Exact Distribution of Eigenvalue Curvatures of Chaotic Quantum Systems

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The parametric sensitivity of complex quantum systems is characterized by the distribution of eigenvalue curvatures k, defined as the second derivative of the eigenvalues with respect to a perturbation parameter. For systems without time-reversal symmetry (unitary ensemble), the *exact* distribution is found to be $P(k) = (2/\pi)[1 + k^2]^{-2}$. This proves a recent conjecture by Zakrzewski and Delande [Phys. Rev. E **47**, 1650 (1993)].

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Statistical properties of eigenvalue spectra of complex quantum systems frequently exhibit universal behavior which depends only on the fundamental symmetries of the Hamiltonian [1]. A large variety of systems can be described by three universality classes: Time-reversal invariant systems belong to the orthogonal ensemble, systems without time-reversal symmetry to the unitary ensemble, and time-reversal invariant systems with strong spin-orbit coupling fall into the symplectic ensemble. While the statistical theory of spectra (random-matrix theory) was originally developed in the context of nuclear physics [2], it has now become clear that it has a much wider range of applicability, including systems such as molecules [3], disordered metals [4–6], strongly correlated electrons [7,8], and systems whose classical analogs are chaotic [9]. Universal spectral correlations described by random-matrix theory have become the hallmark of quantum chaos.

In many physical circumstances, the energy levels are studied as a function of an external parameter λ such as an electric or magnetic field. Recently, it has been established that the parametric motion of eigenvalues also exhibits universality [10–13]. Szafer and Altshuler [10] studied the motion of eigenvalues E_n of a disordered metallic ring threaded by an Aharonov-Bohm flux φ and found that the correlations between the "single-level currents" $dE_n/d\varphi$ at different flux values are universal. Subsequently, Beenakker [12] derived the same correlator from random-matrix theory, and Simons *et al.* [13] found a fascinating relation between the parametric motion of eigenvalues and the imaginary-time evolution of interacting fermions in one dimension.

An important quantity in characterizing the parametric motion of eigenvalues is the distribution of level curvatures

$$K_n = \frac{d^2E_n(\lambda)}{d\lambda^2}. \tag{1}$$

Typically, the curvature becomes large close to avoided level crossings. Hence, one expects that the curvature distribution $P(K)$ for large curvatures K reflects the simple behavior of the spacing distribution $P(S)$ for small eigenvalue spacings S, where $P(S) \sim S^\beta$ with $\beta = 1, 2, 4$ for the orthogonal, unitary, and symplectic ensembles, respectively [1]. Indeed, Gaspard *et al.* [14] developed the statistical mechanics corresponding to the "equations of motion" of the eigenvalues (Pechukas gas [15]) and predicted that the curvature distribution has the universal form $P(K) \sim K^{-(2+\beta)}$ for large K. Subsequently, this prediction was verified numerically for a number of systems including chaotic billiards [16], the kicked top [17], the diamagnetic hydrogen atom [18], and the Anderson model for disordered metals [19]. While the curvature distribution had so far resisted a complete analytical solution except for 2×2 matrices [18,20], Zakrzewski and Delande [18] found that numerical results for the orthogonal, unitary, and symplectic kicked tops are well described for all curvatures by the distributions

$$P(k) = C_\beta[1 + k^2]^{-(2+\beta)/2}, \tag{2}$$

where C_β is the normalization constant and k denotes the dimensionless curvature

$$k = \frac{K}{\beta\pi\langle\rho(0)\rangle\,\langle(dE_n/d\lambda)^2\rangle}. \tag{3}$$

Within their numerical accuracy the distribution (2) appears exact for the unitary ensemble, while small deviations are visible for the orthogonal and symplectic ensembles. It is the purpose of this paper to prove that this is indeed the exact distribution for the Gaussian unitary ensemble (GUE).

Level dynamics in general and the curvature distribution in particular can be studied directly in experiments on the diamagnetic hydrogen atom [21] and in microwave experiments [22]. Also, various thermodynamic effects in mesoscopic systems such as persistent currents [23] and the magnetic susceptibility [24,25] are closely related to the parametric motion of eigenvalues. Another application of the level curvatures in mesoscopic systems concerns the Thouless energy of diffusive systems which has sometimes been defined as the root-mean-square curvature of the levels as function of an Aharonov-Bohm flux [26,27]. The distribution (2) implies that this definition is problematic because the second moment of $P(K)$ diverges in the orthogonal ensemble [19].

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In his semiclassical theory of spectral correlations Berry [28] has shown that while long trajectories give rise to generic behavior, nonuniversal behavior appears due to short trajectories. In particular, short periodic orbits lead to nonuniversal contributions to the density of states and to scarring of the wave functions [29]. Numerical studies for various systems showed that the curvature distribution is more sensitive to nonuniversal features than other spectral statistics such as the spacing distribution [16,18]. For this reason, it has been suggested [18] that the curvature distribution can be employed as a sensitive measure of the degree of scarring of a system. However, to identify nonuniversal features unambiguously, the exact generic distribution needs to be known. In the following, the curvature distribution is computed *exactly* for the unitary ensemble.

