the classical microcanonical average. This theorem is obvious once one has in mind that the Wigner distributions of the eigenstates of a classically ergodic system in the semiclassical limit are just microcanonical distributions (Berry 1977). In order to rederive the Feingold–Peres formula and to generalize it we first point out that the Shnirelman theorem applies also to the states in the regular and mixed regime if the classical average is taken over the relevant classical invariant ergodic component which supports the corresponding semiclassical eigenstate. This can be an invariant torus, a chaotic component, or the entire energy surface.

Following Feingold and Peres (1986) we start by looking at the following sum over eigenstates k of eigenenergies E_k for the transition elements $A_{jk} = \langle j|\hat{A}|k\rangle$:

$$\sum_k \exp\left(\mathrm{i}(E_j - E_k)t/\hbar\right) |A_{jk}|^2 = \sum_k \langle j|\mathrm{e}^{\mathrm{i}E_j t/\hbar}\hat{A}|k\rangle\langle k|\mathrm{e}^{-\mathrm{i}E_k t/\hbar}\hat{A}|j\rangle$$

$$= \langle j|\mathrm{e}^{\mathrm{i}\hat{H}t/\hbar}\hat{A}\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\hat{A}|j\rangle = \langle j|\hat{A}(t)\hat{A}(0)|j\rangle\,. \tag{1}$$

Now we apply the generalized Shnirelman theorem, stating that in the *semiclassical limit* this is equal to the classical average

$$C_j(t) = \{A(t)A(0)\}_j \tag{2}$$

over the invariant ergodic component labelled by j which supports the semiclassical state $|j\rangle$. Using the ergodicity on the given invariant component this two-point autocorrelation function can be expressed as the time average along a classical dense orbit (dense in the given invariant component which, for example, can be an invariant torus, or a chaotic component, or the entire energy surface)

$$C_j(t) = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} \mathrm{d}\tau A(t+\tau)A(\tau)\,. \tag{3}$$

Next we replace the sum $\sum_k$ by the integral $\int \mathrm{d}E_k \rho(E_k)$, where $\rho(E)$ is the density of states, and perform the Fourier transform and obtain

$$\langle |A_{jk}|^2 \rangle_j = \frac{S_j((E_k - E_j)/\hbar)}{2\pi\hbar\rho(E_k)} \tag{4}$$

where the state j is fixed and the average $\langle\cdot\rangle_j$ is taken over states k within a thin energy shell of thickness of a few mean level spacings. Here

$$S_j(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t C(t) \mathrm{e}^{\mathrm{i}\omega t} = \lim_{T\to\infty} \frac{1}{T} \left| \int_{-T/2}^{T/2} \mathrm{d}t A(t) \mathrm{e}^{\mathrm{i}\omega t} \right|^2 \tag{5}$$

is the power spectrum of a dense orbit in the invariant ergodic component j. If A has a non-vanishing mean value $\{A\}_j$ the $S_j(\omega)$ will have a delta spike at $\omega = 0$, and this can be removed by replacing A in the above formulae by $A - \{A\}_j$. To calculate the actual mean values of the intensities $|A_{jk}|^2$ we also perform in the above formula (on the left-hand side) the averaging over the j states microcanonically over the thin energy shell around E_j of sufficient width such that the corresponding semiclassical states uniformly cover the energy surface, whilst on the right-hand side we correspondingly take the microcanonical average over all initial conditions j on the energy surface E_j. So the final formula for the mean generalized intensities is

$$\langle |A_{jk}|^2 \rangle = \frac{\{S((E_j - E_k)/\hbar)\}_E}{2\pi\hbar\rho(E)} \,. \tag{6}$$

By $\{\cdot\}_E$ we denote the microcanonical average over the energy surface E. The apparent asymmetry in jk of this formula disappears in the semiclassical limit $\hbar \to 0$. In the numerical evaluations described below we applied the above formula with $\{S(\omega)\}_E$ and $\rho(E)$ being calculated on the energy surface placed half way between E_j and E_k, i.e. $E = (E_j + E_k)/2$. This choice is met to minimize the error at finite $\hbar$.

