# Spectral autocorrelation function in the statistical theory of energy levels

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The spectral autocorrelation function is evaluated analytically for the Gaussian ensembles of Hamiltonian matrices. A direct comparison of the prediction of these ensembles with experimentally measured spectra is thereby possible. Also computed is the time autocorrelation function of an initially prepared nonstationary state. The repulsion of eigenstates in the time domain is clearly manifested in the analytic result.

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There is a very extensive literature [1–11] on the statistical limit in quantal systems of discrete levels and its possible relation to classical chaos. Even so, the experimental signature of this limit is not yet clear. The problem is not one of definition. A variety of considerations, including extensive numerical tests [4,9], have established the Gaussian ensembles of Hamiltonian matrices [1,12,13] as providing a suitable reference. (Even so, there may well be harsher chaos, with more level repulsion [14], than represented by this limit.) The problem is in comparing the predictions of these ensembles with experiment. The statistics of energy spacings [1] are limited by the finite experimental energy resolution which may fail to distinguish nearby levels. The statistics of spectral transition strengths [7,11,15] or other matrix elements are limited both by the finite resolution and by the difficulties of establishing a secure base line and of saturation. In this article we discuss and evaluate an observable, the autocorrelation of the spectrum, which depends on both the level spacings and the transition strengths, yet it is less sensitive to experimental noise because it is computed as an autocorrelation function of the raw spectrum. In this convolutionlike computation, different transitions contribute to each frequency interval thereby reducing the noise level. This article provides analytic expressions for the Gaussian ensemble average of the spectral autocorrelation function and its Fourier transform [16], the survival probability.

The spectral autocorrelation function $G(\omega)$ is defined in terms of the spectrum $S(\omega)$ by [16]

$$G(\omega)=\int_{-\infty}^{\infty} S(\omega')S(\omega'+\omega)d\omega' \ . \tag{1}$$

If the spectrum is normalized to unit strength, $G(\omega)d\omega$ is the joint probability of two transitions separated by the frequency interval $\omega,\omega+d\omega$. We refer to Ref. [16] for the motivation to introduce $G(\omega)$ and for its important role in establishing the repulsion of eigenstates in the time domain. In the Hamiltonian ensembles the spectral lines are sharp so that (1) can be written as

$$G(\omega)=\sum_n \sum_m p_n p_m \delta(\omega-(\omega_m-\omega_n)) \ . \tag{2}$$

Here, the $p_n$'s are the strengths of the different transitions and the $\omega_n$'s the transition frequencies. Equation (2) shows explicitly that $G(\omega)$ is not determined by the level spacings (i.e., $\omega_m-\omega_n$) alone. Rather, the spacing between every pair of levels is weighted by the spectral strength of the two respective transitions.

The transition strengths $p_n$ are given by $p_n=|\langle\psi_n|T|0\rangle|^2$. Here, $\psi_n$ is the $n$th eigenstate of the Hamiltonian with eigenvalue $\hbar\omega_n$. $T$ is the transition operator and $|0\rangle$ is the initial state. Normalization of the spectrum is equivalent to $\sum_n p_n=1$ and hence to the normalization $\langle\phi|\phi\rangle=1$ where $|\phi\rangle=T|0\rangle$. In the Gaussian ensembles a convenient set of variables is the scalar products of $\psi_n$ onto some fixed basis [12,13]. We take that basis to be the eigenstates of a zeroth-order separable Hamiltonian $H_0$. Because $H_0$ is separable its spectrum is regular [17]. This basis is strongly mixed by the coupling $H-H_0$. This interpretation is, however, not necessary for the mathematical development. We similarly expand $|\phi\rangle$ in the zeroth-order basis and collect the expansion coefficients as a column vector $\phi$. Then, if $\mathbf{a}^{(n)}$ is the row vector whose components are the expansion coefficients of $\psi_n$, $p_n=(\mathbf{a}^{(n)}\cdot\boldsymbol{\phi})^2$.

