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Transition-Strength Fluctuations and the Onset of Chaotic Motion

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The maximum-entropy formalism is used to characterize the fluctuations in transition strengths for a bound quantum-mechanical system. In the chaotic limit only one, ever present, sum rule is required as a constraint. The resulting distribution is that of Porter and Thomas, which can also be derived from random-matrix theory. For nonchaotic systems the distribution of transition strengths has a lower entropy. A possible additional constraint, operative during the onset of chaos, is proposed. The distribution of maximal entropy subject to both constraints accords with computed intensities in a system of two degrees of freedom.

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The onset of chaos in nonintegrable conservative classical systems of few degrees of freedom is by now well characterized.[1] Recently[2,3] there has been considerable interest in determining whether the corresponding quantum systems carry a signature of the classical chaos. Much of this effort has concentrated on the features of the energy spectrum, both eigenstates[4] and eigenvalues, and especially on the energy-level–spacing distribution.[5-8] The conclusion was that as the classical motion was changing from regular to chaotic, the nearest-neighbor level-spacing distribution was changing from a Poisson[9] to a Wigner[8,10,11] distribution. It was further suggested[5,6] that the chaotic system has the statistics derived for the Gaussian orthogonal ensemble (GOE) of random matrices.[12-14] It is well known that the GOE provides a realistic description of the statistical properties of complex heavy nuclei with a large number of degrees of freedom.[12] More incisive tests, however, are required before such a description is adopted for systems with a few degrees of freedom in the chaotic regime.

This Letter examines the signature of classical chaos in the fluctuations of the transition strengths in the corresponding quantum system. In the extreme chaotic limit we expect to obtain a Porter-Thomas[15] distribution. This distribution is known to describe successfully the resonance-width distribution of complex nuclei[12,13] and can be derived from the GOE *Ansatz*. This *Ansatz* refers, however, to an ensemble of Hamiltonians while the system under study has a single, well-defined Hamiltonian. We therefore present an alternative derivation of the Porter-Thomas distribution which avoids the use of an ensemble of Hamiltonians. The derivation offers the further advantage that the procedure we use is not restricted to the chaotic limit. Indeed, we shall suggest one possible extension. The general procedure that we propose is to maximize the entropy of the strength distribution. The Porter-Thomas distribution is obtained when the only constraint that is imposed during the maximization is an ever-present sum rule on the total strength of the transition. Additional constraints, if warranted, lead to other distributions, which necessarily have lower entropy. As an example we derive a χ^2 distribution with ν degrees of freedom ($\nu=1$ for a Porter-Thomas distribution) for a system that is not fully chaotic.

The analytical results are examined for a concrete model: a system with two degrees of freedom with a bounded, Hénon-Heiles–type potential.[16] The transitions we consider can be thought of as optical transitions (in the Condon approximation) to an electronically excited state of the same system but with a different equilibrium position.[17-19] This physical motivation is important because the experience with regular spectra would suggest that such spectra are very structured with definite propensity rules. Indeed, it is only for the subset of higher-lying final states that we find evidence for chaotic behavior.

The transition strength for a quantum system of a given Hamiltonian and a particular probe[20] (operator) T is defined by

$$y = |\langle f | T | i \rangle|^2 = |x|^2. \tag{1}$$

Here $|i\rangle$ is a fixed initial eigenstate and $|f\rangle$ is any final eigenstate. The magnitude of y will differ for different final states and, hence, one can construct the density function, $P(y)$, of y such that $P(y)\,dy$ is the probability to locate the transition strength in the interval dy around y. Of course, the bound quantum system has discrete eigenstates so that the continuous density function $P(y)$ is an idealization and, in practice, the distribution of y is obtained as a histogram on the y axis. It is important to note that such a histogram makes no reference to the energy of the final state f. The aspect that we are examining is fluctuations in the magnitude of y. This is a different manifestation of the nature of the spectrum than the nature of the intensity variations as the energy of the final state is being systematically increased. In fact, as will be explicitly noted below, we remove the secular variations in the intensity prior to the construction of $P(y)$ for our model system.

The strength function is constrained by the completeness condition in the eigenstates to satisfy the following sum rule:

$$\textstyle\sum_f |\langle f | T | i \rangle|^2 = \langle i | T^\dagger T | i \rangle. \tag{2}$$

For a Hamiltonian that is time-reversal invariant the eigenstates can be chosen to be real. If T is also time-reversal invariant then the amplitude $x = \langle f | T | i \rangle$ is real and the sum rule (2) can be written as

$$\int_{-\infty}^{\infty} x^2 P(x)\,dx = (1/N)\langle i | T^\dagger T | i \rangle, \tag{3}$$

where N is the total number of quantum states. The amplitude density $P(x)$ is related to $P(y)$ as usual, $\sum P(x)\,dx = P(y)\,dy$, where the summation is over the two values of x such that $y = x^2$. In rewriting (2) as (3) we have grouped the transition strengths into bins according to their size and thus replaced the summation over final states by summation (i.e., integration) over the bins.