Within random-matrix theory the problem can be formulated in terms of a one-parameter family of Hamiltonians

$$H(\lambda) = (\cos\lambda)H_1 + (\sin\lambda)H_2 \tag{4}$$

with eigenvalues $E_n(\lambda)$. Here H_1 and H_2 are both random $N\times N$ matrices with probability distribution

$$P_N(H_1,H_2) \sim \exp\{-\tfrac{1}{2}N\mathrm{tr}(H_1^2+H_2^2)\}. \tag{5}$$

For the GUE considered here, the measure is $dH_1dH_2 = \prod_{i,j}(dH_1)_{ij}(dH_2)_{ij}$. In the limit $N\to\infty$, the average density of states $\rho(E) = \langle \mathrm{tr}\,\delta(E-H(\lambda))\rangle_{H_1,H_2}$ is given by the well-known semicircle law $\rho(E) = (N/\pi)[1-(E/2)^2]^{1/2}$. Hence, with these definitions the width of the spectrum is of order N^0, while the typical level spacing is of order $1/N$. Furthermore, it turns out that the curvature distribution becomes independent of λ and hence, only the case $\lambda=0$ is considered in the following. An *exact* expression for the eigenvalue curvatures follows from second-order perturbation theory,

$$K_n = -E_n(0) + 2\sum_{m\neq n}\frac{|(H_2)_{n,m}|^2}{E_n(0)-E_m(0)}, \tag{6}$$

where $(H_2)_{n,m}$ denotes the matrix elements of H_2 in the basis in which H_1 is diagonal. From now on, the argument of $E_n(0)$ will be suppressed and it is understood that the E_n denote the eigenvalues of H_1.

The curvature distribution is defined by

$$P(K) = \frac{1}{\rho(0)}\left\langle\sum_{n=1}^{N}\delta(E_n)\,\delta(K-K_n)\right\rangle_{H_1,H_2}, \tag{7}$$

where the brackets denote the average with the distribution function (5). Spectral statistics become universal only if density-of-states effects are eliminated. Numerically, this is usually achieved by unfolding the spectrum. Here the analogous procedure is to consider only levels at a fixed location within the semicircle spectrum. This is the origin of the first δ function in (7). The prefactor in (7) ensures that the curvature distribution is properly normalized. Using the Fourier representation of the second δ function in (7), the average over H_2 can be performed. One obtains

$$P(K) = \frac{1}{\rho(0)}\sum_{n=1}^{N}\int_{-\infty}^{\infty}\frac{d\alpha}{2\pi}e^{iK\alpha} \times\left\langle\delta(E_n)\prod_{m\neq n}\frac{iNE_m/2}{\alpha+iNE_m/2}\right\rangle_{H_1}. \tag{8}$$

The integral over α can be done by contour integration [30],

$$P(K) = \frac{N}{\rho(0)}\frac{N}{2}(N-1)\left\langle\delta(E_1)[\theta(K)\theta(-E_2)+\theta(-K)\theta(E_2)]|E_2|e^{NKE_2/2}\prod_{m=3}^{N}\frac{E_m}{E_m-E_2}\right\rangle_{H_1}. \tag{9}$$

Here, $\theta(x)$ denotes the unit-step function, and it was used that the average over H_1 is symmetric under relabeling of the eigenenergies E_n [cf. Eq. (10) below]. Since Eq. (9) depends only on the eigenvalues of H_1, the average can be performed using the well-known joint eigenvalue distribution of the GUE [1],

$$P_N(\{E_n\}) = C_{\beta=2,N}\prod_{i<j}(E_i-E_j)^2\exp\left\{-\frac{1}{2}N\sum_{j=1}^{N}E_j^2\right\}. \tag{10}$$

The constant $C_{\beta=2,N}$ is defined by the normalization condition $\int dE_1\cdots dE_N P_N(\{E_n\}) = 1$. While it appears to be a formidable task to do the integrals over the E_i directly, progress can be made by considering the integrals over E_1 and E_2 in Eq. (9) separately and rewriting the remaining integrals as an average over an $(N-2)$-dimensional random-matrix ensemble. One finds

$$P(K) = A_N\int_0^\infty dE_2\,E_2^3\exp\{-\tfrac{1}{2}[N(N-2)]^{1/2}|K|E_2-\tfrac{1}{2}(N-2)E_2^2\}\langle[\det H]^3\det(H-E_2)\rangle_H^{(N-2)}. \tag{11}$$

Here, the prefactor is

$$A_N = \frac{N}{\rho(0)}\frac{N}{2}(N-1)\frac{C_{\beta=2,N}}{C_{\beta=2,(N-2)}}\left(\frac{N-2}{N}\right)^{\frac{1}{2}N^2+3}, \tag{12}$$

and H now denotes a random $(N-2)\times(N-2)$ matrix as indicated by the superscript $(N-2)$ on the average.