To compute the ensemble average of $G(\omega)$, we first remove from (2) its diagonal or "self" part, $\delta(\omega)\sum_n p_n^2$. For the $N$ level Gaussian ensembles [12,18], $\langle\sum_n p_n^2\rangle=N\langle p_n^2\rangle$. It remains to average the $N(N-1)$ off-diagonal terms in (2) where each spacing $\omega_m-\omega_n$ is

 

weighted by $p_m p_n$. For this purpose we use a very essential property of the Gaussian ensembles [12,13]. The probability density $P(H)$ of any Hamiltonian depends only on the energy levels $\hbar\omega_n$'s. The measure factorizes into a measure depending only on the energy levels and a measure depending only on the eigenvectors. It follows that in the limit of the Gaussian ensembles

$$\langle G(\omega)\rangle = \sum_n \langle p_n^2\rangle \delta(\omega) + \sum_n \sum_m{}' \langle p_n p_m\rangle \langle \delta(\omega-(\omega_m-\omega_n))\rangle \ . \tag{3}$$

The average over the spacing distribution is computed using Dyson's [12] two-level correlation function

$$\begin{aligned}\langle \delta(\omega-\omega_m+\omega_n)\rangle &= \int \delta(\omega-\omega_1+\omega_2)P(\omega_1,\ldots,\omega_N)d\omega_1\cdots d\omega_N \\ &= \frac{(N-2)!}{N!}\int \delta(\omega-\omega_1+\omega_2)R_2(\omega_1,\omega_2)d\omega_1 d\omega_2 \\ &= \frac{(N-2)!}{N!D}\int \delta\left[\frac{\omega}{D}-\frac{\Delta\omega}{D}\right]\left[1-Y_2\left[\frac{\Delta\omega}{D}\right]\right]d(\Delta\omega/D)d(\omega_1+\omega_2)/2D \\ &= \frac{(N-2)!}{N!}\left[\frac{N}{D}\right]\left[1-Y_2\left[\frac{\omega}{D}\right]\right] .\end{aligned} \tag{4}$$

Here $D$ is the mean spacing in frequency and $Y_2(x)$ is Dyson's two-level cluster function [1,13], given, for practical purposes, by [1]

$$Y_2(x)=(\beta/2)\,\mathrm{sinc}^2(\beta\pi x/2) \ , \tag{5}$$

where $\mathrm{sinc}(x)=\sin(x)/x$. Exact expressions for $Y_2(x)$ are also available [13]. The parameter $\beta$ in $Y_2$ designates the particular Gaussian ensemble, $\beta=1$, 2, and 4, respectively, for the orthogonal, unitary, and symplectic cases. One expects [4,9,12] the Gaussian-orthogonal-ensemble (GOE) limit, $\beta=1$, for most systems of physical interest.

The intermediate result is

$$\left\langle G\left[\frac{\omega}{D}\right]\right\rangle = N\langle p_n^2\rangle \times\left\{\delta\left[\frac{\omega}{D}\right]+\frac{\langle p_n p_m\rangle}{\langle p_n^2\rangle}\left[1-Y_2\left[\frac{\omega}{D}\right]\right]\right\} . \tag{6}$$

As expected in general [16], there are three contributions to the joint spectral density: The "self" spike at the origin, the asymptotic density, and the deviance, $Y_2(\omega/D)$, of the probability density of two different transitions from its uniform value. Note also, cf. (5), the low value of $1-Y_2(\omega/D)$ for $\omega<D$ showing the rarity of nearby strong transitions.

We evaluate $\langle p_n p_m\rangle$ first in the often used Gaussian approximation [12], which yields results correct to order $1/N$, and then exactly. We shall find that by introducing an effective number of states $N_{\text{eff}}$, the two results can be brought to the same form. The explicit results quoted below are for the case of just one state $|\phi\rangle$ such that $p_n=|\langle\psi_n|\phi\rangle|^2$. In the language of reaction theory this corresponds to the single-channel case.

In the Gaussian approximation the joint probability of $p_n=|x_n|^2$ and $p_m=|x_m|^2$ is a Gaussian of width $(N\beta)^{-1}$, $P(x_n,x_m)\propto\exp[-\beta N(|x_n|^2+|x_m|^2)/2]$. Here, $\beta=1,2,4$ for the orthogonal, unitary, and symplectic ensembles, respectively. Then

$$\langle p_n p_m\rangle = \begin{cases} 1/N^2, & n\neq m \\ [(\beta+2)/\beta]/N^2, & n=m \ . \end{cases} \tag{7}$$

If, for the Gaussian approximation, we define $N_{\text{eff}}$ by $N_{\text{eff}}\equiv(N\langle p_n^2\rangle)^{-1}=[\beta/(\beta+2)]N$, we have

$$\left\langle G\left[\frac{\omega}{D}\right]\right\rangle = \frac{1}{N_{\text{eff}}}\left\{\delta\left[\frac{\omega}{D}\right]+\frac{\beta}{\beta+2}\left[1-Y_2\left[\frac{\omega}{D}\right]\right]\right\} . \tag{8}$$

The exact results, to be derived below, also lead to (8) but with $N_{\text{eff}}=(N+2)/3$ for the GOE or $=(\beta N+2)/(\beta+2)$ in general. One needs the exact results since in the Gaussian approximation

$$\sum_n \sum_m \langle p_n p_m\rangle = 1+(2/\beta N)$$

so that the integral of $G(\omega)$ is not quite unity.

