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Some elementary questions in the theory of quasiperiodic heterostructures

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Abstract

The characterization of the spectrum of eigenstates of quasiperiodic heterostructures is discussed by focusing on three questions. Arguments are advanced to justify the often indiscriminate use of different approximants in the calculation of the eigenvalue spectra. It is stressed that the calculation of the fractal dimension may be rather inaccurate if the high eigenvalue range is not included, even if physically the interest is limited to the low range. The question of self-similarity is critically examined and found to have a very limited range of validity in practice. The unique properties of the Rudin–Shapiro sequence are also stressed.

1. Introduction

Quasiperiodic, or quasiregular, heterostructures (henceforth QH) follow an algorithmic sequence S based on some self-replicating rule like, say, the Fibonacci sequence and many others. There is a great deal of current work on QH and numerous references can be found in two recent reviews [1, 2]. This article is actually not concerned with any specific case, but with some broad issues, and for this it will suffice to consider mathematically simple problems described by a single, linear, ordinary, second-order differential equation. The problem is actually three dimensional, but with a sequence of planar interfaces, after two-dimensional in-plane Fourier transformation, it becomes mathematically a one-dimensional problem. This will be commented on later.

Having thus simplified the situation we address three elementary questions. Firstly, in practice, both theoretically and experimentally, one does not form the full infinite sequence S_∞, but reaches only up to some finite generations S_N in the repeated application of the self-replicating rule. It is reasonable to expect that, for sufficiently large N, S_N will display essentially the features of the ideal infinite sequence, and thus one takes S_N as an acceptable

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numerical approximation. But this raises the question of boundary conditions (BC) at the extremes of the finite heterostructure. The second question concerns some technical aspects related to the fractal analysis of the spectra of these systems and the third one concerns the question of self-similarity.

The main point of this paper is to stress that some of the claims often made lack a formal mathematical justification and to demonstrate how a fractal analysis may require considerable care in order to ensure correct results. However, while often it is not possible to provide formal conclusive proofs, one can design some suggestive numerical experiments. These are presented in section 2, together with the discussion of the first question. Furthermore, the question of the often-claimed self-similarity is examined in section 3. Final comments are made in section 4.

2. Fractal analysis of the spectra of QH

We shall consider two elementary problems, namely, (i) electronic states described by a one-band effective-mass model and (ii) pure shear elastic waves propagating along a symmetry direction of cubic materials—the vibration amplitude, along an equivalent cubic symmetry axis, is perpendicular to the propagation direction, which is the growth direction of the heterostructure, and parallel to the interfaces. The differential equation is the same in both cases but they may admit different BC. Moreover, while the long-wavelength Debye model for shear waves in a solid crystal requires an upper bound in the spectrum in order for the model to be physically meaningful, the spectrum of electronic states has no upper bound, a fact with an implication for the fractal analysis which will be presently discussed.

We have studied two types of QH, one based on the Fibonacci sequence, which is the most commonly studied, and the other one on the Rudin–Shapiro sequence, which presents some intriguing features. We thus have four different systems, namely:

(1) Electronic states. Fibonacci sequence. A = $Al_{0.35}Ga_{0.65}As$, B = GaAs, $m_A = 0.096m_0$, $m_B = 0.067m_0$, $V_A = 379$ meV, $V_B = 0$, $d_A = 8.4$ Å, $d_B = 16.8$ Å. This system was studied in reference [3].

(2) Elastic shear waves. Fibonacci sequence. A = AlAs, B = GaAs, $d_A = 17$ Å, $d_B = 42$ Å. Mass densities and stiffness coefficients in table 1.

Table 1. Mass densities and stiffness coefficients employed in the calculations concerning elastic shear waves for the systems described in the text.

