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Quantum spectrum as a time series: Fluctuation measures

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The fluctuations in the quantum spectrum could be treated like a time series. In this framework, we explore the statistical self-similarity in the quantum spectrum using the detrended fluctuation analysis (DFA) and random matrix theory (RMT). We calculate the Hausdorff measure for the spectra of atoms and Gaussian ensembles and study their self-affine properties. We show that DFA is equivalent to the Δ_3 statistics of RMT, unifying two different approaches. We exploit this connection to obtain theoretical estimates for the Hausdorff measure.

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The fluctuations in physical systems carry important information about the system. In the context of quantum systems, the spectral fluctuations reveal whether the corresponding classical dynamics is regular or chaotic or a mixture of both [1]. It is well known that for the classically regular systems, the quantum eigenvalues are uncorrelated, while for the chaotic systems the eigenvalues tend to display a certain degree of correlation, which is dictated by the symmetry properties of the system such as the presence or absence of rotational and time reversal invariance. Typically, the spectrum of high dimensional quantum systems such as atoms, molecules, and nuclei belong to the latter class. This equivalence between the nature of classical dynamics and spectral fluctuations in the corresponding quantized system is generally through an analogy with random matrix ensembles [1] and has been verified in many simulations and experiments [2].

Recently a different approach has been suggested. It is possible to consider suitably transformed eigenvalues of a quantum system as a time series. Then, using time series analysis methods, it was shown that the quantum systems display $f^{-\gamma}$ noise where $1 \leqslant \gamma \leqslant 2$ depends on the classical dynamics in the system [3]. In particular, for the chaotic systems the level fluctuations display $1/f$ noise. So do the levels of complex nuclei [3]. In contrast, for the regular systems we get $1/f^2$ noise. Hence, the spectral fluctuations can be characterized without reference to random matrix models.

This is reminiscent of the following types of time series. In the Brownian motion or random walk time series $x_t, t=1,2,\ldots,N$, the successive increments of the series are uncorrelated. The variance of this process is $\mathrm{var}(x) \propto t^{2H}$, $(H=1/2)$, where H is the Hausdorff measure. In this case, the power spectrum gives rise to $1/f^2$ noise [4]. Thus, *regular* classical systems with uncorrelated quantum levels are analogous to a series of Brownian motion path. On the other hand, one could also imagine a time series with $1/f$ noise. There are many mechanisms and processes that produce $1/f$ noise [5]. In a chaotic system, the eigenvalues of the corresponding quantum system contain certain degrees of correlation and they display $1/f$ noise. In this case, $H=0$ and corresponds to a variance being time independent. In general, for $0<H<1$, $\gamma=2H+1$. In terms of the exponent H, our interest is in the regular $(H=1/2)$ and chaotic limits $(H=0)$ for the fluctuations of the spectral time series. This region $0<H<1/2$ corresponds to an antipersistent time series, i.e, the one that has opposing trends at successive time steps. Visually an antipersistent time series presents a very rough profile as compared to the $H=1/2$ series. In fact, H is also used to characterize the roughness of surfaces and profiles.

Such an antipersistent series is also a self-affine fractal and displays a statistical self-similarity that scales differently in different directions. Mathematically, it implies $y(Ht) \approx t^{-H} y(t)$, where the symbol $\approx$ represents statistical equality. Note that the power spectrum is a measure of the strength of frequencies in Fourier space but the fluctuation function and the Hausdorff measure, taken together, indicate the structure of the spectrum at various spectral scales. This structure is related to the classical periodic orbits of the system through semiclassical theories such as Gutzwiller's trace formula [6]. Hence it is important to understand the self-affine properties of the spectrum since they have implications at the level of classical dynamics of the system.

The idea of characterizing fluctuations and their scaling is of interest in other areas as well. For instance, the surface-height fluctuations in the surface growth processes reflect the morphological changes that determine the physical and chemical processes such as crystal growth, metal deposition, etc. [7]. Fluctuations in the Electroencephalogram series might tell us about the nature of physiological processes taking place [8]. In all these cases, fluctuations and how they scale provide important clues to the physical processes under study. Hence, the results presented here have relevance in fields beyond quantum physics.

In this paper, we take the time series point of view for the quantum spectrum and compute the exponent H for levels of lanthanide atoms (Sm, Pm, and Nd) and random matrix theory (RMT) ensembles using detrended fluctuation analysis (DFA) method [9]. Note that the value of γ does not necessarily guarantee a self-affine nature [10]. We show that the DFA of order 1 is related to the Δ_3 statistics of RMT and exploit it to obtain theoretical fluctuation functions and H. We show that the time series of level sequences and a random time series both with the same value of H have the same fluctuation properties.

