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Reliability of Small Matrices for Large Spectra with Nonuniversal Fluctuations

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We study the change of quantum spectra under two types of perturbations. One of them corresponds to the breaking of classical integrability and amounts to a crossover from level clustering to level repulsion. The second type of perturbation breaks time-reversal invariance; under conditions of classical chaos the degree of level repulsion then grows from linear to quadratic. To characterize the spectral changes we propose, for each type of transition, a distribution of nearest-neighbor spacings. Both of these "generalized Wigner surmises" are rigorous for suitable ensembles of 2×2 matrices but prove reliable for dynamical systems with many levels.

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For several decades now fluctuations in the energy spectra of atomic nuclei have been characterized by the distributions of nearest-neighbor spacings. Typically, those distributions are closely approximated by a simple function which was proposed by Wigner [1] and which has come to be called Wigner's surmise. It is now understood that Wigner's original proposition applies not only to nuclear spectra but also to a whole universality class of dynamical systems. That class, referred to as "orthogonal," is characterized by Hamiltonians which (i) generate globally chaotic motion in the classical limit and (ii) are time-reversal invariant. Two other quantum-mechanical universality classes are associated with global classical chaos [2], the "unitary" and the "symplectic" ones. Wigner's surmise for the orthogonal class has been extended to the other two classes. The three probability densities read

$$P_{\mathrm{O}}(S)=(\pi S/2)\exp(-S^2\pi/4),\ \text{orthogonal}, \tag{1a}$$

$$P_{\mathrm{U}}(S)=(32S^2/\pi^2)\exp(-S^2 4/\pi),\ \text{unitary}, \tag{1b}$$

$$P_{\mathrm{S}}(S)=(2^{18}S^4/3^6\pi^3)\exp(-S^2 64/9\pi),\ \text{symplectic}. \tag{1c}$$

Here, as well as in all other spacing distributions below, the energy scale is chosen such that the mean spacing is unity. Because of the small-S behavior, $P(S)\sim S^\beta$, one speaks of linear, quadratic, and quartic level repulsion in the orthogonal, unitary, and symplectic cases, respectively.

The Wigner surmise in its three forms (1a)–(1c) is a rigorous result for the Gaussian orthogonal, unitary, and symplectic ensembles (GOE, GUE, and GSE) of Hermitian 2×2 matrices [1,2]. Their success for dynamical systems is amazing in two respects. First, Hamiltonians of dynamical systems for the most part do not appear to be random; in fact, the equivalence of spectral fluctuations for random and "nonrandom" Hamiltonians has been understood only recently [2–4]. Second, the number N of discrete levels of a given spectrum must be large for the spacing distribution to assume a reasonably smooth form, while Eqs. (1) are based on random matrices with $N=2$. The spacing distributions for the Gaussian ensembles of $N\times N$ matrices can be worked out for arbitrary N [2,4,5]. One finds that $P(S)$ for the Gaussian ensembles depends only weakly on the dimension N.

A fourth universality class we need to mention here comprises classically integrable systems with two or more degrees of freedom [2,6]. In that case levels do not repel but rather cluster so as to give rise to an exponential distribution of nearest-neighbor spacings, $P(S)=e^{-S}$. In that respect the levels behave like the uncorrelated events of a Poissonian random process.

We shall here be concerned with Hamiltonians "in between" universality classes,

$$H(\lambda)=\sqrt{f(\lambda)}(H_0+\lambda V),\ \ f=1/(1+\lambda^2), \tag{2}$$

where H_0 and V belong to different classes [7]. For instance, H_0 might be time-reversal invariant but V not so restricted. As the coupling constant λ increases from zero to infinity the Hamiltonian (1) executes a continuous transition from one class to another. The path through matrix space followed by $H(\lambda)$ given by (2) may be called deterministic since for a fixed pair of "initial" and "final" matrices H_0 and V, the interpolating matrix $H(\lambda)$ is uniquely determined for any value of λ. However, as we have shown in a previous paper [7], a certain bundle of such deterministic paths is equivalent to a certain other bundle of Brownian-motion paths. The latter bundle constitutes Dyson's Brownian-motion model [8]. From our point of view, that model arises when a family of Hamiltonians (2) is defined by the matrix density [7]

$$P(H,\lambda)=\langle\delta(H-\sqrt{f}(H_0+\lambda V))\rangle . \tag{3}$$

Here the average $\langle\cdots\rangle$ is over both H_0 and V with weights $P_0(H_0)$ and $P_\infty(V)$ chosen as the initial and final densities for the transition in consideration.