	ρ (kg m^{-3})	C_{44} (10^{10} N m^{-2})
GaAs	5316.9	5.94
AlAs	3721.8	5.42

(3) Electronic states. Rudin–Shapiro sequence. The constituent slabs A and C are as in system 1, with the same parameters. We generate the successive generations by starting with an alphabet of four letters, A, B, C, D and applying the substitution rules

$$\xi(\mathrm{A}) = \mathrm{AC} \qquad \xi(\mathrm{B}) = \mathrm{DC} \qquad \xi(\mathrm{C}) = \mathrm{AB} \qquad \xi(\mathrm{D}) = \mathrm{DB} \qquad (1)$$

corresponding to this sequence [2, 4–7]. The constituent slabs A and B are as in system 1 and then we make C = A and D = B.

(4) Elastic shear waves. Rudin–Shapiro sequence constructed as in system 3, with constituent slabs A and B as in system 2.

Now, consider a finite realization S_N of a given sequence S for N—the generation—finite though largish. We then define as an *approximant* the problem defined by S_N with given BC at both extremes—not to be confused with the matching boundary conditions to be imposed at the interfaces. The *periodic approximant*, defined by Born–von Karman periodic boundary conditions at the extremes of S_N, is actually a superlattice in which S_N is the period. The term *Fibonacci superlattice*, for instance, is often—though not always—used in this sense, but at other times it denotes simply the finite generation F_N without being too explicit about BC. Given any sequence S_N we shall consider three different approximants defined by the BC, namely:

(i) Periodic BC. This is the periodic approximant, just defined. This can serve to model the case of propagating states. An approximant in the same spirit would assume semi-infinite media—A or B—at both ends of S_N.
(ii) Dirichlet BC, in which the amplitude vanishes at the boundaries. This corresponds to infinite barriers for electronic states or rigid walls for elastic waves.
(iii) Von Neuman BC, in which the derivative vanishes at the boundaries. This corresponds to freely vibrating surfaces.

The calculations were performed by using a full transfer matrix which transfers amplitudes and derivatives [8].

Now, consider the fractal analysis of the spectra of such systems. We concentrate on the *generalized box-counting dimension* $D(q)$, where q is a continuous parameter ranging from $-\infty$ to $+\infty$, which is related to the function $f(\alpha)$, which describes the spread of values of the scaling index α over the different regions of the spectrum [9–14]. It is proved quite generally that $D(q)$ varies between the values

$$D_{max} = D(-\infty) \leqslant 1 \qquad D_{min} = D(+\infty) \geqslant 0. \tag{2}$$

Moreover, α spans a range of values—where $f(\alpha) > 0$—with lower and upper bounds [12]

$$\alpha_{min} = D_{min} \qquad \alpha_{max} = D_{max}. \tag{3}$$

Practical aspects of the numerical computation of $D(q)$ and $f(\alpha)$ were discussed in reference [2], where it was stressed that in the case of electronic states this requires special care for q large and negative, which is precisely the region for which thorough knowledge is needed in order to evaluate $f(\alpha)$ correctly as α approaches α_{max}.

Now, in the study of electronic spectra of QH, attention is often focused on the low-energy range, but an accurate evaluation of $D(q)$ for q negative and large depends critically on including a sufficiently large range of the high-energy part of the spectrum. In fact [2], since the energy of the electronic states has no upper bound,

$$\lim_{q \to -\infty} D(q) = 1 \tag{4}$$

which is intuitively to be expected because for increasingly high energies the electronic states tend to behave increasingly like free electrons, with a spectrum which is absolutely continuous and has therefore a fractal dimension equal to unity [4–7].

Figure 1 gives $D(q)$ for system 1—full line. The calculations were done for the generation $N = 18$ and in a few cases checked up to $N = 20$ without any significant numerical changes. The energy range included values from V_B up to $V_B + 50(V_A - V_B)$, close to 19 eV above the bottom of the well material (GaAs). It is seen that, as expected, the upper bound of $D(q)$ is 1. Thus the curve $f(\alpha)$ reaches up to $\alpha = 1$, as expected.

