Rapid Communications

Local box-counting dimensions of discrete quantum eigenvalue spectra: Analytical connection to quantum spectral statistics

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(Received 12 November 2017; published 13 March 2018)

Two decades ago, Wang and Ong, [Phys. Rev. A **55**, 1522 (1997)] hypothesized that the local box-counting dimension of a discrete quantum spectrum should depend exclusively on the nearest-neighbor spacing distribution (NNSD) of the spectrum. In this Rapid Communication, we validate their hypothesis by deriving an explicit formula for the local box-counting dimension of a countably-infinite discrete quantum spectrum. This formula expresses the local box-counting dimension of a spectrum in terms of single and double integrals of the NNSD of the spectrum. As applications, we derive an analytical formula for Poisson spectra and closed-form approximations to the local box-counting dimension for spectra having Gaussian orthogonal ensemble (GOE), Gaussian unitary ensemble (GUE), and Gaussian symplectic ensemble (GSE) spacing statistics. In the Poisson and GOE cases, we compare our theoretical formulas with the published numerical data of Wang and Ong and observe excellent agreement between their data and our theory. We also study numerically the local box-counting dimensions of the Riemann zeta function zeros and the alternate levels of GOE spectra, which are often used as numerical models of spectra possessing GUE and GSE spacing statistics, respectively. In each case, the corresponding theoretical formula is found to accurately describe the numerically computed local box-counting dimension.

DOI: 10.1103/PhysRevE.97.030202

I. INTRODUCTION

In fractal geometry [1], scale invariance is quantified through the so-called fractal dimension. A *constant* fractal dimension is often defined as the scaling exponent of a geometric power law. The box-counting dimension is the simplest and most pervasive example of a fractal dimension (see, for example, Ref. [2] for definitions and review). "Fractal analysis," which is a term that is frequently used in many different contexts throughout the sciences, in practice, often means to seek out scaling behavior and ultimately deduce a fractal dimension from a log-log plot of the box-counting function. Except for special mathematical sets such as the classical fractals, log-log plots of the box-counting function are never perfect straight lines. In other words, the box-counting dimension is generally nonconstant and a function of the measurement or observation scale and is strictly constant only in special cases (e.g., the classical fractals) [3].

The box-counting dimension has in fact quite often been observed to be a smooth or discontinuous function of the measurement scale. An example of the former case is fluid interfaces in turbulence [4] and an example of the latter is fracture networks in geophysics [5]. There are, however, very few examples for which the scale dependence of the box-counting dimension is understood analytically. One well-known theoretical example is the family of statistical mechanical models involving randomly distributed spheres, rods, and disks [6].

Interestingly, the box-counting dimensions of discrete quantum energy-level spectra have also been found to be smooth functions of the measurement scale [7]. The exact scale-dependent behaviors of the box-counting dimensions are not known analytically, and it is this particular problem that we wish to address in this Rapid Communication. Before we begin, it is important to establish the background to this problem.

In 1985, Cederbaum *et al.* [8] (CHP) defined a scale-dependent generalization of the box-counting dimension, which they called the "fractal dimension function," that depends on both the measurement scale and the number of elements in a given set. They applied it to discrete quantum spectra and found that different spectra (of a prescribed length) had different scale-dependent behaviors and that certain statistical properties of spectra essentially determined the behavior of their scale-dependent fractal dimension. CHP were also able to derive an analytical formula for the "fractal dimension function" of a finite discrete quantum spectrum, which interestingly they found depended on the nearest-neighbor spacing distribution (NNSD) of the spectrum *and* on the length of the spectrum (i.e., the number of energy levels in the sample). There are, however, serious problems that arise from the dependence on the number of energy levels, and some of these problems were pinpointed and discussed 12 years later in a paper by Wang and Ong (WO) [7].

WO argued that, for a discrete eigenvalue spectrum, the function $D_b(r)$ defined in the next section [see Eq. (3)], which is a formal scale-dependent generalization of the box-counting dimension, should only depend on the NNSD of the spectrum [9]. Although reasonable, their hypothesis lacked analytical proof in the sense that they could not give an explicit formula (exact or otherwise) for $D_b(r)$ in terms of the spacing distribution. WO computed $D_b(r)$ numerically for spectra having Poisson and Wigner spacing distributions and also for the vibrational spectra of the SO_2 molecule. The authors also stated that box-counting methods are amenable

to numerical implementation, but "will encounter difficulties when one attempts to search for an analytical solution." There is, in principle, no difficulty in seeking out an analytical solution, and in this Rapid Communication, we will derive an exact general formula for the (scale-dependent) box-counting dimension $D_b(r)$ of a discrete quantum spectrum using only elementary results from the statistical theory of spectra [10]. As we shall see, $D_b(r)$ does indeed depend only on the NNSD of the spectrum.