Knowing the average value of intensities as a function of ω we can now separate the smooth part from its fluctuating part by renormalizing the matrix elements as follows:

$$X_{jk} = \frac{A_{jk}}{\sqrt{\langle |A_{jk}|^2 \rangle}} \,. \tag{7}$$

The renormalized matrix elements X_{jk} are now regarded as random variable whose probability distribution is denoted by $D(X)$, which by definition has unit dispersion, and naturally is expected to be an even function of X, $D(X) = D(-X)$, and so it has zero mean. In the classically ergodic case we expect that quite generally the matrix elements of a given operator are very well modelled by the GOE of random matrix theories (Brody *et al* 1981) which predict a Gaussian distribution for $D_{\mathrm{PT}}(X) = \exp(-X^2/2)/\sqrt{2\pi}$, which is equivalent to the so-called Porter–Thomas distribution for the intensities $I = X^2$, namely $P(I) = \exp(-I/2)/\sqrt{2\pi I}$, see Porter and Thomas (1956). In integrable cases one expects a vast abundance of at least approximate selection rules which render most X to become zero, implying that $D(X)$ approaches a delta function $\delta(X)$ in the semiclassical limit. This can be seen by considering the matrix representation of an operator in the basis of the torus-quantized eigenstates of an integrable system, as explained in detail by Prosen and Robnik (1993a). In the mixed-type dynamics (KAM) in the transition region between integrability and chaos we expect a continuous transition from $\delta(X)$ towards $D_{\rm PT}(X)$. More precisely, we have derived a semiclassical formula for $D(X)$ in such a transition region by taking into account the fact that the only broadening of $D(X)$ stems from the transitions between chaotic initial and chaotic final states belonging to the same family of the invariant ergodic components (continuously parametrized by the energy), while all other transitions are almost forbidden. This work in progress rests upon a more detailed analysis of higher autocorrelation functions and will be reported on in a separate paper (Prosen 1992).

We illustrate the above theoretical considerations in the numerical study of a 2D billiard system with analytic boundaries covering the range between integrability and chaos, namely the quadratic conformal image $w(z) = z + \lambda z^2$ of the unit disk $|z| \leqslant 1$, which has been introduced by Robnik (1983, 1984) and has been extensively studied recently by Prosen and Robnik (1992, 1993b). At $\lambda = 0$ we have the integrable case of a circular billiard, whilst for λ between 0.25 and 0.5 we observe numerically almost ergodicity, in the sense that the tiny islands of stability predicted by Hayli *et al* (1987) have negligible area on the SOS. Our object of study are the dipole matrix elements for transitions between the eigenstates of even parity with respect to the reflection symmetry. In order to have a uniform covering of the transition region we have chosen the parameter values $\lambda = 0.1, 0.15, 0.2$ and 0.375. The relative fraction of volume of the regular regions covered by the invariant tori on the energy surface are 0.88, 0.36, 0.05 and 0.00, respectively. We considered all transitions between the even eigenstates of sequential number between 2001 and 2400, which offers 80 000 matrix elements—a number sufficiently large to warrant high-quality statistics.

In figure 1(*a*)–(*d*) we plot the intensities (squared matrix elements) as functions of frequency measured in units of the mean level spacing divided by $\hbar$, for the above mentioned values of λ. The obvious common feature is the fact that the transitions are effectively limited to a relatively narrow frequency range within which the intensities are significant, while outside this frequency range the transitions are virtually forbidden. In the ergodic case (figure 1(*a*)) the fluctuations around the smooth average value are quite random, but as we approach the integrable case (the volume of the regular component on the energy surface increases) the presence of regular–regular transitions becomes more and more obvious. Its signature is manifested in a small number of very large intensities which are typically organized as a systematical line series clearly visible in the diagrams (figure 1(*b*)–(*d*). Of course, such systematics is a consequence of a well defined geometry of families of classical invariant tori, which support the semiclassical regular states between which the transitions take place. This behaviour is predicted to be generic for the systems in the transition region.

It is now most interesting to calculate the average values of the intensities versus the frequency (by binning the lines of figure 1(*a*)–(*d*) into small frequency intervals and averaging over them) and to compare this quantum results with the semiclassical prediction of the generalized Feingold–Peres formula (6). This is shown in figure 2(*a*)–(*d*) for the corresponding values of λ. We plot the quantum curve (thick curve) and the ± 1 sigma band around the expected theoretical value. The agreement is really

