Fractal potentials from energy levels

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We analyze the reconstruction by Wu and Sprung [Phys. Rev. E 48, 2595 (1993)] of a fractal onedimensional potential, the quantum spectrum of which reproduces the first 500 nontrivial zeros of the Riemann ζ function. Our construction is based on a spectrum with Gaussian unitary ensemble statistics as far as the nearest-neighbor spacing distribution is concerned. Our results show that a reliable estimate of the fractal dimension of the potential necessitates a very large number of levels.

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In a previous publication [1], Wu et al. have addressed the problem of quantum chaos from a novel and interesting angle. The common lore in the domain is that (classically) nonintegrable Hamiltonians show level repulsions in their quantum spectrum and the conjecture of Bohigas. Giannoni, and Schmit [2] has made this statement more specific, relating the spectral statistics to that of an appropriate ensemble of random matrices. Sprung and collaborators have challenged this statement by exhibiting one-dimensional (1D) Hamiltonians (which by definition are classically integrable) which show the same level repulsion as the one expected in the case of quantum chaos. This last point is intriguing, since any smooth 1D potential would lead to a spectrum that would locally look as that of a harmonic oscillator, i.e., exhibiting evenly spaced levels. The key word in the preceding remark is "smooth." Indeed, the statements concerning the spectral behavior of a given potential are based on a smoothness assumption (that is sometimes only implicitly made). Wu et al. have shown that if one relinquishes this requirement one has considerable freedom and can obtain practically any spectral behavior in 1D Hamiltonians. They have thus shown that Gaussian orthogonal ensemble (GOE)-type statistics for the nearest-neighbor spacing distribution (NNSD) can be obtained from a 1D nonsmooth potential provided the curve V(x) is appropriately fractal. In a recent publication, they have addressed the question of reconstructing the fractal potential that would have its energy levels at the position of the zeros of the Riemann ξ function [3]. They have estimated the fractal dimension from a reconstruction of the potential from N=100, 300, and 500 levels and obtained the value D = 1.5 for N = 500.

In this Comment we examine the problem of the estimation of the fractal dimension of the potential from a finite number N of fitted levels. We show that the convergence of the value of the fractal dimension as a function of N is very slow. Thus, a realistic estimate necessitates a

very large number of levels (and correspondingly large computing time). The all important ingredient of our approach is the method for the solution of the inverse problem, namely, the reconstruction of the potential from a given sequence of energy levels. We have explained this method in [4] but we summarize it below for the sake of completeness. It is based on the techniques developed in relation to integrable nonlinear evolution (soliton) equations, although this statement has only a historical significance: the "dressing" transformation we shall introduce in the next paragraph is obviously related to the quantum inverse problem.

We start with the 1D stationary Schrödinger equation for the motion of a particle in a potential V(x) (in units $\hbar^2/2m=1$):

$$-\Psi'' + V(x)\Psi = \epsilon \Psi . \tag{1}$$

When ϵ is the deepest eigenvalue ϵ_0 in the potential V(x), then $\Psi_0(x)$ is decreasing exponentially at both $\pm \infty$ without any node in between. If we choose now some $\epsilon < \epsilon_0$ then if we consider the solution Ψ_\pm of Eq. (1) with asymptotic behavior exponentially decreasing as $x \to \pm \infty$ we find that it diverges exponentially as $x \to \mp \infty$ without any node in between. Then from the Ψ_\pm we can obtain a function Ψ diverging at both $\pm \infty$ with no nodes in between simply through a linear combination of the Ψ_\pm with positive coefficients. Inverting Ψ , we obtain a finite (non-normalized) wave function $\Phi=1/\Psi$ decreasing at both infinities. Thus Φ can be considered as the lowest eigenfunction of some potential W with eigenvalue ϵ

$$-\Phi'' + W(x)\Phi + \epsilon\Phi . (2)$$

Thus, starting from a given potential V(x) one computes the diverging solution Ψ associated with some energy ϵ and through the relation $\Phi=1/\Psi$ one obtains an eigenfunction of a new potential (at precisely energy ϵ). This is the essence of the dressing transformation and we shall show how it can be explicitly obtained. First we introduce the logarithmic derivatives $f = -\Psi'/\Psi$ and $g = -\Phi'/\Phi = -f$. Equations (1) and (2) become

$$f' - f^2 + V(x) = \epsilon , \qquad (3a)$$

$$g'-g^2+W(x)=\epsilon. (3b)$$

Adding (3a) and (3b), given that g = -f, we obtain

$$W(x) = 2\epsilon + 2f^2 - V(x) . \tag{4}$$

The dressing transformation (4) is well-known in the domain of nonlinear evolution equations. In fact, it allows us to construct the multisoliton solutions of the Korteweg-de Vries (KdV) equation, starting from the vacuum solution [5]. The main advantage of this transformation is that the addition of each soliton does not modify all the previous eigenvalues.