The calculations were done with (a) infinite barriers and (b) periodic approximants, with apparently the same results. This is easy to understand if we define a 2-vector Ψ and 2×2

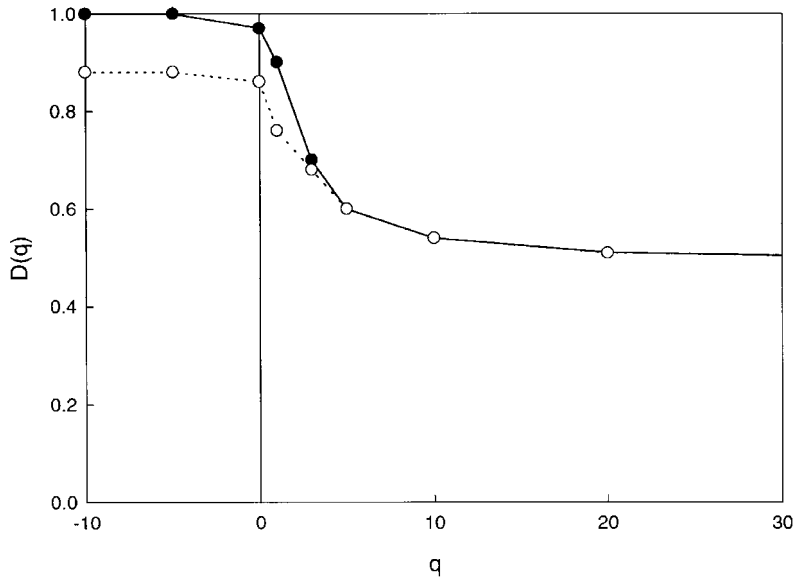

Figure 1. The generalized box-counting fractal dimension $D(q)$ for system 1—see the text. Full line: results obtained by covering the energy range from $V_B + 50(V_A - V_B)$. Dashed line: results obtained by including only the energy range from V_B to V_A.

real energy-dependent transfer matrix $\mathbf{T}$ by [8]

$$\Psi(z) = \begin{bmatrix} \varphi(z) \\ \varphi'(z)/m \end{bmatrix} \qquad \Psi(z) = \mathbf{T}(z, z_0) \cdot \Psi(z_0). \tag{5}$$

Then the two-component 'vector' transferred by $\mathbf{T}$ is continuous across the heterostructure extending from $z = 0$ to $z = L$, the length of the finite realization S_N of the QH under study. Infinite barriers at the boundaries require $\varphi(L)$ to vanish which, by (5), requires

$$T_{12}(L, 0) = 0. \tag{6}$$

This is the secular equation yielding the eigenvalues if this approximant is used. Now consider the periodic approximant. Then the Born–von Karman BC read, putting $\mathbf{T} \equiv \mathbf{T}(L, 0)$,

$$\begin{aligned} &(T_{11} - \mathrm{e}^{\mathrm{i}kL})\Psi_{1k}(0) + T_{12}\Psi_{2k}(0) = 0 \\ &T_{21}\Psi_{1k}(0) + (T_{22} - \mathrm{e}^{\mathrm{i}kL})\Psi_{2k}(0) = 0. \end{aligned} \tag{7}$$

If we solve this problem, then we find the minibands of the superlattice formally defined and, in each miniband, E is a function of k. We now ask whether there are any solutions of equation (6), the infinite-barrier approximant, for which equations (7) are satisfied. Then, since $\varphi_k(0)$ vanishes and, by assumption, this happens for an energy at which T_{12} also vanishes, we are led to

$$T_{22} = \mathrm{e}^{\mathrm{i}kL}. \tag{8}$$

But the matrix $\mathbf{T}$ is real and this leaves two possibilities. One is that kL is real and a multiple of π. Then the energy eigenvalue is at a band edge of the minibands. The other one is that kL is complex, the real part being a multiple of π. Then E is a forbidden energy value corresponding to that complex value of k for which (8) is satisfied in a real energy loop spanning a gap of the miniband spectrum of the periodic approximant.