We shall first treat the transition GOE$\rightarrow$GUE. In that case the averages in (3) can be carried out and yield a Gaussian form for $P_{\mathrm{O}\rightarrow\mathrm{U}}(H,\lambda)$. A lot is known about the interpolating density $P_{\mathrm{O}\rightarrow\mathrm{U}}(H,\lambda)$ from the work of Pandey and Mehta [9]. Unfortunately, however, no explicit form is available for the spacing distribution $P_{\mathrm{O}\rightarrow\mathrm{U}}(S,\lambda)$ for large N. It is only for $N=2$ that a closed form of the interpolating spacing distribution can be worked out,

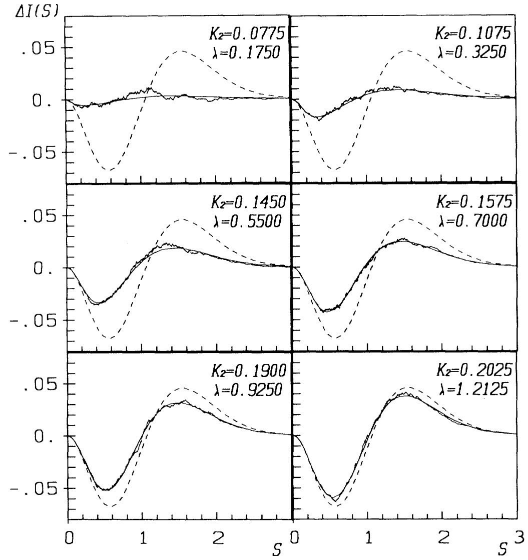

FIG. 1. Gradual breaking of time-reversal invariance for a succession of values of the symmetry-breaking parameter K_2 or λ. The curves describe spacing distributions through the function $\Delta I(S)$ defined in the text. [Rugged curve: kicked top according to (5); smooth: optimal generalized Wigner surmise (4); dashed: completely broken symmetry according to (1b).]

$$P_{\mathrm{O}\rightarrow\mathrm{U}}(S,\lambda)=[\tfrac{1}{2}(2+\lambda^2)]^{1/2}D(\lambda)^2 S e^{-S^2D(\lambda)^2/2}\,\mathrm{erf}[SD(\lambda)/\lambda]\,,$$
$$D(\lambda)=\left(\frac{\pi(2+\lambda^2)}{4}\right)^{1/2}\left\{1-\frac{2}{\pi}\left[\arctan\left(\frac{\lambda}{\sqrt{2}}\right)-\frac{\sqrt{2}\lambda}{2+\lambda^2}\right]\right\}. \tag{4}$$

As it must, this distribution interpolates between (1a) for $\lambda=0$ and (1b) for $\lambda\rightarrow\infty$.

The derivation of (4) is an elementary task since for $N=2$ the density (3) depends on H through only four real variables. Two of the latter may be chosen as the spacing and the sum of the eigenvalues of H; the remaining two as the angles defining the unitary transformation which diagonalizes H. By integrating out the last three variables we arrive at (4).

As already pointed out above, the limiting forms of the interpolating density (4) at $\lambda=0$ and $\lambda\rightarrow\infty$ give excellent approximations to the spacing distributions for "large" ($N\gg1$) energy spectra of autonomous dynamical systems of the appropriate symmetries. We should add that the distribution of quasienergy spacings of periodically driven systems are similarly well represented by those limiting cases of (4). One would hope that our $P_{\mathrm{O}\rightarrow\mathrm{U}}(S,\lambda)$ also works for the (quasi) energy spectra of dynamical systems with partially broken time-reversal invariance, provided the value of λ is properly adjusted.

The hope just expressed is indeed born out by an investigation of the kicked top with the Floquet operator [2]

$$F=e^{ipJ_z}e^{iK_1J_x^2/2j}e^{iK_2J_y^2/2j}. \tag{5}$$

Here the $J_{x,y,z}$ are angular momentum operators, made dimensionless by referral to Planck's constant $\hbar$ as a unit; p, K_1, and K_2 are dimensionless coupling constants. The stroboscopic motion generated by this Floquet operator conserves the squared angular momentum, $(\mathbf{J})^2=j(j+1)$, where the quantum number j may take on integer or half-integer values. For fixed j, the Floquet operator F may be represented as a $(2j+1)\times(2j+1)$ matrix. In the classical limit, attained for $j\rightarrow\infty$, the motion is globally chaotic if at least two of the three coupling constants take on values of order unity. As long as one coupling constant vanishes the kicked top has a time-reversal invariance, $[T,F]=0$, and (for integer j) F then is a member of the circular orthogonal ensemble (COE) [2]. As the third coupling constant is switched on, time-reversal invariance is broken and F crosses over into the circular unitary ensemble (CUE).