II. LOCAL BOX-COUNTING DIMENSION

To define the box-counting dimension, we first consider a uniform partition of the embedding space of a given set into a grid of nonoverlapping boxes of side length r. (The embedding space for an energy spectrum is $\mathbb{R}$, in which case the boxes are actually line segments of length r.) This grid of boxes is often called an r-mesh. Let $N(r)$ denote the number of boxes needed to cover the set, that is, the number of boxes that have a nonempty intersection with the set. The box-counting dimension D_b of a set can be defined as follows [2,3]:

$$D_b = -\lim_{r\to 0}\frac{d\,\log_a[N(r)]}{d\,\log_a(r)}, \tag{1}$$

where the base $a > 1$ is arbitrary. For a given set, the box-counting function $N(r)$ may or may not follow a power law of the form

$$N(r) \sim r^{-D_b}. \tag{2}$$

In the latter case, the given set possesses a scale-dependent geometry and the interest then lies in understanding the behavior of the box-counting dimension as a function of the measurement or observation scale r. In other words, the object of interest in such cases is the function

$$D_b(r) = -\frac{d\,\log_a[N(r)]}{d\,\log_a(r)}. \tag{3}$$

The above function is well defined provided $N(r)$ is a smooth function of the measurement scale. Note that $D_b(r)$ will be constant only when $N(r)$ is an exact power law and is nonconstant otherwise. The function $D_b(r)$ has several different names in the physics literature. For instance, in the well-known and often cited text by Takayasu [3], it is referred to as the "effective fractal dimension," so called after Mandelbrot, who in his book [1] discussed the notion of an "effective dimension" that depends on the resolution or the scale of measurement. We shall refer to $D_b(r)$ as the local box-counting dimension, which is the terminology used in Ref. [11].

III. DISCRETE EIGENVALUE SPECTRA

Suppose we are given a countably-infinite discrete spectrum for which the spacing s between adjacent energy levels is described by a probability density function $P(s)$ with mean $\bar{s} = \int_0^\infty s\,P(s)ds$. Consider the subset of the spectrum that lies in the interval $[\mathsf{E}_{\min},\mathsf{E}_{\max}]$ and partition this interval into $(\mathsf{E}_{\max} - \mathsf{E}_{\min})/r \equiv L/r$ intervals (boxes) of size r. Let $N(r)$ denote the number of these intervals that contains one or more eigenvalues. The fraction $N(r)/(L/r) = (r/L)N(r)$ of boxes that contain eigenvalues is equivalent to the probability $Q(r)$ that one of the boxes chosen at random contains one or more eigenvalues. This probability can alternatively be expressed as $Q(r) = 1 - E(r)$, where $E(r)$ is the probability that an arbitrary interval of length r (i.e., a box of length r chosen at random) contains *no* eigenvalues. Thus, the number of boxes needed to cover the subset of the spectrum lying in $[\mathsf{E}_{\min},\mathsf{E}_{\max}]$ is the number of intervals L/r multiplied by $Q(r)$:

$$N(r) = \frac{L}{r}[1 - E(r)]. \tag{4}$$

Using definition (3) and the fact that

$$\log_a[N(r)] = \log_a(L) - \log_a(r) + \log_a[1 - E(r)], \tag{5}$$

the local box-counting dimension $D_b(r)$ for a discrete energy-level spectrum is therefore

$$D_b(r) = 1 + \frac{r}{[1 - E(r)]}\frac{dE(r)}{dr}. \tag{6}$$

All that remains to determine is $E(r)$ and $dE(r)/dr$. Given $P(s)$, it is a relatively simple matter to write down an expression for $E(r)$.

In the statistical theory of spectra, the function $E(x)$ is known as the "gap probability" [12]. The link between $E(x)$ and $P(s)$ can be quickly established using elementary results from the statistical theory of spectra. We shall here simply quote the following identity from Ref. [10]: $dE(x)/dx = -(1/\bar{s})F(x)$, where $F(x)$ is the probability that there are no eigenvalues within a distance x of an eigenvalue chosen at random, or equivalently, the probability that the distance to the nearest neighbor is *greater* than x [13]. The complementary probability $\Psi(x) \equiv [1 - F(x)]$ is the probability that the nearest neighbor (to an eigenvalue chosen at random) is within a distance x. In other words, $\Psi(x)$ is the probability that the nearest-neighbor distance is *less* than or equal to x, which, by definition, is given by $\int_0^x P(s)ds$. Combining these two results yields the following identity relating $E(x)$ and $P(s)$:

$$\frac{dE(x)}{dx} = -\left(\frac{1}{\bar{s}}\right)[1 - \Psi(x)] = -\left(\frac{1}{\bar{s}}\right)\int_x^\infty P(s)ds. \tag{7}$$