Whether inside the gaps or just at their boundaries, the two sets of eigenvalues are topologically equivalent among themselves and equivalent to the spectrum of eigenvalues yielded by equation (8). It is easily seen that the same analysis holds for approximant (iii) with φ' instead of φ and T_{21} instead of T_{12}. Thus the result of the fractal analysis is the same irrespective of the choice of approximant provided that the calculation employing (i) is carried out just for one reduced value of k, say, $k = 0$ in a folded scheme with all minibands in the first 1D Brillouin zone, so one picks out a sequence of successive band-edge levels. Note that one may even choose approximant (iii) for electrons, although it is in itself physically meaningless. Studies of QH are very abundant in the literature and results are often reported without always specifying the type of approximant involved. The point of this analysis is to stress that all commonly employed approximants are formally acceptable and yield topologically equivalent results provided that the high-energy range—in the case of electrons—is properly covered.

In an interesting study of optical spectra of a Fibonacci heterostructure [3], corresponding to system 1 described above, the analysis focuses on the low-energy range involved experimentally in optical transitions. The scaling factor α appears to attain a maximum value short of unity. Figure 1—dashed line—shows $D(q)$ calculated by taking only the part of the spectrum of energy states between V_B and V_A—that is, in the wells of the heterostructure. This yields $D(+\infty) = 0.50$, $D(0) = 0.76$ and $D(-\infty) = 0.88$, quite in line with the results of reference [3], which illustrates the importance of the high-energy range for an accurate characterization of the topological properties of the spectrum, even if one analyses experiments involving only lower energies.

We now consider the Rudin–Shapiro (henceforth R–S) sequence, which is in some respects rather special. For all other self-replicating sequences commonly studied, the conditions for the application of the Bovier–Ghez theorem hold [6,7] and one can then prove that the spectrum is singular continuous, and therefore with fractal dimension <1. Then $D(q)$ takes values between 0 and 1. It was pointed out in reference [2] that this does not hold for the R–S sequence. Now, the fact that the Bovier–Ghez theorem cannot be applied only means that it cannot be proved that the spectrum must be singular continuous, but the possibility is not excluded. It only means that the issue is uncertain and the spectrum may be singular continuous—with values of $D < 1$—or absolutely continuous with all $D = 1$.

In the absence of a formal mathematical foundation one can only carry out some numerical experiments. In one, reported in reference [2], D was found to be constant and equal to unity within the attainable numerical accuracy, which is not a conclusive proof, but it is a very striking example of a QH which is based on a self-replicating sequence but appears to have an absolutely continuous spectrum. We have performed another two numerical experiments on R–S heterostructures. One is for system 3 (electronic states), generation $N = 11$, and the other one for system 4 (elastic waves), generation $N = 16$. The full $D(q)$ curve was calculated and some results again checked by—partial—independent calculation employing a different approximant. It is clear that a calculation reaching up to the very high part of the spectrum may become physically meaningless for elastic waves if the Debye cut-off is exceeded, but in any case it is a legitimate formal system for a numerical experiment. Table 2 gives the key

Table 2. Characteristic values of the generalized box-counting fractal dimension obtained for systems 3 and 4 described in the text.

System	$D(-\infty)$	$D(0)$	$D(+\infty)$
3: electrons	1	0.97	0.65
4: shear waves	1	0.92	0.87

results for the two systems. In both cases the spectrum is fractal, which again is a possibility which cannot be ruled out.

We note that in both of these cases, while the sequence is R–S, only two different constituent slabs are involved, as in both we have taken C = A and D = B, while in the numerical experiment of reference [2] A, B, C and D were all different. Whether or not this is significant, it does suggest that the R–S case deserves a great deal more detailed study.