The sum rule (3) imposes a given value for $\langle x^2 \rangle$. We take it that when the quantum system is fully chaotic, its states are so complicated and devoid of any individual characteristics[21] that no other constraint except the sum rule (3) is carried by the strength function.[22] The distribution can then be found by maximizing its entropy[23]

$$S[P] = -\int_{-\infty}^{\infty} dx\, P(x) \ln P(x), \tag{4}$$

subject to the constraint (3) and to normalization of $P(x)$. It follows by the usual procedure[24] that $P(x)$ is given by

$$P(x) = (2\pi\langle x^2 \rangle)^{-1/2} \exp(-x^2/2\langle x^2 \rangle). \tag{5}$$

The entropy of this distribution is $\frac{1}{2}\ln(2\pi e\langle x^2 \rangle)$. In terms of the intensity, $y = x^2$, we have

$$P(y) = (2\pi\langle y \rangle)^{-1/2} y^{-1/2} \exp(-y/2\langle y \rangle), \tag{6}$$

which is the Porter-Thomas distribution or, in statistical terms, a χ^2 distribution with one degree of freedom.

The usual derivation of (6) in the present context is via random-matrix theory.[14] In that derivation, the collection of different final states $|f\rangle$ of a particular Hamiltonian is assumed to be represented by the nth eigenstate (n fixed), but for a GOE of different Hamiltonians. If $|\alpha\rangle$ is a fixed normalized vector then the distribution (in the ensemble) of the amplitude $x \equiv \langle n | \alpha \rangle$ is[12]

$$[\Gamma(N/2)/\pi^{1/2}\Gamma((N-1)/2)](1-x^2)^{(N-3)/2} \underset{N\ \text{large}}{\longrightarrow} (N/2\pi)^{1/2}\exp(-Nx^2/2), \tag{7}$$

where N is the dimension of the Hilbert space. If we choose for the normalized fixed state $|\alpha\rangle = T|i\rangle/\langle i | T^\dagger T | i \rangle$ the distribution (7) reduces to (6). The derivation of (6) by maximal entropy therefore has the advantage of being more directly related to the typical physical situation in which the Hamiltonian is known. A second advantage, which we shall now make use of, is that the derivation can be extended to those situations which are not fully chaotic and, hence, additional constraints are required. The sum rule (3) is, of course, valid irrespective of the character of the classical motion. It is therefore always imposed. Say now that we impose additional constraints, but at the same value for $\langle x^2 \rangle$. Whatever these additional constraints are, the procedure of maximal entropy will predict a strength distribution whose entropy (4) is lower than or equal to that of the (Porter-Thomas) distribution (6).

Why would one expect additional constraints for an intermediate situation? One obvious reason is that for a system which is more regular we expect that propensity rules for the transition-matrix elements become operative. A simple *Ansatz* for such additional constraints is thus the averaged magnitude of the deviance of the intensity y from its averaged value, $\langle y \rangle = \langle i | T^\dagger T | i \rangle / N$. This suggests a constraint on this deviance,

$$I = -\int_0^{\infty} dy\, P(y) \ln(y/\langle y \rangle). \tag{8}$$

Subject to a given value of $\langle y \rangle$ and of the averaged value I of the surprisal, the distribution whose entropy is maximal is

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

Here $(\nu-1)/2$ is the Lagrange multiplier conjugate to the constraint (8). The distribution (9) is normalized and satisfies the sum rule (3). The value of ν is determined from the magnitude of I. By use of the explicit form (9) in (8) the required relation is $I=\ln(\nu/2)-\psi(\nu/2)$, where $\psi(x)$ is the digamma function. Generally $I>0$ and increases as ν decreases.

The distribution (9) is a χ^2 distribution with ν degrees of freedom. Its width is given by $(2/\nu)^{1/2}\langle y\rangle$ and is thus decreasing as ν increases. It should be emphasized, however, that we do not necessarily expect (9) to describe the strength distribution for intermediate situations. Rather, we use it to illustrate the deviation from the limiting case of the Porter-Thomas distribution, parametrized in a manner which allows a simple control of the width.