Figure 1 describes the gradual breaking of time-reversal invariance for the kicked top. The series of graphs refers to a sequence of values of K_2 while K_1 and p are kept fixed ($p=1.642$, $K_1\approx14.5$). Each rugged curve represents a spacing distribution for the quasienergies of F with $j=700$. For the sake of convenience we have plotted $\Delta I(S)=\int_0^S dS'\Delta P(S')$, where $\Delta P(S)$ is the difference of the numerically obtained spacing distribution of the top and Wigner's surmise (1a). The smooth curve close to each rugged one also depicts such a difference $\Delta I(S)$, with the spacing distribution of the top replaced by the optimal interpolating distribution (4); optimized is the value of λ, by minimizing the integrated rms deviation between the rugged $\Delta I(S)$ and the one based on (4) and (1a). Figure 2 displays the optimal integrated rms deviation just mentioned as a function of the coupling constant K_2, as the full curve with the label GWS−Top. That curve is meant to show that the generalized Wigner surmise (4) remains as good an approximation to the data for the top throughout the transition as it is for the limiting cases (1a) and (1b) at, respectively, $K_2=0$ and K_2 large. Figure 3, finally, shows that the optimal value of λ is related to the coupling constant K_2 as $\lambda \sim K_2^2$; the slope of the curve is consistent with $\lambda/K_2^2 \sim N^{3/2} \sim j^{3/2}$. This relation between λ, K_2, and N is not fully understood right now. It is important to realize, though, that the K_2 scale on which the symmetry breaking becomes manifest is $\sim N^{-3/4}$, i.e., very small for large N.

Of great interest are transitions from level clustering to level repulsion, where the spacing distribution changes from the exponential e^{-S} to the form characteristic of, say, the GOE. Several interpolating distributions have been proposed [10], and we shall now add one more. Ours will be based on a certain ensemble of random 2×2 matrices. We again start from Hamiltonians of the structure (2) and proceed to the family (3). The final matrix density $P_\infty(V)$ is now taken from the GOE of 2×2 matrices while for the initial one we assume the "Poissonian" density of real symmetric 2×2 matrices

$$P_{\rm P}(H)=\{({\rm tr}H)^2-4\det H\}^{-1/2}e^{-({\rm tr}H)^2}\times\exp\{-[({\rm tr}H)^2-4\det H]^{-1/2}\}. \qquad (6)$$

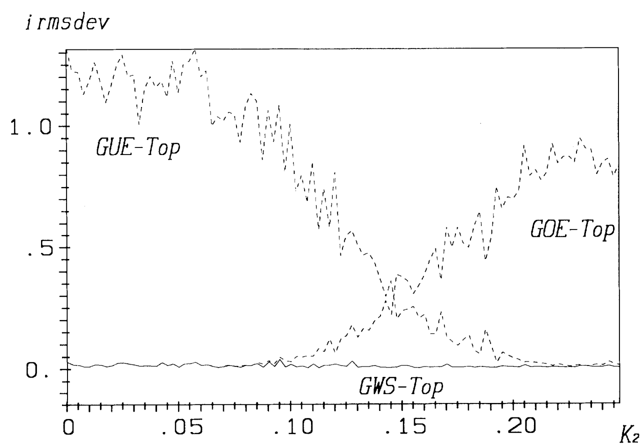

FIG. 2. Integrated rms deviations between the level staircases of the kicked top and the optimal generalized Wigner surmise (4) (labeled GWS−Top), plotted against the symmetry-breaking parameter K_2. For reference, the analogous deviations between the top and the GOE and the GUE are also shown.

The latter ensemble is easily seen to imply an exponential distribution of the spacing between the two eigenvalues. Again, the averages in (3) can be done explicitly. The resulting matrix density now depends on H through three real variables, H_{11}, H_{22}, and H_{12}. By a suitable double integral we arrive at the spacing distribution, which can be expressed in terms of the Bessel function $I_0(x)$ and the Kummer function $U(a,b,x)$ as

$$P_{\rm P\to O}(S,\lambda)=\{Su(\lambda)^2/\lambda\}\exp\{-u(\lambda)^2S^2/4\lambda^2\}\times\int_0^\infty d\xi\, e^{-\xi^2-2\xi\lambda}I_0(\xi Su(\lambda)/\lambda), \qquad (7)$$

$$u(\lambda)=\sqrt{\pi}U(-\tfrac{1}{2},0,\lambda^2).$$

Of course, $\lambda=0$ pertains to the exponential e^{-S} while the Wigner surmise (1a) is approached for sufficiently large values of λ. For all intermediate values of λ we encounter linear repulsion, $P(S,\lambda)\sim S$, at small S; the slope decreases monotonically as λ grows.