The exact joint distribution of the amplitudes $x_n, x_m$ is computed, for the GOE, as

$$P(x_m,x_m)=C\int \prod_{\nu=1}^{N} da_\nu^{(n)} da_\nu^{(m)} \delta(x_n-\mathbf{a}^{(n)}\cdot\boldsymbol{\phi})\delta(x_m-\mathbf{a}^{(m)}\cdot\boldsymbol{\phi})\delta(\mathbf{a}^{(n)}\cdot\mathbf{a}^{(n)}-1)\delta(\mathbf{a}^{(m)}\cdot\mathbf{a}^{(m)}-1)\delta(\mathbf{a}^{(n)}\cdot\mathbf{a}^{(m)}) \ . \tag{9}$$

Here the vector $\mathbf{a}^{(n)}$ is as defined above (i.e., $x_n=\mathbf{a}^{(n)}\cdot\boldsymbol{\phi}$) and the integration in (9) imposes the normalization and or-

thogonalization of the vectors **a**. $C$ is a normalization coefficient. The final result is

$$P(x_1,x_2)=\pi^{-1}\frac{\Gamma(N/2)}{\Gamma((N-2)/2)}(1-x_n^2-x_m^2)^{(N-4)/2}\ , \tag{10}$$

leading to

$$\langle p_n p_m\rangle=(1+2\delta_{n,m})/N(N+2)\ . \tag{11}$$

Now, $\sum_{n,m}\langle p_n p_m\rangle=1$ so that $G(\omega)$ is strictly normalized. Note, however, that for $n\neq m$, the exact result (11) shows that the orthogonality condition $\mathbf{a}^{(n)}\cdot\mathbf{a}^{(m)}=0$ imposed in (9) leads to a slight anticorrelation in that $\langle p_n p_m\rangle-\langle p_n\rangle\langle p_m\rangle=-2/N^2(N+2)$. With $N_{\rm eff}=(N+2)/3$, the exact GOE results also lead to (8).

$G(\omega)$ is the Fourier transform of the so-called survival probability [3,5,8,19] $|C(t)|^2=|\langle\phi(t)|\phi(0)\rangle|^2=\mathrm{Tr}[\rho(t)\rho(0)]$, where $\phi(t)=\exp(-iHt/h)\phi(0)$ and $\rho(0)$ is the density of the initial nonstationary state $\phi(0),\rho(0)=|\phi(0)\rangle\langle\phi(0)|$. Taking the Fourier transform of (8), we have

$$\langle|C(t)|^2\rangle=\frac{1}{N_{\rm eff}}\left\{1+\frac{\beta}{\beta+2}\left[\delta\left[\frac{t}{2\pi\bar\rho}\right]-b_2\left[\frac{t}{2\pi\bar\rho}\right]\right]\right\}=\frac{1}{N}\left[2\pi\bar\rho\delta(t)+\frac{\beta+2}{\beta}-b_2\left[\frac{t}{2\pi\bar\rho}\right]\right]\ . \tag{12}$$

Here $b_2(t)$, the Fourier transform of $Y_2(\omega)$, is the so-called [13] two-level form factor and $\bar\rho=1/D$ is the average density of states. The result (12) is similar but not identical to the inspired estimate of Leviandier *et al.* [5]. The key difference is in the role of the fluctuations in the transition strengths $p_n$. Equation (12) has been derived taking a full and exact accord of these fluctuations in the limit of Gaussian ensembles. See also the derivation of Guhr and Weidenmüller [20]. The Fourier transform of Eq. (5), with $\bar t=t/2\pi\bar\rho$,

$$b_2(\bar t)=\begin{cases}1-2|\bar t|/\beta, & |\bar t|\le\beta/2\\ 0, & |\bar t|\ge\beta/2\end{cases} \tag{13}$$