We denote a spectrum of discrete levels, belonging to either a random matrix or a given atomic system, by

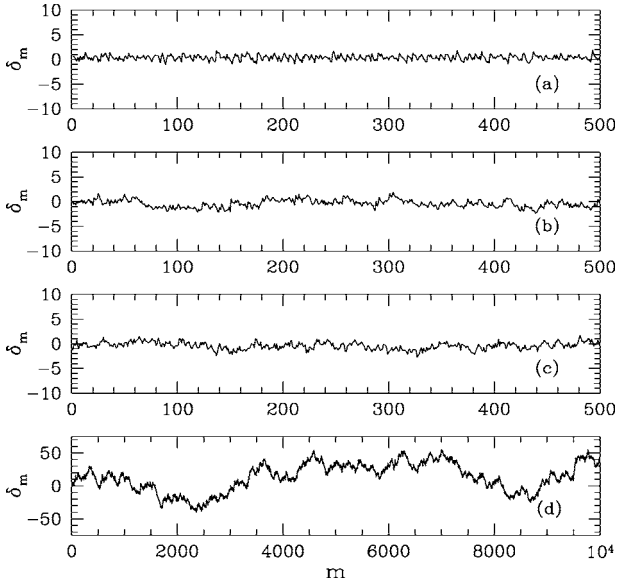

FIG. 1. $\delta_m - m$ curve for (a) Sm I atomic levels, (b) GOE levels, (c) time series with $H=0$, and (d) GDE levels. Note that (a), (b), (c) have qualitatively similar features as opposed GDE levels in (d).

$E_i, i=1,2,\ldots,n+1$. Then, its integrated level density, i.e, the total number of levels below a given level, can be decomposed into an average part plus an oscillatory contribution, $N(E)=N_{av}(E)+N_{osc}(E)$. Spectral unfolding is affected by the transform, $\lambda_i=N_{av}(E_i)$, such that the mean level density of the transformed sequence $\{\lambda\}$ is unity. All further analysis is carried out using $\{\lambda\}$. For instance, the level spacing is $d_i=\lambda_{i+1}-\lambda_i$, $i=1,2,\ldots,n$. The main object of interest in this paper is the fluctuations in the time series of levels given by

$$\delta_m = \sum_{i=1}^{m} (d_i - \langle d \rangle) \equiv - N_{osc}(E_{m+1}); \quad m = 1, \ldots, n. \quad (1)$$

Note that δ_m is formally analogous to a time series with the time index denoted by m [3]. The power spectrum $S(f)$ of δ_m displays a power law, i.e, $S(f) \sim f^{-\gamma}$, where $1 \leqslant \gamma \leqslant 2$ [3]. In particular, if the system is regular, $\gamma=2$, and for Gaussian ensembles and the chaotic systems, $\gamma=1$. Thus, $1/f$ noise should correspond to $H=0$. A $H=0$ random time series should have a profile similar to levels of Gaussian ensembles and atoms as seen in Figs. 1(a)–1(c).

To obtain δ_m, we needed to unfold the spectrum. This puts the spectra from various systems on the same footing amenable to direct comparison. For the atomic systems, unfolding was done using an empirical function to fit the given levels. For the Gaussian ensembles the Wigner semicircle law [2] was used for unfolding.

First, we show the results from lanthanide atoms. The atoms in this series exhibit complex configuration mixing and spectra. Recently, a series of studies on the statistical properties of these levels from the RMT point of view were reported [11]. All the calculations for levels of Sm, Nd, and Pm were done using the GRASP92 code, and for details we refer to [12]. In Fig. 1(a), we show δ_m for levels obtained from Sm. Note that the profile is similar to levels from the Gaussian orthogonal ensemble (GOE), shown in Fig. 1(b), and a random time series with $H=0$ [Fig. 1(c)]. This is in contrast to the level profile of the Gaussian diagonal ensemble (GDE) [Fig. 1(d)] defined as an ensemble of diagonal matrices whose elements are Gaussian distributed random numbers.

TABLE I. Numerical estimates of H_1 and H.