The average over the determinants can be computed after representing them in terms of integrals over anticommuting (Grassmann) variables [31],

$$\langle[\det H]^3\det(H-E_2)\rangle_H^{(N)} = \int\prod_{\sigma=1}^{4} d\bar{\xi}_\sigma d\xi_\sigma \left\langle \exp\left[-\sum_{\sigma,\sigma'}\bar{\xi}_\sigma(H\delta_{\sigma,\sigma'}-E_{\sigma,\sigma'})\xi_{\sigma'}\right]\right\rangle_H^{(N)}. \tag{13}$$

Here, ξ_σ denotes an N-dimensional vector whose entries $\xi_{i,\sigma}$ are Grassmann numbers and the measure is $d\bar{\xi}_\sigma d\xi_\sigma = \prod_{i=1}^{N} d\bar{\xi}_{i,\sigma}d\xi_{i,\sigma}$. E denotes the diagonal matrix $E=\mathrm{diag}[0,0,0,E_2]$. Performing the average over H, one obtains

$$\langle[\det H]^3\det(H-E_2)\rangle_H^{(N)} = \int\prod_{\sigma=1}^{4} d\bar{\xi}_\sigma d\xi_\sigma \exp\left\{\sum_{\sigma,\sigma'}\left[\bar{\xi}_\sigma E_{\sigma,\sigma'}\xi_{\sigma'} - (1/2N)(\bar{\xi}_\sigma\xi_{\sigma'})(\bar{\xi}_{\sigma'}\xi_\sigma)\right]\right\}. \tag{14}$$

The quartic term in the exponent is decoupled by a Hubbard-Stratonovich transformation which introduces an integration over a Hermitian 4×4 matrix μ. Finally performing the Gaussian integral over the Grassmann variables one finds the integral representation

$$\langle[\det H]^3\det(H-E_2)\rangle_H^{(N)} = \left(\frac{N}{2\pi}\right)^8\int d\mu\exp\left\{-\frac{1}{2}N\mathrm{tr}\mu^2 + N\mathrm{tr}\ln(E+i\mu)\right\}. \tag{15}$$

Here, $d\mu=\prod_{i,j=1}^{4}d\mu_{ij}$. It is convenient to change variables to the eigenvalues and eigenvectors of μ by writing $\mu=T\Lambda T^\dagger$, where $\Lambda=\mathrm{diag}[\lambda_1,\lambda_2,\lambda_3,\lambda_4]$ contains the eigenvalues λ_j of μ, and T denotes the SU(4) matrix which diagonalizes μ. The corresponding Jacobian is

$$d\mu = \frac{2\pi^6}{9}dm(T)\prod_{i=1}^{4}d\lambda_i\prod_{i<j}(\lambda_i-\lambda_j)^2, \tag{16}$$

where $dm(T)$ denotes the invariant measure of SU(4) [the group volume is normalized to $\int dm(T)=1$].

So far, the calculation is exact for any N. In the following, the limit $N\to\infty$ is taken, so that the integral (15) can be computed by the saddle-point method. Further simplifications arise in this limit because the curvature K is $\mathcal{O}(N^0)$. Hence, the leading contribution to the E_2 integral in (11) comes from the region $E_2=\mathcal{O}(1/N)$. First, this implies that one can neglect the term quadratic in E_2 in the exponent of Eq. (11). Second, the action in (15) may be expanded to first order in E. Then the saddle-point equation becomes $\Lambda=\Lambda^{-1}$, independent of E and T. One finds that the dominant saddle points are $\Lambda_0=\mathrm{diag}[+1,+1,-1,-1]$ and its permutations. Performing the saddle-point integration over Λ gives

$$\langle[\det H]^3\det(H-E)\rangle_H^{(N)} = \frac{4N^4}{3}e^{-2N}\int dm(T)\exp\{-iN\mathrm{tr}[T\Lambda_0T^\dagger E]\}. \tag{17}$$

A general formula for integrals of this form over the SU(n) manifold was obtained by Itzykson and Zuber [32]. Here it is sufficient to note that the integrand depends only on a single column of the SU(4) matrix T, and hence the integration reduces to one over the unit sphere in $\mathbb{C}^4$. One finds

$$\langle[\det H]^3\det(H-E)\rangle_H^{(N)} = 4N^4e^{-2N}\frac{\sin(NE_2)-NE_2\cos(NE_2)}{(NE_2)^3}. \tag{18}$$

Inserting this expression into Eq. (11), performing the integral over E_2, and noting that $k=K/2$ from Eqs. (3) and (5), one obtains the final result for the curvature distribution of the GUE,

$$P(k) = \frac{2}{\pi}\left[1+k^2\right]^{-2}. \tag{19}$$

This expression is asymptotically exact for $N\to\infty$.

In conclusion, the *exact* curvature distribution of chaotic quantum systems has been calculated for the unitary ensemble. The result proves a recent conjecture of Zakrzewski and Delande [18] which was based on a careful examination of numerical results. It is interesting to compare the curvature distribution to the well-known spacing distribution. While the exact spacing distribution for large random matrices is not known, the result for 2×2 matrices (Wigner surmise) appears to be an excellent approximation [1]. By contrast, it has been found that the curvature distribution of 2×2 matrices does not give a good description of numerical results [18], but fortunately, the exact distribution for large matrices can be obtained analytically.

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