Onset of Chaos and Its Signature in the Spectral Autocorrelation Function

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The signature of chaos in the spectral autocorrelation function and in its Fourier transform, the survival probability, is shown to be in good agreement with the predictions of random matrix theory. An expression is proposed for the survival probability of an experimentally prepared nonstationary state when the dynamics are intermediate between chaotic and regular. Its validity is tested through the study of a model Hamiltonian. Two parameters can be extracted from the above observable, one which characterizes the level statistics and one which characterizes the distribution of transition intensities.

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The signatures of classical chaos in associated quantum systems are of great current interest [1–4]. Commonly used signatures are the various level statistics; for a chaotic system they are derived from random matrix theory (RMT) [5,6], while for a regular spectrum they are generally Poisson. Another signature is the transition intensities distribution [7,8]. From an experimental point of view the problem with such measures of quantal chaos is that they require an accurate knowledge of a complete set of energy levels and/or transition intensities. Because of finite resolution and background noise one might fail to separate adjacent levels and miss weak transitions. It is therefore highly desirable to have a quantity which can be directly extracted from the observed spectrum and which is less sensitive to finite resolution. The Fourier transform of the experimental spectrum has been suggested as such a quantity [9,10]. A related observable is the spectral autocorrelation function [11]. Its Fourier transform may be interpreted as a survival probability [10,12] of a certain nonstationary state. Recent studies [13,14] of the survival probability averaged over random initial states showed a distinct [14] difference between chaotic and regular systems. Analytic expressions were derived for the survival probability in the chaotic limit by using random matrix theory either directly [15] or in the framework of a scattering model [16]. An important qualitative feature is the existence of a correlation hole [9] where the probability decreases below its asymptotic value at intermediate times. We will show that the theoretical result for the survival probability can be generalized to situations where the dynamics are intermediate between regular and chaotic. Two features are observed as the dynamics become more regular, the time over which the hole is visible decreases, and the asymptotic value of the probability increases. The validity of the theoretical result is tested through a numerical study of a model Hamiltonian. The survival probability associated with the actual spectrum depends on the joint distribution of energy eigenvalues and eigenvectors. We are therefore able to extract two parameters from this survival probability; one which characterizes the level statistics and one which characterizes the intensity distribution. They are shown to be well correlated with measures of classical chaos.

The normalized strength function $S(\omega)$ (spectrum) of a transition operator T is given by

$$S(\omega)=\sum_n p_n\delta(\omega-\omega_n)\,, \tag{1}$$

where

$$p_n=|\langle n|T|i\rangle|^2/\langle i|T^\dagger T|i\rangle\,. \tag{2}$$

$|n\rangle$ are the eigenstates with frequencies ω_n and $|i\rangle$ is an initial (fixed) eigenstate (e.g., the ground state). If, for example, one measures the absorption spectrum of laser light on a molecule, then T is the dipole operator of the molecule. The spectral autocorrelation function $G(\omega)$ is obtained by [11]

$$G(\omega)=\int_{-\infty}^{\infty}S(\omega')S(\omega+\omega')d\omega'\,. \tag{3}$$

The Fourier transform of the spectrum $S(\omega)$ is the amplitude

$$C(t)=\langle\phi(0)|\phi(t)\rangle\,, \tag{4}$$

where the initial normalized nonstationary state $\phi(0)$ is $\phi(0)\propto T|i\rangle$. It then follows that the Fourier transform of the power spectrum (3) is the survival probability $P(t)\equiv|C(t)|^2$ of the initially prepared state $\phi(0)$. For a general nonstationary state $\phi(0)=\sum_n a_n|n\rangle$ (a_n is real assuming time-reversal symmetry) we have

$$P(t)=\sum_n p_n^2+\sum_{n\neq m}p_np_me^{i(\omega_n-\omega_m)t}\,, \tag{5}$$

where $p_n=a_n^2$. Before discussing the survival probability associated with the experimental spectrum, we calculate an average survival probability for an initial state that is randomly distributed [13,14] over the unit sphere $\sum a_n^2=1$. We have

$$P_{\rm av}(t)=\frac{3}{N+2}\left[1+\frac{1}{3N}\sum_{n\neq m}e^{i(\omega_n-\omega_m)t}\right]\,, \tag{6}$$

where N is the number of eigenstates. Note that $P_{\rm av}(t)$ depends on the energy eigenvalues alone. Using random matrix theory one can further evaluate the ensemble average [9,15,16]

$$\langle P_{av}(t)\rangle = \frac{3}{N+2}\left\{1+\frac{1}{3}\Delta_N * [\delta(\tau)-b_{2\beta}(\tau)]\right\}, \quad (7)$$