System	Hausdorff measure (H)	H_1
Sm	0.045	1.045±0.031
Pm	−0.025	0.975±0.024
Nd	−0.003	0.997±0.013
GOE	0.0003	1.0003±0.0083
GUE	0.0047	1.0047±0.0089
GSE	0.0025	1.0025±0.0125
GDE	0.5080	1.5080±0.0044

To quantitatively obtain the exponent H, we compute it using the detrended fluctuation analysis technique, which has become a popular tool to study long-range correlations in time series [9]. DFA is based on the idea that if the time series contains nonstationarities, then the variance of the fluctuations can be studied by successively detrending using linear, quadratic, cubic,…, higher-order polynomials in a piecewise manner. The entire time series is divided into segments of length s, and in each of them detrending is applied and variance $F^2(s)$ about the trend is computed and averaged over all the segments. This exercise is repeated for various values of s. For a self-affine fractal, we have,

$$F(s) \propto s^H, \quad (2)$$

where $0<H<1$. In Table I, we show the numerical estimates of H obtained for various atomic and Gaussian ensemble cases. The results tabulated alongside represent the average of $F(s)$ taken over an appropriate ensemble. For instance, for the Sm levels, the ensemble consists of six sequences, each with 650 levels (similarly for Pm and Nd). In the case of Gaussian ensembles of RMT, the results were obtained from ensemble of 50 level sequences each with 4600, 3900, and 2100 levels, respectively, for the Gaussian orthogonal ensemble, Gaussian unitary ensemble (GUE), and Gaussian symplectic ensemble (GSE). For the uncorrelated levels from GDE, we get $H=0.508$ in good agreement with the expected value of 1/2. For the atomic and Gaussian ensembles, the value of H is close to zero. In such cases, standard DFA becomes inaccurate, and DFA is performed after integrating δ_m once more so that the new exponent is $H_1=H+1$. Table I shows that H_1 is close to unity for atomic and Gaussian ensembles. Thus, the GDE levels are a self-affine fractal with $H=1/2$ but those of atomic and Gaussian ensembles ($H=0$) do not fall in this class.

In order to obtain an analytical estimate for the value of H, we appeal to the $\Delta_3(s)$ statistic widely studied in RMT to quantify the rigidity of spectrum, i.e, given a level, a rigid spectrum will not allow any flexibility in the placement of

the next level. $\Delta_3(s)$ is a measure of this flexibility or conversely the rigidity. It is defined by

$$\Delta_3(\bar{\lambda},s) = \frac{1}{2s} \min_{a,b} \int_{\bar{\lambda}-s}^{\bar{\lambda}+s} [n(\lambda) - a\lambda - b]^2 d\lambda, \tag{3}$$

where $n(\lambda)=n_{av}(\lambda)+n_{osc}(\lambda)$ is the integrated level density for the unfolded spectrum $\{\lambda\}$ and a and b are the parameters from linear regression and $\bar{\lambda}$ is any reference level. Now, $\Delta_3(s)$ is an average over various choices of $\bar{\lambda}$. Notice that $n(\lambda)=N(E)$ and due to the unfolding procedure, $n_{av}(\lambda)=\lambda$. This implies that $n_{osc}(\lambda)=N_{osc}(E)$. Then, we could rewrite Eq. (3) as

$$\Delta_3(\bar{\lambda},s) = \frac{1}{2s} \min_{a,b} \int_{\bar{\lambda}-s}^{\bar{\lambda}+s} [n_{osc}(\lambda) - (a-1)\lambda - b]^2 d\lambda. \tag{4}$$

Now we discretize this equation to relate $\Delta_3(s)$ with the standard fluctuation function $F(s)$ obtained by DFA. Substituting from Eq. (1) for $n_{osc}(\lambda)$, we get

$$\Delta_3(s) = \frac{1}{M}\sum_{j=0}^{M} \frac{1}{2s} \sum_{m=j+1}^{j+2s} [\delta_m - Y(\lambda_m)]^2 = \frac{1}{M}\sum_{j=0}^{M} F^2(s,j) = F^2(s), \tag{5}$$

where $Y(\lambda_m)=(a^*-1)\lambda_m+b^*$ with best fit parameters a^* and b^*, and j indexes M different choices of $\bar{\lambda}$. Since the DFA is applied with linear detrending on segments of length s, then Eq. (5) boils down to $\Delta_3(s)=F_1^2(s)$, and the subscript denotes DFA(1). Then, ensemble averaging and writing $F_1(s)$ in terms of $\Delta_3(s)$, we have,