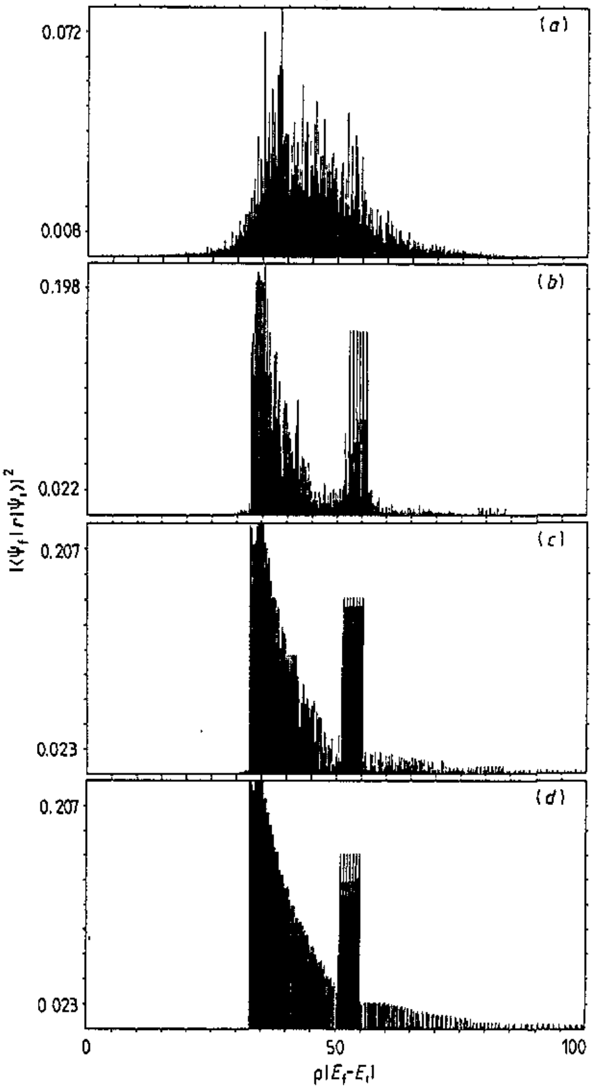

Figure 1. The transition probabilities (squared dipole matrix elements) are plotted against the frequency of the photon in units of the mean level spacing divided by $\hbar$, for the four values of the parameter $\lambda = 0.375$ (a), 0.2 (b), 0.15 (c) and 0.1 (d). The range of the ordinate values and its units are adapted to the maximal value, which in (a) is about three times smaller than in (b)–(d).

excellent in view of the fact that the two curves cover the range of several orders of magnitude (4 in 2(a) through 8 in 2(d)). It is readily seen that the fluctuations in the form of delta spikes increase with the approach towards integrability—a consequence of the increasing fraction of the energy surface volume occupied by the invariant tori on which the motion is quasiperiodic having a discrete spectrum.

Using the above information on the smoothed average values of intensities versus the frequency we can now calculate the fluctuation distribution $D(X)$ for the chosen values of λ. The results are shown in figure 3(a)–(d). In the classically ergodic case of $\lambda = 0.375$ we see that the Porter–Thomas distribution $D_{\mathrm{PT}}(X)$ (Gaussian) is perfectly well confirmed (figure 3(a)). With increasing fraction of the regular component we see the gradual emergence of the central delta spike due to the increasing fraction of almost forbidden regular–regular transitions (figure 3(a)–(d)).

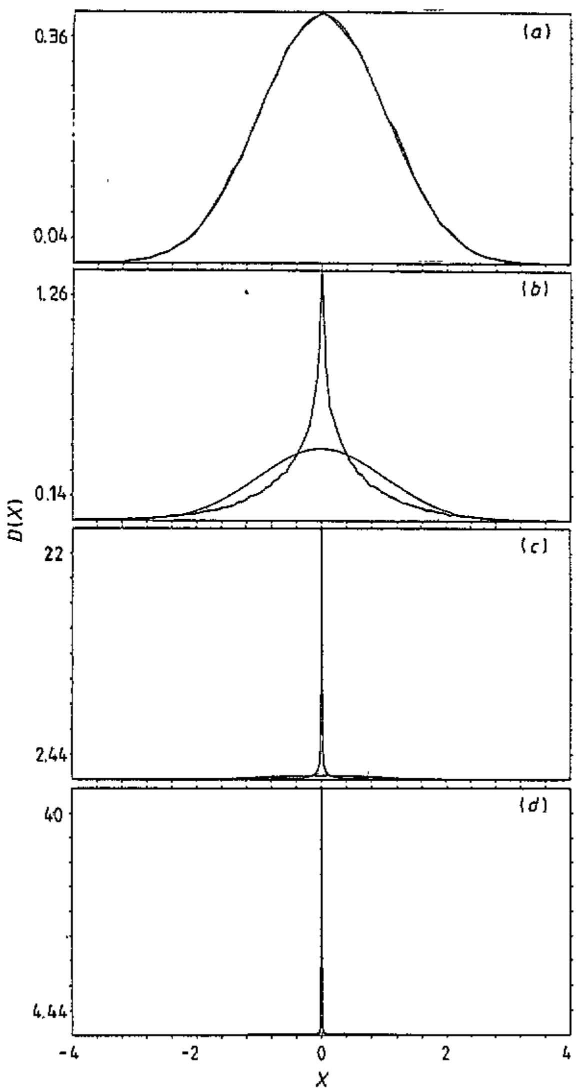

Figure 2. The logarithm of the average values of the intensities versus the frequency in units of the mean level spacing divided by $\hbar$ (thick curve) compared with the ± 1 sigma band (thin curve) around the expected theoretical semiclassical value according to (6) for $\lambda = 0.375$ (*a*), 0.2 (*b*), 0.15 (*c*) and 0.1 (*d*). The range of the ordinate values and its units are adapted to the maximal and the minimal value. The discrepancy at small values of ω (*c*)–(*d*) is a consequence of the finite time evaluation of the power spectra, namely the integration time T in (5) is equal to about 14 times the break time $T_{\mathrm{BREAK}} = 2\pi\hbar\rho(E)$.