3. Morphological aspects: the question of self-similarity

It is known from general theory of fractal objects [11, 12] that strict self-similarity, which requires that the entire object be reproduced by magnification of any chosen segment, is not entirely possible if the system is multifractal—that is to say, if different scaling factors are involved. Now, in all physical models commonly studied, even in the simplest ones, the spectra are actually multifractal [2]—leaving aside for the time being the R–S sequence. This suggests severe reservations as regards unproved claims to having found self-similarity, a concept which is not usually defined in a precise manner and largely remains in essence a matter of visual appreciation. The integrated density of states (IDOS) is usually claimed to be a self-similar devil's staircase, but this was critically scrutinized for a simple Fibonacci heterostructure by detailed examination of different magnifications and shown to hold only approximately and for the lowest part of the spectrum only [2]. We have encountered the same situation for the IDOS of system 2—shear waves—calculated with a periodic approximant.

In view of the fractal structure obtained for the R–S heterostructures of systems 3 and 4—table 2—we have calculated the IDOS for the low part of the spectrum in both of these cases. The results are shown in figure 2. One expects the R–S sequence, being as it is a self-replicating one, to have properties different from those of a regular periodic sequence—a superlattice—especially after inspecting the results shown in table 2 for systems 3 and 4, but the results of figure 2 show that the IDOS is definitely not self-similar, even approximately.

The ground-state wavefunction is often presented as evidence of self-similarity. Figure 3(a) shows the ground-state ($n = 1$) wavefunction for system 1 obtained with a type (ii) approximant. Although the term requires more precise definition, one could say that this has some self-similar appearance in the usual somewhat loose sense, but this is totally lost as soon as we go up to any higher state. Figure 3(b) shows the wavefunction for $n = 10$, with no trace of self-similarity. Finally, figure 3(c) shows the ground-state wavefunction for the R–S heterostructure of system 3. The difference between figures 3(c) and 3(a) is quite striking. All one can say is that this R–S heterostructure localizes the ground state rather strongly, with again no trace of self-similarity. A similar result is obtained with tight-binding models [15].

4. Final comments

We have seen that if the purpose is to perform a fractal analysis, different approximants have topologically equivalent spectra and thus can be alternatively chosen. Some approximants might be intrinsically inadequate for studying a specific physical problem—like infinite barriers for the transmittance across the QH, for instance—but they are all valid alternatives for the fractal analysis.

We have verified that an accurate evaluation of the $f(\alpha)$ function requires $D(q)$ to be reliably estimated for q large and negative and this, for a spectrum with no upper bound, like that of electronic states, requires including up to a rather high range of the spectrum even if one