Integrating Eq. (7), and noting that $E(0) = 1$, the probability that an arbitrary interval of length r does not contain any eigenvalues is

$$E(r) = 1 - \left(\frac{1}{\bar{s}}\right)\int_0^r [1 - \Psi(x)]dx. \tag{8}$$

Substituting (7) and (8) into (6) then immediately yields the following general formula for $D_b(r)$ in terms of $P(s)$:

$$D_b(r) = 1 - \frac{r\int_r^\infty P(s)ds}{\int_0^r\int_x^\infty P(s)ds\,dx}. \tag{9}$$

The above formula is the main theoretical result of this Rapid Communication [14]. Note that although $N(r)$ depends on L (and hence on the size of the sample spectrum), $D_b(r)$ is independent of L. Armed with formula (9), we are now in a position to derive the local box-counting dimension of specific sequences of levels.

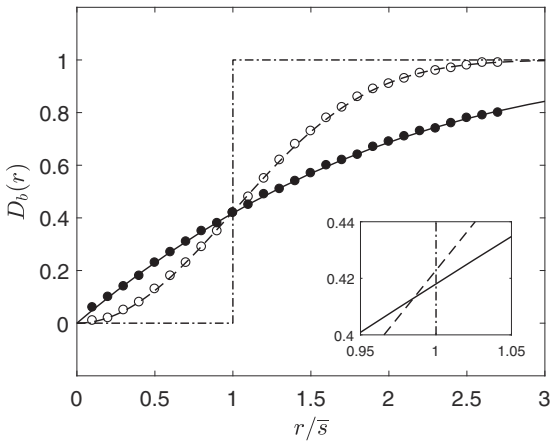

FIG. 1. The local box-counting dimension $D_b(r)$ versus $r/\bar{s}$ for energy-level spectra having Poisson and Wigner spacing distributions. The solid and open circles are the numerical values of the "effective fractal dimension" obtained by WO [7] for levels having Poisson and Wigner spacing distributions, respectively. The solid and dashed curves are the theoretical $D_b(r)$ formulas (11) and (13) obtained for levels having Poisson and Wigner spacing distributions, respectively. The dashed-dotted lines are for reference only and correspond to the special case of equally spaced levels. The inset shows a close-up view around the intersection of the two theoretical curves from which it is obvious that the Poisson and Wigner curves do not intersect at $r = \bar{s}$ (contrary to the observations of WO [7]).

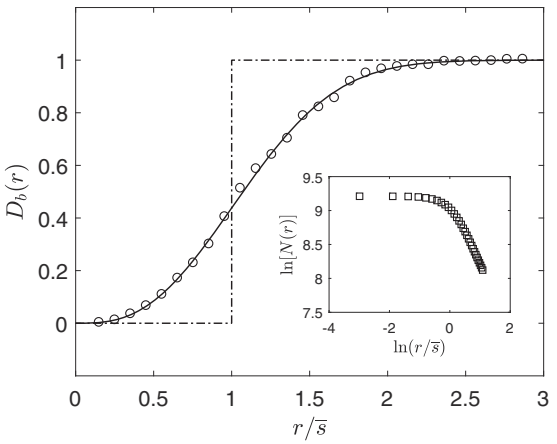

FIG. 2. $D_b(r)$ versus $r/\bar{s}$ for 10 000 high-lying zeros of the Riemann zeta function. The open circles are numerical derivatives calculated from the $\ln[N(r)]$ versus $\ln(r/\bar{s})$ data, which is shown as open squares in the inset. The solid curve is the theoretical $D_b(r)$ formula (15) obtained for levels having GUE spacing statistics. The dashed-dotted lines are for reference only and correspond to the special case of equally spaced levels.

IV. APPLICATIONS

A. Poisson spectra

The NNSD for an ordered sequence of independent random levels is given by [10]

$$P_P(s) = (1/\bar{s})\exp(-s/\bar{s}), \tag{10}$$

where again $\bar{s}$ is the mean spacing. Substituting (10) into (9) and performing the straightforward algebra yields

$$D_b(r) = 1 - \frac{(r/\bar{s})\exp(-r/\bar{s})}{1-\exp(-r/\bar{s})}. \tag{11}$$

This is displayed in Fig. 1, and for comparison, we also plot the "effective fractal dimension" data obtained numerically by WO for a Poisson spectrum. Note that 100 000 levels were used by WO to numerically compute $D_b(r)$. The WO data is in excellent agreement with formula (11).