In analysis of experimental or computational data it is first necessary to factor our the secular variation of the strength along the energy spectrum. For a pure initial state, the strength function at the final energy E is defined by

$$\langle y\rangle(E)=\frac{\sum_f|\langle f|T|i\rangle^2\delta(E-E_f)}{\sum_f\delta(E-E_f)}. \tag{10}$$

That, however, is the proper form only for a very long time resolution.[18] In practice, the δ function in (10) must be taken as a Gaussian with a finite width. The width chosen should be such that one obtains a smooth variation of $\langle y\rangle(E)$ with energy. The scaling of y by $\langle y\rangle(E)$ has been carried out for the results shown in Fig. 1.

To illustrate our argument we use a two dimensional system with a bound Hénon-Heiles–type potential,[16]

$$V(X,Y)=\tfrac{1}{2}(X^2+Y^2)+\varepsilon(X^2Y-Y^3/3)+C(X^2+Y^2)^2.$$

This potential has a C_{3v} symmetry. The eigenstates were found numerically by diagonalization of the Hamiltonian in a harmonic-oscillator basis and classified according to A or E symmetry.[16] Transition strengths to eigenstates of the same potential (but with equilibrium points in X and Y shifted by α and β, respectively), and of a given symmetry, were computed. For any given initial state, the distribution of transition strengths was determined separately for the two groups of final states with energies below and above E_c (the energy at which classical chaos sets in[16]), respectively. The derivation of (6) assumes real matrix elements. For final states of E symmetry we have either considered separately the real and imaginary parts of $\langle f|T|i\rangle$ or considered that $\nu=2$ in the chaotic limit.[24] Figure 1 shows typical results for complex am-

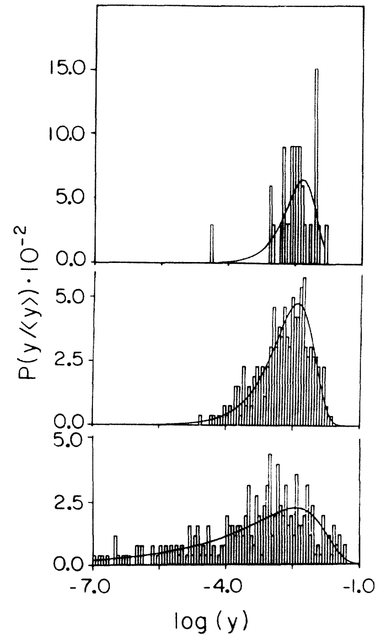

FIG. 1. Three histograms of computed transition strengths and their fits (continuous curves) by (9). Note that ν decreases towards 2 (the Porter-Thomas value for complex amplitude[24]) as the corresponding classical system becomes more chaotic ($\nu=4.4$, 3.6, and 2.5 going from top to bottom). Computations are for $\alpha=\beta=0.5$ with intensities scaled by the secular variation with energy prior to binning. The plot is vs log$y$ because even after scaling the intensities span a wide dynamic range.

plitudes. When the initial state lies above E_c and so do the final states, the computed distribution is well fitted by (9) with $\nu\simeq 2.5$. For an initial state with an energy just above E_c and final states with energy above E_c, the fit by (9) is still reasonable but with $\nu\simeq 3.6$. With an initial state above and final states below E_c, the fit is not quite acceptable and $\nu\simeq 4.4$. For initial and final states both below E_c, i.e., in the regular regime, there are many small matrix elements and $P(y)$ is strongly increasing as $y\rightarrow 0$. This behavior is reproduced by the distribution (9) when $\nu<1$ (if we assume real matrix elements). It falls off as x increases from zero faster than a Gaussian; cf. (5), which has the same width $\langle x^2\rangle$. That effect is best seen for initial and final states of comparable energy.[19] It should be noted, however, that the strength in the regular regime usually has more structure than what (9) can describe.

In closing, we note that the chaotic limit as used here is similar in its information-theoretic characterization to the equilibrium limit of macroscopic physics: It is the limiting situation where entropy is maximal, subject only to the ever-present constraints. Deviations from that limit can then be accounted for by use of additional constraints. Work is in progress on relating these constraints to the nature of the system and of the probe.

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[22]If there are rigorous constraints of the motion which are conserved by T (e.g., discrete symmetries) then, of course, the discussion applies within a subspace of final states with given values of these constraints.

[23]That it is the entropy of $P(x)$ [rather than, say, that of $P(y)$] that is relevant follows also from the requirement that the entropy be invariant under a proper orthogonal transformation of the states.

[24]This conclusion depends on $\langle x^2\rangle$ being about the same for the real and imaginary parts. Otherwise there will be an effective value of ν as discussed in Ref. 13.