We have tested the reliability of our proposition (7) for large matrices by diagonalizing random matrices of the form (2) with various values of N and λ. The matrices V were drawn from the GOE with $\langle V_{ij}^2\rangle=1/4N$. A Poissonian ensemble was realized by choosing diagonal matrices H_0 with independent diagonal elements drawn from a Gaussian distribution with $\langle H_{0ii}\rangle=0$, $\langle H_{0ii}^2\rangle=1$. In order to compare the data with the interpolating spacing distribution (7) we have used only the central parts (width $\Delta E\approx0.5$ around $E=0$) of the numerically determined spectra. The latter precaution proved necessary since fluctuations in different parts of the spectrum undergo the transition from level clustering to level repulsion with different speeds [11]; that inhomogeneity of the matrix ensemble in consideration is least pronounced near $E=0$, where the level density depends most weakly on E. To further reduce the effect of such inhomogeneities on $P(S)$ we have unfolded the spectra to unit mean spacing throughout the range ΔE. In order to obtain smooth

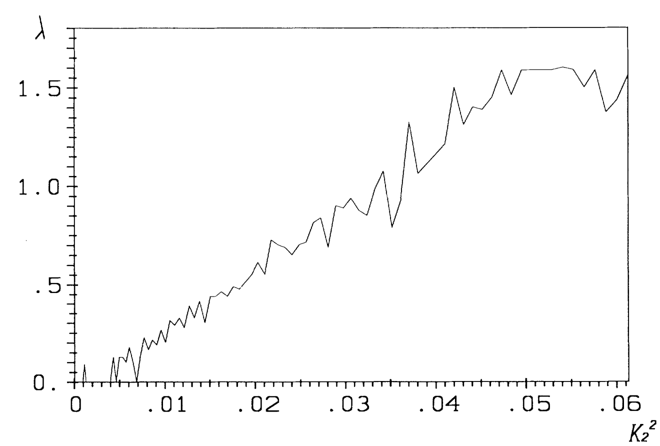

FIG. 3. Relation between the symmetry-breaking parameters K_2 and λ.

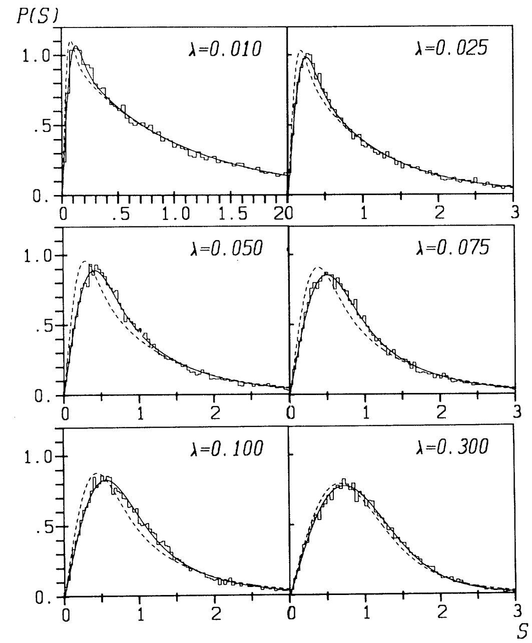

FIG. 4. Nearest-neighbor spacing distributions for the transition from a Poissonian ensemble to the GOE. [Histograms: from central parts of spectra of random matrices; full smooth curves: our proposition (7); dashed curves: data from the wings of the spectra where the transition proceeds more slowly.]

spacing histograms we have collected 15000 levels within the range ΔE for each value of λ. With all these precautions taken, we have found the numerically determined spacing distributions to be faithful to our proposition (7) to an amazing degree of accuracy, throughout the transition. Figure 4 illustrates our findings for $N=500$.

Unfortunately, we have nothing much to say about *why* the spacing distributions of large spectra *should* be so well represented by the spacing distributions of ensembles of 2×2 matrices, within as well as in between universality classes. The power law $P(S)\sim S^{\beta}$ for the GOE, COE, GUE, CUE, GSE, and CSE (circular symplectic ensemble) can in fact be obtained from symmetry arguments and nearly degenerate perturbation theory, i.e., by considering close encounters of pairs of levels [2,3]. The Gaussian falloff of $P(S)$ at $S\gg 1$ for the GOE, GUE, and GSE may be looked upon as a trivial consequence of the assumed Gaussian nature of the respective matrix densities. Given these behaviors for $S\ll 1$ and $S\gg 1$ one appreciates the weak N dependence of the spacing distribution as not counterintuitive, at least for the three classic Gaussian ensembles. As for the quasienergy spectra with $N\gg 1$ of Floquet operators from the three classic circular ensembles one may argue as follows. The N quasienergies can be visualized as the positions of particles on a circular ring. Imagine a nearest-neighbor spacing S much larger than a mean spacing. Any further increase ΔS will then be resisted by a force $\sim\Delta S$, due to the pressure of the remaining $N-2$ particles; the linear (in ΔS or S) force entails a quadratic potential and thus a Gaussian distribution of S. Incidentally, no such pressure arises for classically integrable systems, since for these the quantum levels tend to be independent from one another, i.e., have no repulsive interaction.

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