$$\langle F_1(s)\rangle = \langle \Delta_3(s)^{1/2}\rangle \tag{6}$$

This main result of the paper shows DFA(1) to be equivalent to a Δ_3 statistic. From RMT, the averages for $\langle\Delta_3(s)\rangle$ are well known. For the GDE, we have $\langle\Delta_3^{\mathrm{GDE}}(s)\rangle=s/15$. Then, the result for uncorrelated set of levels is

$$\langle F_1(s)\rangle \sim s^H \sim \left(\frac{s}{15}\right)^{1/2}. \tag{7}$$

On a log-log plot we expect a slope of $H=1/2$. This is amply verified in Fig. 2(d) for GDE with slope of 0.508. In our numerical simulation, GDE consists of 50 level sequences of 15 000 levels each.

The numerical results for atomic levels and Gaussian ensembles in Table I show that $H\approx 0$ $(H_1\approx 1)$. To make correspondence with H_1, we consider modified Δ_3 statistics given by

$$\Delta(\bar{\lambda},s) = \frac{1}{2s} \min_{a,b} \int_{\bar{\lambda}-s}^{\bar{\lambda}+s} [\lambda n(\lambda) - a\lambda - b]^2 d\lambda, \tag{8}$$

which corresponds to integrating the δ_m once more before performing DFA on it. We obtain the asymptotic random matrix average to be [13],

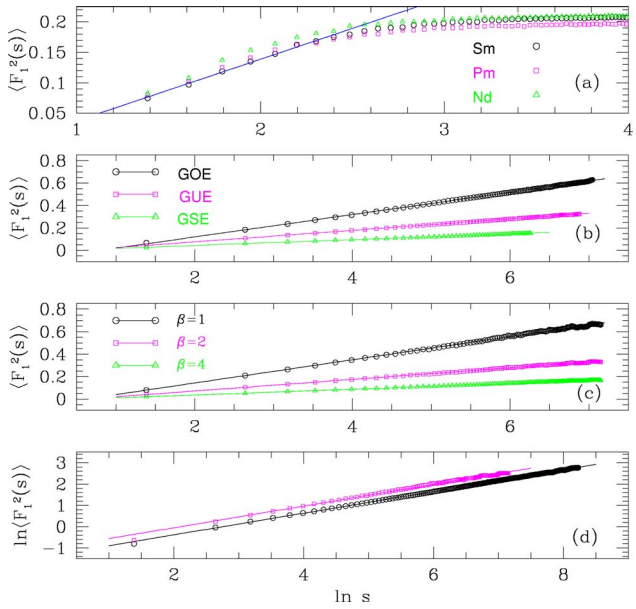

FIG. 2. (Color online) The fluctuation function $\langle F_1^2(s)\rangle$ in a semilogarithmic plot for (a) atomic levels, (b) Gaussian ensembles, and (c) a random time series with $H=0$ and power spectrum $1/\beta f$. (d) shows $\ln\langle F_1^2(s)\rangle$ vs $\ln s$ for GDE and a random walk time series. The slopes of best fit (solid) lines are quoted in the text.

$$\langle \Delta(s)\rangle \sim s^{2H_1} \propto s^2 \tag{9}$$

for all the three ensembles. Then, using Eq. (6), $\langle F_1(s)\rangle \propto s$ and hence the theoretical slope $H_1=1$ and corresponds to the standard Hausdorff measure $H=0$. The numerical values in the last column of Table I confirm this RMT-based result. For Pm and Nd, note that the small negative values for H are in the error bar as seen by the error estimates provided.

Using the time series analogy, we explore the nature of fluctuations at $H=0$ for Gaussian ensembles. This, in turn, throws further light on the fluctuation properties of the $H=0$ time series. From RMT we have $\langle\Delta_3(s)\rangle_\beta \approx \ln 2\pi s/\beta\pi^2$, where $\beta=1,2,4$ for GOE, GUE, and GSE, respectively. Substituting this in Eq. (6), the fluctuation function at $H=0$ is

$$\langle F_1(s)\rangle \sim \left(\frac{\ln 2\pi s}{\beta\pi^2}\right)^{1/2}. \tag{10}$$