shows that past the peak at the origin, $\langle|C(t)|^2\rangle$, drops to a minimal value of $\approx 2/\beta N$ at $t\approx(2\pi/D)(\beta/\pi^2N)^{1/3}$ which is below its asymptotic value of $1/N_{\rm eff}$ (see Fig. 1). This asymptotic value of $\langle|C(t)|^2\rangle$ is reached for times longer than the recurrence time $t_{\rm rec}=2\pi\beta/D$. Notice that the three ensembles differ in both the minimal value of $\langle|C(t)|^2\rangle$ and the rate of recovery of $\langle|C(t)|^2\rangle$ towards its first recurrence. The known [1,13] exact form of $b_2(t)$ does not change the qualitative conclusion based on (13) except that for $\beta=1$, $b_2(t)$ is finite beyond the first recurrence.

Equation (12), cf. Fig. 1, distinguishes two contributions to the time autocorrelation function. The first is the initial fast ($\delta$-function-like) decay which has an effective width of $2/DN$, where $N$ here and before is the number of levels. The fast component describes the rapid dephasing of the initial state $\phi(0)$. For $N\gg1$ this dephasing time is very short compared to the recurrence time $2\pi\beta/D$. The initial dephasing is expected to be rather similar for both regular and chaotic systems [2,3,21], and will be well described by classical mechanics. For longer times, of the order of up to $2\pi/D$, it is the second part in Eq. (12), $(\beta+2)/\beta-b_2(t/2\pi\bar\rho)$, that characterizes the time evolution. Due to the $b_2$ term, $\langle|C(t)|^2\rangle$ drops below its asymptotic value and it is the recovery from this "correlation hole" [2,5] that reflects the level statistics.

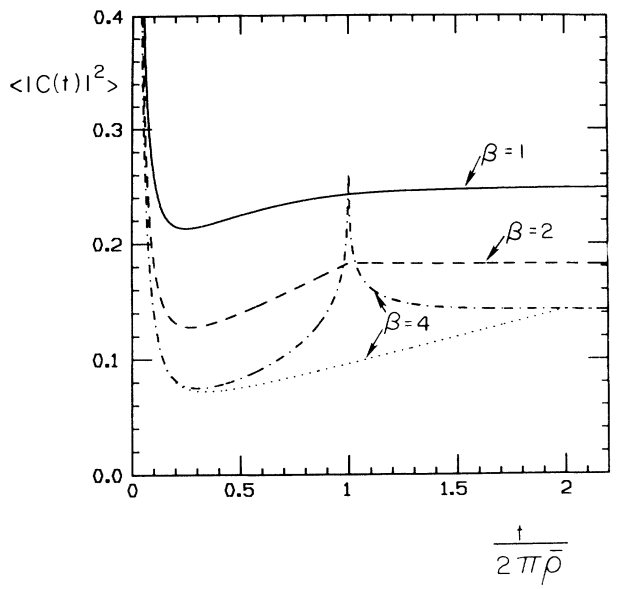


FIG. 1. The average survival probability $\langle|C(t)|^2\rangle$ vs time $t/2\pi\bar\rho$ for the three Gaussian ensembles: GOE ($\beta=1$, solid line), Gaussian unitary ensemble (GUE) ($\beta=2$, dashed line), and Gaussian symplectic ensemble (GSE) ($\beta=4$, dashed-dotted line). The exact two-level form factor $b_2(t)$ is used in Eq. (12) and the number of levels is $N=10$. The $\delta$ function in (12) is represented by $(\epsilon/\pi)/[(t/2\pi\bar\rho)^2+\epsilon^2]$, where $\epsilon=1/\pi N$ is chosen so that $\langle|C(0)|^2\rangle=1$. Notice that as $\beta$ increases, the minimal value of $\langle|C(t)|^2\rangle$ at short times is lower and the rate of recovery to the asymptotic limit is slower. The exact $\langle|C(t)|^2\rangle$ for $\beta=4$ has a spike at $t/2\pi\bar\rho=1$ which disappears in the linear approximation (13) to $b_2(t)$ (see dotted line).

The parameter $\beta$ can be regarded as a measure of the above level repulsion. The limit $\beta \to 0$ does not quite correspond to the regular regime although it does give a useful indication. As $\beta \to 0$ it follows from (13) that $b_2(t) \approx 0$, so that $\langle |C(t)|^2 \rangle$ does not drop below its limit $1/N_{\text{eff}}$ in the regular regime. Level repulsion is thus clearly manifested in the time domain.

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