B. GOE spectra

We seek here to obtain a closed-form approximation to $D_b(r)$ in the case of spectra that follow Gaussian orthogonal ensemble (GOE) statistics. In order to do so, we shall use the Wigner surmise for the GOE:

$$P_W(s;\beta=1) = \frac{\pi}{2\bar{s}}(s/\bar{s})\exp\left(-\frac{\pi}{4}(s/\bar{s})^2\right). \tag{12}$$

Although the above distribution (commonly referred to as the Wigner distribution) is an exact result only for real symmetric 2×2 random matrices, it serves as an excellent analytical approximation to the asymptotic Mehta-Gaudin distribution appropriate for arbitrarily large random matrices from the GOE [10]. Substituting (12) into (9) and performing the necessary algebra yields

$$D_b(r) = 1 - \frac{(r/\bar{s})\exp\left[-\frac{\pi}{4}(r/\bar{s})^2\right]}{\mathrm{erf}\left[\frac{\sqrt{\pi}}{2}(r/\bar{s})\right]}, \tag{13}$$

where $\mathrm{erf}(z)$ is the error function [16]. This result is displayed in Fig. 1 along with the "effective fractal dimension" that was calculated numerically by WO [7] for a spectrum possessing a Wigner spacing distribution (12). Once again, the WO data is in excellent agreement with formula (13).

C. GUE spectra

In the case of spectra that follow Gaussian unitary ensemble (GUE) statistics, a nonelementary closed-form approximation to $D_b(r)$ can be obtained by using the Wigner surmise for the GUE:

$$P_W(s;\beta=2) = \frac{32}{\pi^2\bar{s}}(s/\bar{s})^2\exp\left(-\frac{4}{\pi}(s/\bar{s})^2\right). \tag{14}$$

Although (14) is exact only for Hermitian 2×2 random matrices, it serves as an excellent analytical approximation to the asymptotic Mehta-Gaudin distribution appropriate for arbitrarily large random matrices from the GUE [10]. Substituting (14) into (9) and performing the necessary algebra yields

$$D_b(r) = 1 - \frac{(r/\bar{s})\left\{\mathrm{erfc}\left[\frac{2}{\sqrt{\pi}}(r/\bar{s})\right] + \frac{4}{\pi}(r/\bar{s})\exp\left[-\frac{4}{\pi}(r/\bar{s})^2\right]\right\}}{1-\exp\left[-\frac{4}{\pi}(r/\bar{s})^2\right] + (r/\bar{s})\mathrm{erfc}\left[\frac{2}{\sqrt{\pi}}(r/\bar{s})\right]}, \tag{15}$$

where $\mathrm{erfc}(z)$ is the complementary error function [16].

As a numerical example, we examine the local box-counting dimension of 10 000 high-lying zeros of the Riemann zeta function, in particular, the $(10^{22}+1)$th zero to

the $(10^{22}+10^{4})$th zero [17]. It is conjectured that (asymptotically) the zeta zeros have the same statistical properties as the eigenvalues of arbitrarily large random matrices from the GUE, and numerical observations so far corroborate this conjecture [18]. We computed the local box-counting dimension of the above-specified 10 000 zeros by calculating the average slope at each point of the numerically determined $\ln[N(r)]$ versus $\ln(r/\bar{s})$ plot. This is shown in Fig. 2. The theoretical $D_b(r)$ curve [Eq. (15)] accurately describes the numerically computed local box-counting dimension.

D. GSE spectra

In the case of spectra that follow Gaussian symplectic ensemble (GSE) statistics, a nonelementary closed-form approximation to $D_b(r)$ can be obtained by using the Wigner surmise for the GSE:

$$P_W(s;\beta=4)=\frac{2^{18}}{3^6\pi^3\bar{s}}(s/\bar{s})^4\exp\left(-\frac{64}{9\pi}(s/\bar{s})^2\right). \quad (16)$$

Substituting (16) into (9) and performing the necessary algebra yields

$$D_b(r)=1-\frac{(r/\bar{s})\left\{\mathrm{erfc}\left[\frac{8}{3\sqrt{\pi}}(r/\bar{s})\right]+\left[\frac{16}{3\pi}(r/\bar{s})+\frac{2048}{81\pi^2}(r/\bar{s})^3\right]\exp\left[-\frac{64}{9\pi}(r/\bar{s})^2\right]\right\}}{1-\left[1+\frac{16}{9\pi}(r/\bar{s})^2\right]\exp\left[-\frac{64}{9\pi}(r/\bar{s})^2\right]+(r/\bar{s})\mathrm{erfc}\left[\frac{8}{3\sqrt{\pi}}(r/\bar{s})\right]}. \quad (17)$$