where $\tau = t/2\pi\langle\rho\rangle$ ($\langle\rho\rangle$ is the average level density) and $\beta=1,2,4$ for the Gaussian orthogonal, unitary, and symplectic ensembles, respectively. $b_{2\beta}(t)$ is the two-level form factor [5,18] which is the Fourier transform of the two-point cluster function $Y_{2\beta}(\omega)$. The asterisk denotes a convolution $\Delta_N * f(t) \equiv \int dt' \Delta_N(t') f(t-t')$ and $\Delta_N(t) = N^{-1}[\sin(\pi N t)/\pi t]^2$. The convolution with Δ_N appears because the number of levels N is finite. In the limit $N\to\infty$, $\Delta_N(t)\to\delta(t)$ and the result of Ref. [15] is recovered. A chaotic system with time-reversal symmetry is characterized by a Gaussian orthogonal ensemble (GOE) level statistics so that $\langle P_{av}(t)\rangle$ should be given by Eq. (7) with $\beta=1$. The δ function in (7) describes the rapid dephasing of the initial state at the short time scale $t\sim 2\pi/ND$ (D being the average level spacing). This short time behavior is dominated by classical dynamics [19] and is not universal. The other part of (7) characterizes the long time behavior $t\sim 2\pi/D$. As a result of this term, $\langle P_{av}(t)\rangle$ drops below its asymptotic value and saturation occurs for $T\gg 2\pi/D$.

What is the corresponding expression for $P_{av}(t)$ when the dynamics are intermediate between chaotic and regular? In such a case only a fraction of the classical phase space is chaotic. Following Ref. [20] we assume that a corresponding fraction β of the quantum levels obeys the GOE statistics while a fraction $1-\beta$ is Poisson. Using the rule [21] for calculating b_2 of a superposition of spectra with different statistics and that for an M level Poisson spectrum $b_2(t)=M^{-1}\delta(t)$, we find

$$b_{2\beta}(t)=\beta b_2(t/\beta)+[(1-\beta)/N]\delta(t), \quad (8)$$

where b_2 on the right-hand side is the GOE one. Equation (7) with $b_{2\beta}$ ($0\le\beta\le 1$) given by (8) provides an expression for $P_{av}(t)$ where the dynamics is intermediate between chaotic and regular.

To test the above predictions we studied a nuclear model, known as the interacting boson model [22], whose classical and quantal chaotic properties were recently investigated [17,23]. The solid lines in Fig. 1 show the calculated average survival probability for three cases: chaotic, intermediate, and regular dynamics. It is important to remark that since the predictions of RMT assume a constant $\langle\rho\rangle$, the initial state $\phi(0)$ should be chosen on a subspace spanned by N eigenstates in a narrow energy window. We chose $N=10$ and to obtain better statistics we averaged over all successive groups of ten levels between the 20th and 200th levels of spin $J=10$. According to (7) the relevant time scale is determined by the average level density $\langle\rho\rangle$. Since $\langle\rho\rangle$ is different for each group of levels, it is important to scale t by $\langle\rho\rangle$ before the group average is done, if a quantitative agreement with the prediction of RMT is desired.

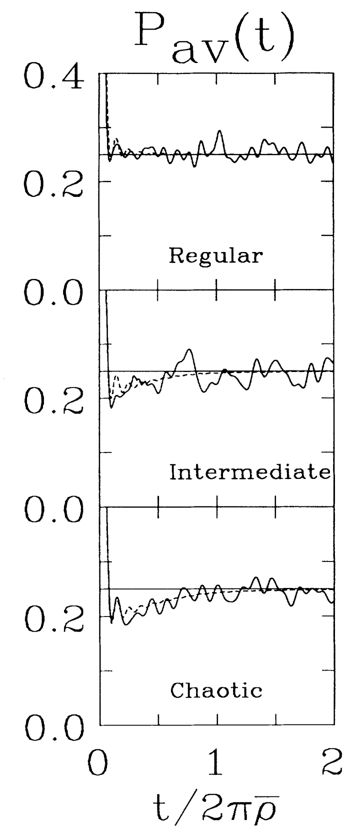

FIG. 1. The survival probability $P_{av}(t)$ averaged over random initial states with $N=10$ levels. The solid lines are $P_{av}(t)$ calculated for the spin $J=10$ levels of a nuclear model Hamiltonian [17] with parameters χ,η. Shown are regular ($\chi=-1.1$, $\eta=0.3$), intermediate ($\chi=-0.9$, $\eta=0.3$), and chaotic ($\chi=-0.65$, $\eta=0$) cases. The dashed lines are $\langle P_{av}(t)\rangle$ of Eq. (7) [and (8)] with $\beta=\sigma$. We have (from top to bottom, respectively) $\beta=0.24$, 0.80, and 0.96. The horizontal lines correspond to the asymptotic value of $P_{av}(t)$.