Now let us describe our method of construction of the potential. First, we give a spectrum $\epsilon_0, \epsilon_1, \ldots, \epsilon_{N-1}$. The important point is that the potential will be constructed "top down" in such a way as to have exactly N negative eigenvalues ϵ_0 , ϵ_1 , ..., ϵ_{N-1} and $\epsilon_N = 0$. We start with an initial potential V(x)=0 and solve Eq. (3a) for f with $\epsilon = \epsilon_{N-1}$. The only free parameter in the Riccati (3a) is f(0) and taking f(0)=0 guarantees that Ψ is the even solution that has no nodes. Once f is obtained (numerically) one constructs W(x) from (4). Starting with this as a new potential one adds a further eigenvalue ϵ_{N-2} , and so on. The choice f(0)=0 has for consequence that the final V(x) is even. The efficiency of the dressing transformation for the reconstruction of the potential has been largely tested in [4]. We should also point out that, since no parameters' search is involved in this construction, the computations involved are most economical.

The great advantage of the method is that it allows a step by step reconstruction of the potential, although, admittedly, since this is a top-down construction, the number of levels must be fixed in advance (unless the statistics of the states is independent on the energy). The numerical precision is thus optimal and since the computations involved are moderate we can easily achieve an improvement by orders of magnitude over the result of Wu and Sprung as far as the number of levels is concerned.

The main aim of this Comment is not to present an accurate estimate of the fractal potential with a spectrum corresponding to the zeros of the Riemann ζ function, but rather to show that such an estimate is very difficult to obtain from numerical evaluations. Thus we need not include the fine details of the spectrum, i.e., use the precise zeros of the Riemann ζ function, but may restrict ourselves to their statistical properties, and in particular on the behavior of the fluctuating part of the spectrum. For the latter, it is known that the NNSD obeys Gaussian unitary ensemble (GUE) statistics, i.e., the levels show quadratic repulsion [6,7]. Although the full GUE result cannot be given in closed form, a simple representation of a GUE-type distribution can be obtained from a 2×2 unitary matrix model and reads [8]:

$$p(s) = \frac{32}{\pi^2} s^2 e^{-4s^2/\pi}$$
.

This estimate will be sufficient for our study. The setting is now fixed. We start with a spectrum with level spacing equal to unity. This would lead to a smooth harmonic potential, which is indeed the dominant behavior of the smooth potential related to the Riemann ξ zeros (up to logarithmic corrections). Next, we perturb this spectrum so as to obtain a GUE spacing distribution. We thus obtain a set of levels and solve the inverse problem for the potential using the dressing transformation. The result for the reconstructed potentials are given in Fig. 1. A blowup of the region around the origin is shown for three different numbers of levels 500, 4000, and 32 000. The building up of the fractality is clear.

This becomes even clearer when a qualitative estimate of the fractal dimension is obtained. For this we use the

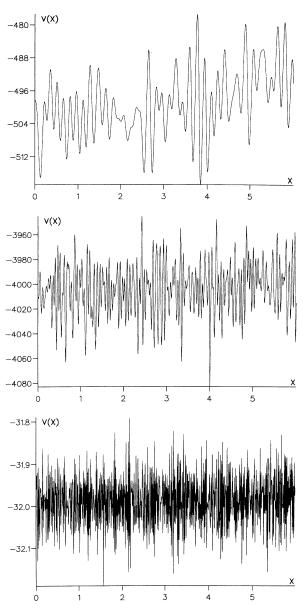


FIG. 1. Blowup of the potential (around its minimum) reconstructed with (a) N=500, (b) N=4000, and (c) $N=32\,000$ levels.

same box-counting techniques as in [1]. We start by considering a region over which the curve oscillates in (roughly) the same way. Practically, this means that we are limiting ourselves to x close to the origin. We choose a rectangular region just high enough to include all the oscillations of the potential and we normalize the axes so that this rectangle becomes a square with side length equal to 1. Next, we cut our square into n^2 elementary squares of size dx = 1/n and count the number P of squares that contain a portion of the curve of the potential. Finally, we plot ln(P dx) as a function of ln(dx). The typical result is a curve with the aspect of a hyperbolic tangent: constant values for very small or very large dx and a region with roughly constant slope in between. The slope of this intermediate region is just 1-Dwhere D is the fractal dimension. Figure 2 contains the results for all the numbers of levels examined from N=250 to 32 000. The steepening of the slope with increasing N is evident, indicating that the fractal dimension grows. This is better seen in Fig. 3, where we show the fractal dimension D as a function of $\ln N$. We remark that, although a large number of levels has been used, no convergence has been attained. Thus we cannot assign a precise value to the fractal dimension of the potential; all the more so, since the determination of D with the boxcounting technique somewhat depends on the size of the region under analysis. Still, it is clear that the value 1.5 of the fractal dimension obtained by Wu and Sprung, although fairly accurate for N=500, is far from the asymptotic $(N \rightarrow \infty)$ value.