At $H=0$, the ensemble averaged fluctuations display logarithmic scaling with length of level sequence s considered. For convenience, we plot $\langle F_1^2(s)\rangle$ in a semilogarithmic plot. Then we expect slopes for level sequences from GOE, GUE, and GSE to be $1/\beta\pi^2$. In Fig. 2(a), we show results from the atomic levels of Sm, Pm, and Nd. In all three cases, the straight line obtained shows that the DFA fluctuation function is in good agreement with the theoretical result based on $\Delta_3(s)$ statistics. Their slopes, 0.105, 0.104, and 0.109 for Sm, Pm, and Nd agree closely with $1/\pi^2$. The deviations for $\ln s > 2.2$ occur due to the breakdown of universality in the presence of system-specific information. This is related to the period of the short periodic orbits in the atomic system [14]. Thus, the quantum spectrum of complex atoms can be

characterized by $H=0$ and display logarithmic scaling. Similar results are obtained for the Gaussian ensembles. Figure 2(b) shows the linear relationship in a semilogarithmic plot for levels from GOE, GUE, and GSE. The measured best fit slopes 0.0995 ($\beta=1$), 0.0511 ($\beta=2$), 0.0257 ($\beta=4$) closely approximate the theoretical value $1/\beta\pi^2$. The DFA applied to spectral levels can distinguish between the three ensembles. This is not possible with the power spectrum method unless one measures the slope and the intercept together. Intercept measurement is often difficult due to deviations from scaling for small frequencies.

What happens to an antipersistent time series at $H=0$? We generate random time series with $H=0$ and power spectrum $S(f)=1/2\beta\pi^2 f$. The technique is to generate Gaussian random numbers u and take their Fourier transform to obtain $\tilde{u}$. Then, take the inverse Fourier transform of $\tilde{u}\sqrt{|S(f)|}$ to obtain a time series with the required properties [15]. By varying β, we get a synthetic random time series that will mimic level fluctuations of GOE, GUE, and GSE. The DFA applied to 10 member ensembles of such time series (each of length 5000) is shown in Fig. 2(c). On a semilogarithmic plot, they produce the expected linearity, and slopes 0.1035, 0.0517, and 0.0258 agree quite well with the theoretically expected result $1/\beta\pi^2$. We conclude that an appropriate time series with $1/f$ noise is similar to a level spectrum from random matrix ensembles and complex atoms and both display fluctuations that scale in a logarithmic manner at $H=0$. These results, viewed in conjunction with the Bohigas *et al.* conjecture [1], mean that we can expect the spectrum of classically regular systems to be characterized by $H=1/2$ and chaotic systems by $H=0$.

Even though we motivated our work using quantum systems, we emphasize that if the spectrum is viewed as a time series, then we can apply our main results to any classical system where self-affinity of the time series is relevant; for instance, in studies of surface roughness, growth models where surface morphology determines the properties of the physical and chemical processes. Examples of surface growth are the evolution of landscapes, vapor deposition, propagation of flame fronts, and growth of bacterial colonies, etc. [7]. In these cases, a relevant quantity of interest is the correlation function for the surface heights $h(\mathbf{x})$, $C(\mathbf{r})=\langle|h(\mathbf{x})-h(\mathbf{x}+r)|^2\rangle^{1/2}$. In many cases, $C(r)\sim r^H$ over a large range of length scales, i.e, many such growing surfaces are self-affine fractals. In Ref. [16] a modified form for the correlation function of rough surfaces is studied that gives logarithmic fluctuations, similar to Eq. (10) obtained above, as $H\rightarrow 0$. This has been confirmed by numerical simulations of surfaces as well as from experimental results of thin-film evaporation [16]. Another feature of surface growth is the existence of a roughening transition for certain critical parameter values. At the roughening transition, the exponent is $H=0$ and $C(r)$ displays logarithmic fluctuations as experimentally verified for the Ag(115) sample [17]. We have also shown that $H=0$ corresponds to logarithmic fluctuations using random matrix methods. Hence taking the time series perspective and RMT could be beneficial for various other problems.

To summarize, we treat the quantum spectrum like a time series. In this picture, the uncorrelated spectral levels behave like a random walk series with a Hausdorff measure $H=1/2$ and is a self-affine fractal. For the spectrum of complex atoms and Wigner-Dyson random matrix ensembles, $H=0$, an antipersistent time series. We show that the DFA is equivalent to the Δ_3 statistics of RMT and we exploit this connection to obtain theoretical estimates for H. This shows that at $H=0$ the spectral fluctuations display logarithmic behavior, a feature seen in many experimental and model simulations in surface growth studies. Thus, $H=0$ is an unusual and interesting limit and will require further investigation.

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