As a numerical example, we computed the local box-counting dimension of 10 000 alternate levels of a GOE spectrum (consisting of 20 000 eigenvalues) by calculating the average slope at each point of the numerically determined $\ln[N(r)]$ versus $\ln(r/\bar{s})$ plot. This is shown in Fig. 3. As before, the theoretical $D_b(r)$ curve [Eq. (17)] accurately describes the numerically computed local box-counting dimension.

V. CONCLUSION

To summarize, we have provided an analytical theory for the local box-counting dimension of discrete quantum eigenvalue spectra. Our main formula [Eq. (9)] explicitly shows that the local box-counting dimension of a discrete spectrum depends only on its NNSD, as was first hypothesized two decades ago by Wang and Ong [7]. In fact, according to Eq. (9), the local box-counting dimension of a discrete spectrum is simply an integral transformation of its NNSD.

As applications of our theory, we derived an analytical formula for Poisson spectra and closed-form approximations to the local box-counting dimension for spectra having GOE, GUE, and GSE spacing statistics. In the Poisson and GOE cases, we compared our theoretical formulas with the published numerical data of WO [7] and observed impeccable agreement between their data and our theory. We also studied numerically the local box-counting dimensions of the Riemann zeta function zeros and the alternate levels of GOE spectra, which are often used as numerical models of spectra possessing GUE and GSE spacing statistics, respectively. In each case, the corresponding theoretical formula [Eq. (15) for GUE spectra and Eq. (17) for GSE spectra] was found to accurately describe the numerically computed local box-counting dimension.

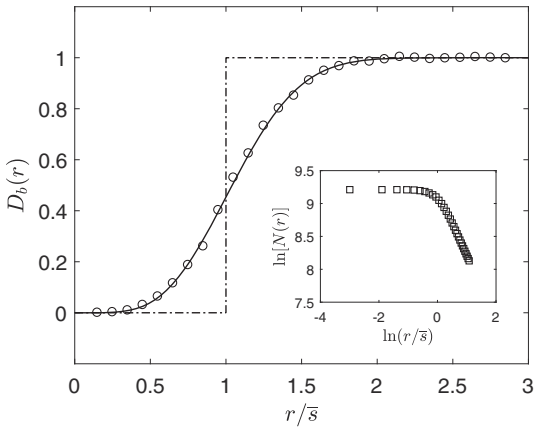

FIG. 3. $D_b(r)$ versus $r/\bar{s}$ for 10 000 alternate levels of a GOE spectrum (of length 20 000). The open circles are numerical derivatives calculated from the $\ln[N(r)]$ versus $\ln(r/\bar{s})$ data, which is shown as open squares in the inset. The solid curve is the theoretical $D_b(r)$ formula (17) obtained for levels having GSE spacing statistics. The dashed-dotted lines are for reference only and correspond to the special case of equally spaced levels.

Quantum eigenvalue spectra might appear to be just another mathematical playground for the tools of fractal geometry, and from the standpoint of the more general discussion given in the Introduction, discrete quantum spectra are indeed cited as just another example of point sets having a scale-dependent geometry. However, in quantum mechanics itself, the geometric scaling properties of energy-level spectra have a much more profound significance (see, for example, Refs. [19–23]). So, unlike in many lines of research where fractal geometry has been adopted mainly as a descriptive tool, applying the concepts of fractal geometry to quantum eigenvalue spectra is not merely for descriptive purposes.

We conclude with the following clarification, which is important in the above context. WO think of discrete spectra as "sets of a series of discrete points that exhibit fractal properties," or more simply, as "fractal sets." Unless it is made absolutely clear *in what sense* discrete spectra are fractal sets, it is ambiguous (and even wrong) to refer to them as such [24]. By merely computing $D_b(r)$ for a discrete spectrum, one has not (to quote WO) "investigated the fractal properties" of the spectrum. In fact, the numerical studies of WO clearly demonstrate that discrete quantum spectra do not have box-counting type scaling behavior (i.e., no "fractal structure" defined in terms of a constant box-counting dimension) and thus have a scale-dependent geometry.

ACKNOWLEDGMENT

The authors thank A. M. Odlyzko for providing open access to the Riemann zeta function zeros.

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