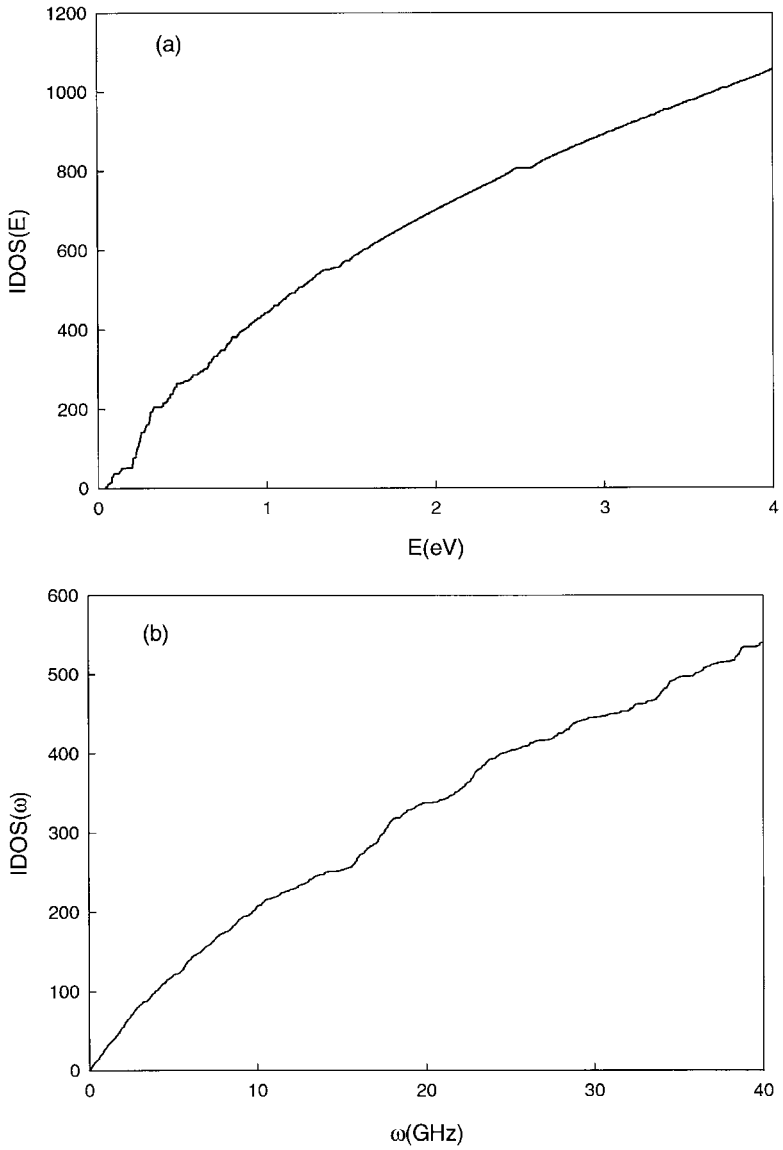

Figure 2. The integrated density of states for the low part of the spectra of (a) system 3—electronic states—and (b) system 4—elastic shear waves.

analyses experiments involving only the lower part. This is a note of caution as regards many calculations encountered in the literature, where only a part of the spectrum is considered.

For all self-replicating sequences commonly studied so far, except for the Rudin–Shapiro one, the Bovier–Ghez theorem establishes that the spectrum is singular continuous and, whenever $D(q)$ has been evaluated, it has been found that D varies with q. This means that the spectrum is not only fractal, but *multifractal* and therefore there are different scaling factors.

This rules out strict self-similarity, although some partial results, partially considered, might have a self-similar appearance. The ground-state wavefunction is sometimes claimed as evidence of self-similarity, but we have seen that this soon changes as we go up to states