Let us conclude with some general remarks concerning the fractality of the potential related to a GUE level statistics. A visual examination of the potential in Fig. 1 reveals no resemblance to a random walk (which is what we would expect if the fractal dimension were indeed 1.5) [9]. The potential looks more like white noise. This model predicts the value D=2 for the fractal dimension. Indeed, there are reasons to believe that the dimension is that of the white noise.

From the general KdV theory the potential is given by

$$V = \sum a_n |\psi_n|^2 ,$$

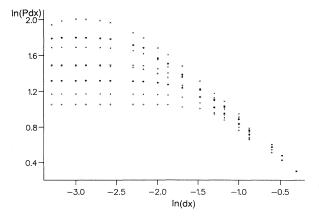


FIG. 2. Box-counting estimate of the fractal dimension for the potential reconstructed with N=250, 500, 1000, 2000, 4000, 8000, 16 000, and 32 000 levels.

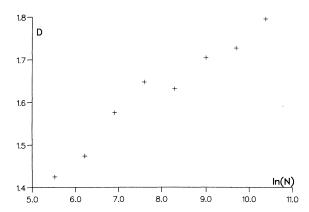


FIG. 3. Fractal dimension D as a function of the number N of levels used in the recontruction of the potential (on a semilogarithmic scale).

where a_n vary slowly with n and ψ_n is the normalized solution of KdV corresponding to the level ϵ_n . This function has an oscillating behavior $\cos\phi_n(x)$ [where $d\phi_n(x)/dx = \sqrt{\epsilon_n - V}$] over a domain of size L_n where $\epsilon_n > V$, and vanishes rapidly outside this domain. Thus the oscillatory part of $|\psi_n|^2$ is of order $\cos 2\phi_n(x)/L_n$. By adding the contributions arising from an unperturbed spectrum one obtains a smooth potential V, i.e., the oscillations in the $|\psi_n|^2$ cancel out. However, if the spectrum is perturbed, for instance by a random component as in the case treated above, the oscillatory part does not vanish but rather becomes, near the minimum V_0 of the potential (with $k_n = \sqrt{\epsilon_n - V_0}$)

$$\delta V = \sum \frac{\delta \epsilon_n}{\Delta \epsilon_n} \frac{1}{L_n} \cos(2k_n x - \varphi_n) ,$$

with φ_n independent of x. The summation can be approximated by an integral,

$$\delta V = \int_{k_{\rm min}}^{k_{\rm max}} \frac{\delta \epsilon}{\Delta \epsilon}(k) \frac{1}{L(k)} \cos[2kx - \varphi(k)] \frac{dn(k)}{dk} dk \ .$$

In fact, since $n(k) \sim kL(k)$, the factor [1/L(k)][dn(k)/dk] is essentially constant. The integration limits k_{\min} and k_{\max} are related to the inherent cutoffs of the problem: k_{\min}^2 is related to the $\Delta \epsilon_n$ for n small and k_{\max}^2 to the total depth of the potential $-V_0$. The factor $\delta \epsilon_n/\Delta \epsilon_n$ is the random factor with a zero mean and a deviation which we may specify as a function of k.

In order to estimate the fractal nature of the potential, we compute the mean value over x of $|\delta V|^2$ and $|\delta V'|^2$ of the square of the potential and of its derivative. We have

$$\frac{|\delta V'|^2}{|\delta V|^2} \sim \frac{\int \left[\frac{\delta \epsilon}{\Delta \epsilon}\right]^2 k^2 dk}{\int \left[\frac{\delta \epsilon}{\Delta \epsilon}\right]^2 dk}.$$

In the present case of a constant deviation $\delta \epsilon/\Delta \epsilon$ the (divergent) integrals are both dominated by $k_{\rm max}$ and thus

$$\frac{|\delta V'|^2}{|\delta V|^2} \sim k_{\max}^2.$$

Thus, qualitatively, $|\delta V'|/|\delta V| \sim k_{\max}$ and the curve V(x) fills the plane up to the smallest scale present, $1/k_{\max}$. In the limit $N \to \infty$, the fractal dimension is thus D=2. This, of course, depends on the behavior of $\delta \epsilon/\Delta \epsilon$. We expect, however, the result D=2 to be valid not only for the GUE-like spectrum analyzed here but for most constant-deviation perturbations of realistic spectra. However, when this factor has a strong k dependence, then the result can be different. For instance, if we

choose $\delta\epsilon/\Delta\epsilon\sim 1/k$, we get the random-walk spectrum proportional to $1/k^2$ and though the integral for $\delta V'^2$ is still dominated by the cutoff at $k_{\rm max}$, it is now the other cutoff at $k_{\rm min}$ which dominates the integral for δV^2 . We thus have $|\delta V'|/|\delta V|\sim (k_{\rm min}k_{\rm max})^{1/2}$ leading to a fractal dimension of D=1.5.

Thus generalizing from our GUE results, we believe that the one-dimensional potentials with a spectrum that reproduces the imaginary part of the nontrivial zeros of the Riemann ζ function has a white-noise aspect and a fractal dimension equal to 2.

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