In each of the cases in Fig. 1 we studied also the classical limit and calculated the fraction σ of phase space which is chaotic. We find $\sigma=0.24$, 0.80, and 0.96 (top to bottom, respectively). The respective values of the Kolmogorov entropy are 0.007, 0.09, and 0.24. According to the definition of the parameter β, one would expect to have $\beta\approx\sigma$ (e.g., the fraction of levels which are GOE-like should be equal to the fraction of phase space which is chaotic). The dashed lines in Fig. 1 are the theoretical prediction [Eqs. (7) and (8)] with $\beta=\sigma$. A least-squares fit to (7) with a single parameter β gives similar values for β. In judging the quality of the fit in Fig. 1 we remark that the observed fluctuations of the calculated $P_{av}(t)$ around its theoretical average [Eq. (7)] are consistent with the theoretical variance of $P_{av}(t)$ estimated from the random matrix ensemble. The combined effect of the initial dephasing [described by the $\Delta_N * \delta(t)$ term in (7)] and the form factor b_2 is to generate a correlation hole [9] in the chaotic case. The most important effect observed as the system makes a transition between the chaotic and regular limits is that the width of the correlation hole shrinks. This effect is nicely described by Eq. (8), where saturation is predicted to occur at $t/2\pi\langle\rho\rangle \sim \beta$.

We now return to the experimental spectrum (1) and (2). The relevant survival probability is that of the experimentally prepared state $\phi(0) \propto T|i\rangle$ and not of a random initial state. Random matrix theory was used in Ref. [15] to calculate the ensemble average $\langle P(t)\rangle$ for a given $\phi(0)$. For that purpose the joint distribution of eigenvalues and eigenstates is required. Since the joint distribution factorizes (in RMT) we get

$$\langle P(t)\rangle = N\langle p_n^2\rangle[1 + (\langle p_n p_m\rangle/\langle p_n^2\rangle)(N-1)e^{\langle i(\omega_n-\omega_m)t\rangle}]\,, \tag{9}$$

where n,m ($n \neq m$) are any two eigenstates. Equation (9) differs from Eq. (6) only by the ensemble averages of $p_n p_m$ and p_n^2. While in (6) we assumed *a priori* a random initial state (i.e., a_n real and uniformly distributed on the sphere), in (9) we calculate the ensemble averages from the appropriate RMT. For the three Gaussian ensembles ($\beta = 1,2,4,$) these averages were calculated in Ref. [15] using the underlying eigenvector distribution. In these ensembles β plays the role of the number of degrees of freedom, where each amplitude a_n is composed of β real components. More generally, for ν degrees of freedom one finds the following distributions:

$$P(p_n) \propto p_n^{\nu/2-1}(1-p_n)^{\nu(N-1)/2-1}\,,$$
$$P(p_n,p_m) \propto (p_n p_m)^{\nu/2-1}(1-p_n-p_m)^{\nu(N-2)/2-1}\,. \tag{10}$$

Using the distributions (10) it is straightforward to show that [24]

$$\langle p_n p_m\rangle/\langle p_n^2\rangle = \nu/(\nu+2); \quad N\langle p_n^2\rangle = (\nu+2)/(N\nu+2)\,. \tag{11}$$

An intermediate situation between chaos and regular dynamics is characterized by $0 < \nu < 1$. Indeed in the limit of large N the distribution $P(p_n)$ in (10) becomes the χ^2 distribution in ν degrees of freedom [7]. The latter was shown [8] to characterize transition intensity distributions whose corresponding ν decreases from 1 towards 0, as a chaotic system becomes more regular. Using (11) the survival probability is then

$$\langle P(t)\rangle = \frac{\nu+2}{\nu N+2}\left\{1 + \frac{\nu}{\nu+2}\Delta_N * \left[\left[\left(1-\frac{1-\beta}{N}\right)\delta(t) - \beta b_2(t/\beta)\right]\right]\right\}. \tag{12}$$

For the random ensembles ($\beta = 1,2,4$), $\nu = \beta$ and Eq. (12) reduces to the result of Ref. [15]. However, for intermediate statistics where $\nu,\beta < 1$ we may have $\nu \neq \beta$. The result (12) is similar but different in detail from the phenomenological estimate of Ref. [10]. The main difference emerges from the role played by the fluctuations in p_n. We also note that the survival probability in Ref. [14] is equivalent to the case $\nu = 2$, since the amplitudes a_n in the initial random state were assumed to be complex.