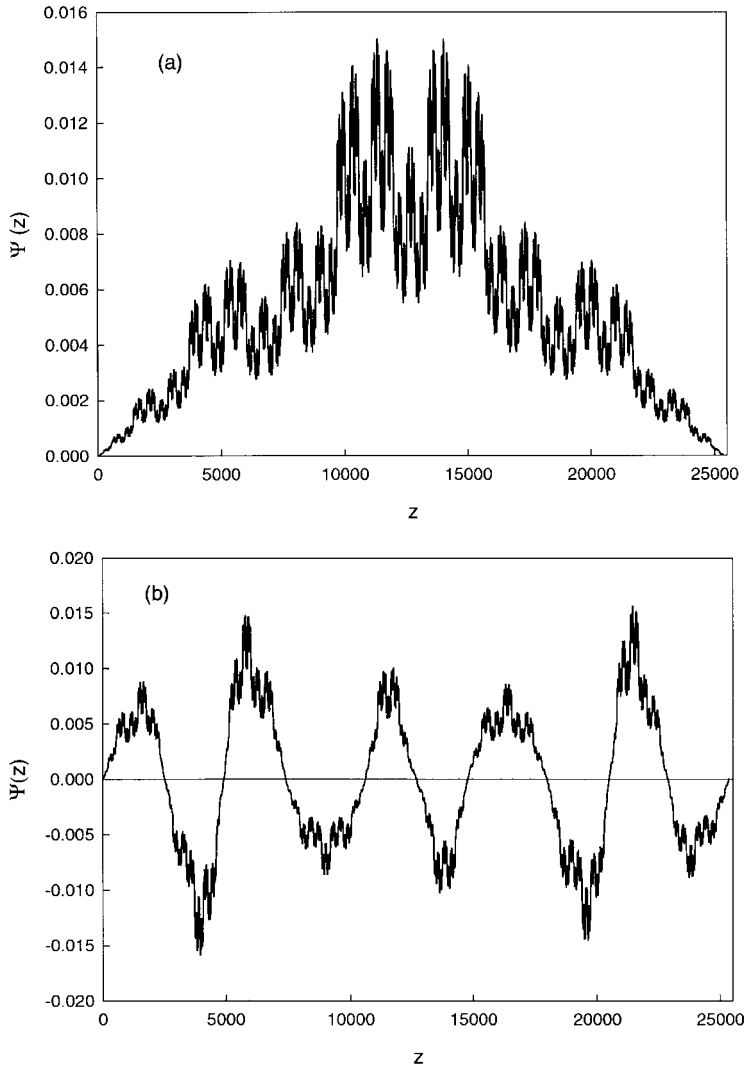

Figure 3. Electronic wavefunctions obtained with a type (ii) approximant. (a) System 1—Fibonacci sequence. Ground state, $n = 1$. (b) System 1. Excited state, $n = 10$. (c) System 3—Rudin–Shapiro sequence. Ground state, $n = 1$. The calculations were performed for the generation $N = 16$ in the first two cases, involving 988 interfaces, and for $N = 11$, involving 1025 in the third case. The amplitudes correspond to normalized bound-state wavefunctions and the distances are given in units of the Bohr radius, 0.5292 Å.

only slightly above. Similarly, only a reduced range of the low-energy part of the spectrum resembles a devil's staircase and there, again, this soon ceases to stand scrutiny when detailed magnifications are critically examined. Furthermore, all of the results so far shown have been obtained for $\kappa = 0$, $\boldsymbol{\kappa}$ being the in-plane 2D wavevector. This is present in the analysis, witnessing to the 3D nature of the actual physical system. If we start from an IDOS obtained for $\kappa = 0$, obtain something resembling a devil's staircase in the low part of the spectrum, and do the calculation for $\kappa \neq 0$, even a small one, then not the slightest semblance of self-similarity survives [2]. If only some very especially chosen results have some self-similar

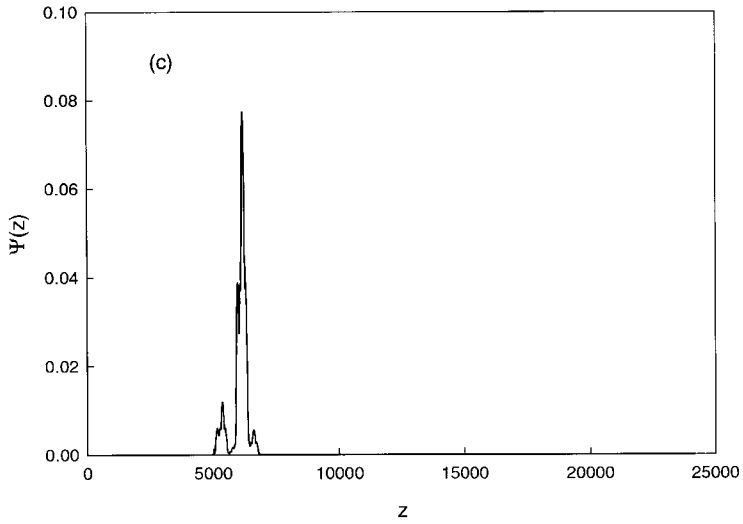

Figure 3. (Continued)

appearance, the question is: what is the relevance of this as regards the physical nature or properties of the QH? This seems to require more detailed attention than it has been given.

The Rudin–Shapiro sequence has intriguing features. We have three numerical experiments; in one the fractal dimension is unity, while in the other two the spectrum is multifractal. It may or may not be significant that in the first case four different constituent slabs are involved while the other two, while being numerically different, have the common feature that in both, C = A and D = B. This might suggest that in a parameter space there may be domains where the sequence has different essential—e.g. topological—properties. The non-applicability of the Bovier–Ghez theorem leaves room for such a speculation and more detailed studies from the point of view of design parameters seem to be suggested. One may also ask whether the R–S sequence is unique or whether there are others in the same class. These questions seem worth pursuing.

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