This circumstance is also well manifested in the increasing value of the kurtosis $K = \langle (X - \langle X \rangle)^4 \rangle / \langle (X - \langle X \rangle)^2 \rangle^2 - 3$, which has the following values: −0.03, 6.7, 42 and 99 for the chosen four values of λ equal to 0.375, 0.2, 0.15 and 0.1, respectively. It is useful to check also whether the dispersion $\sigma^2 = \langle (X - \langle X \rangle)^2 \rangle$ is sufficiently close to its theoretical value of unity; in fact we find σ equal to 0.999, 1.005, 1.034 and 1.038, respectively. Let us also quote the numerical values for the average (which ideally should be zero), $\langle X \rangle$: −0.003, −0.008, −0.006 and 0.002, respectively.

In conclusion we summarize that in the present work we offer a generalized Feingold–Peres approach (based on a generalized Shnirelman theorem) to predict the smooth average dependence of generalized intensities on the frequency in any system between integrability and ergodicity. This is used to define the (unfolded) fluctuation

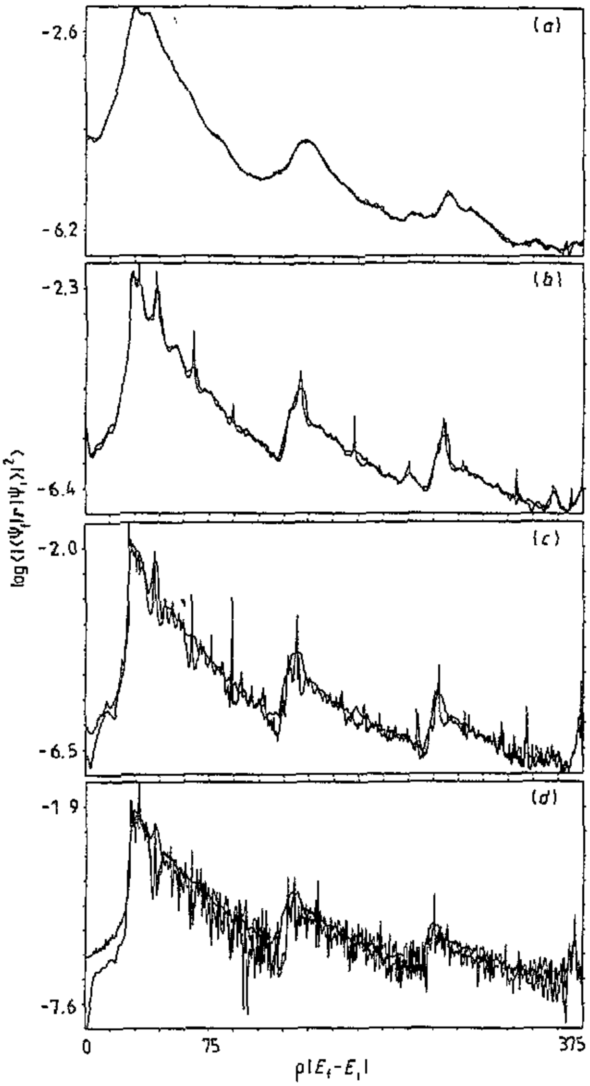

Figure 3. The probability density $D(X)$ for the fluctuations of the matrix elements for $\lambda = 0.375$ (*a*), 0.2 (*b*), 0.15 (*c*) and 0.1 (*d*). For comparison we plot also the Gaussian distribution with the same mean (which should vanish ideally) and with the same dispersion (which after the unfolding should ideally be unity) as the numerically calculated distribution. In (*a*) corresponding to the classically ergodic case we see that $D(X)$ is perfectly well fitted by the Gaussian which confirms the validity of the Porter–Thomas law.

distribution of the matrix elements $D(X)$ which turns out to be universal in classically ergodic Hamiltonian systems and is given by the Gaussian distribution with zero mean and unit dispersion $D_{\mathrm{PT}}(X)$ which is equivalent to the well known Porter–Thomas distribution for the fluctuating intensities. We have numerically demonstrated the surprising accuracy of these theoretical predictions by investigating the dipole matrix elements in a generic family of 2D billiards. Further theoretical work in progress is devoted to a systematic study of higher moments $\langle|A_{jk}|^{2m}\rangle$ and higher correlations and a more complete understanding of the semiclassical description of systems in the transition region (Prosen 1992). Needless to say, our approach is expected to be very useful and practical in the context of nuclear, atomic and molecular physics (Bohigas and Weidenmüller 1988).

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