To test the predictions of (12) we used the nuclear model mentioned above where the transition operator that prepares the initial state is taken to be the electric quadrupole $E2$ operator [17]. We studied the same three causes as in Fig. 1. For a fixed state $|i\rangle$, the states $|n\rangle$ in (1) are chosen in groups of $N = 10$ states (as before), and in each group the sum of the intensities is normalized to one. To improve the statistics we have repeated the above calculation for various initial states $|i\rangle$. The $E2$ intensity distributions are shown in Fig. 2 and are fitted by the distribution $P(p)$ in Eq. (10) with the quoted ν. We

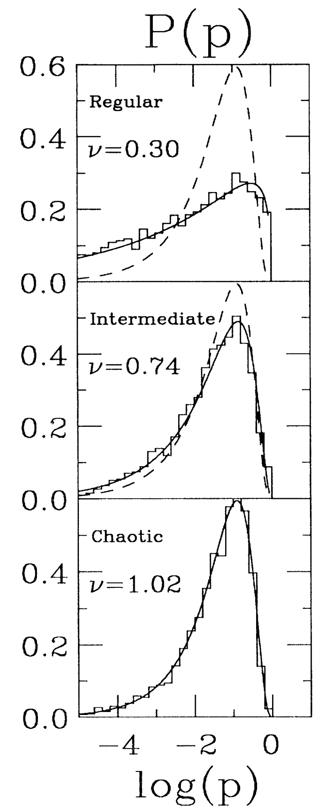

FIG. 2. The distribution (histograms) of the intensities p in Eq. (2) with T chosen to be the electric quadrupole operator [17]. The intensities are normalized within groups of $N = 10$ levels. The three cases shown correspond to the same Hamiltonians as in Fig. 1. The solid lines are the fit to the distribution $P(p)$ in Eq. (10) with the quoted ν, and the dashed lines are the GOE limit $\nu = 1$.

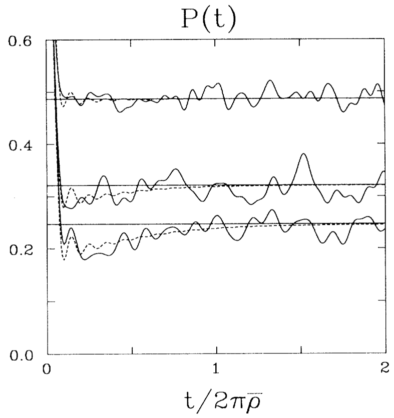

FIG. 3. The survival probability $P(t)$ of an experimentally prepared state $\phi(0)\propto T|i\rangle$. The three cases shown correspond to the same Hamiltonians as in Fig. 1 (from top to bottom: regular, intermediate, and chaotic), and T is the electric quadrupole operator of the model. The dashed lines are $\langle P(t)\rangle$ of Eq. (12) with $\beta=\sigma$ and ν determined by Eqs. (11). We have $\beta=0.24$, $\nu=0.27$ (regular); $\beta=0.80$, $\nu=0.61$ (intermediate), and $\beta=0.96$, $\nu=1.02$ (chaotic). The horizontal lines correspond to the asymptotic value of $\langle P(t)\rangle[(\nu+2)/(N\nu+2)]$.

see that ν is strongly correlated with the measure σ of classical chaos, as is also confirmed in detailed studies of the model [17]. Figure 3 shows $P(t)$ for these cases (solid lines). The dashed lines are the theoretical curves, Eq. (12), with $\beta=\sigma$ and ν determined from Eqs. (11). The values of ν agree with the ones obtained in Fig. 2. A two-parameter fit (β,ν) to Eq. (12) yields similar values for β and ν. $\langle P(t)\rangle$ is still characterized by a correlation hole which saturates at $t/2\pi\langle\rho\rangle\sim\beta$ as did $\langle P_{\rm av}(t)\rangle$. However, two new features arise: (i) The asymptotic value of $\langle P(t)\rangle$, shown by the horizontal lines in Fig. 3 and given by $(\nu+2)/(\nu N+2)$, increases as the system becomes more regular (and ν gets smaller). A similar asymptotic behavior of a related quantity is also discussed in Ref. [25]. (ii) The function $b_{2\beta}(t)$ is multiplied by the factor $\nu/(\nu+2)$ which gets smaller as the system becomes more regular.

In an experimental situation a stick spectrum should be replaced by Lorentzians with typical width Γ due to the finite resolution. The result (12) should then be multiplied by an envelope [16] which for $\Gamma=$const is $\exp(-\Gamma t)$. Thus, as long as $\Gamma\lesssim D$, the exponential decay of $P(t)$ will not mask the effects seen in Fig. 3. A similar conclusion was obtained in Ref. [26].

In conclusion, we have demonstrated that the signatures of the transition from regular to chaotic dynamics are observed in the survival probability of an experimentally prepared nonstationary state. Two parameters (β and ν) characterizing the level and intensity statistics, respectively, can be extracted from such a quantity and are found to be well correlated with classical measures of chaos. The advantage of this observable is that it is less sensitive to finite resolution problems and it can be evaluated directly from the measured spectrum.

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