Localization-delocalization in aperiodic systems

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The question of localization in a one-dimensional tight-binding model with aperiodicity given by substitutions is discussed. Since the localization properties of the well-known Rudin-Shapiro chain is still far from well understood, partly due to the absence of rigorous analytical results, we introduce a sequence that has several features in common with the Rudin-Shapiro sequence. We derive a trace map for this system and prove analytically that the electron spectrum is singular continuous. Despite the extended (non-normalizable) nature of the corresponding wave functions, the states show strong localization for finite approximations of the chain. Similar localization properties are found for the Rudin-Shapiro chain, where earlier results have indicated a pure point spectrum. We compare the properties for two other physical systems, ordered according to the two discussed sequences; stationary electron transmission is studied through finite chains using a dynamical map, optical properties of dielectric multilayer structures are investigated.

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I. INTRODUCTION

The field of localization has in recent years showed interesting development which seem to somewhat contradict the intuitive picture related to Anderson localization. In 1990 Dunlap and co-workers[1] studied a random dimer tight-binding model, where the site energies are distributed randomly in pairs. They showed that $\sqrt{N}$ of the eigenstates are extended, where N is equal to the length of the system. Sil *et al.*[2] gave in 1993 a simple example of a one-dimensional model with all the electronic states extended. Their model has constant site-energies and the hopping matrix elements assume the values t and $-t$ with the probabilities p and $(1-p)$, respectively. It has later been shown,[3] by using ideas from Sil *et al.*, that there exist tight-binding models with a deterministic aperiodic distribution of the off-diagonal matrix elements that give all states extended and one state periodic. Perhaps even more interesting is that a theoretical model with correlated disorder also can have all states extended, one of which is periodic.[4] This is probably as far away as one can get, from what has become almost a folklore, that in a one-dimensional disordered system all states are localized.

Coming from the other end one could ask if there exist perfectly ordered systems that have all states localized. A possible candidate for generating this is the Rudin-Shapiro chain.[5,6] This binary sequence can be generated by a substitutional rule acting on four different letters, which is then reduced to a sequence of two letters. One reason for the interest in the Rudin-Shapiro sequence is that its Fourier transform is an absolutely continuous function such as for a random sequence. It is even so that the Rudin-Shapiro sequence has a Fourier transform which is a constant. This is in sharp contrast to the other well known deterministic aperiodic sequences; the Fibonacci sequence has a Fourier transform that consists of delta peaks, while the Thue-Morse sequence has a Fourier transform which is singular continuous. The importance of the character of the Fourier transform for the properties of the electronic spectra comes from the idea that there ought to exist a connection between energy gaps and singularities in the Fourier spectra. As is well-known from periodic systems, gaps in the energy spectrum correspond to Bragg peaks in the Fourier transform. For smooth enough quasiperiodic potentials the corresponding so called gap-labeling theorem[7,8] has been shown to be valid. However, numerical results indicate, that for the Rudin-Shapiro model the energy spectrum is a dense set of gaps,[9] in spite of the absence of singularities in the Fourier spectrum. This indicates that the above conjectured connection is not clear in the case of general aperiodic sequences.

There are very few rigorous results concerning the electronic spectrum and the associated wave functions for the Rudin-Shapiro system, probably due to the complexity of the sequence. Results based on numerical data indicate[10] that for finite approximations of the Rudin-Shapiro sequence all eigenstates are localized, for almost any value of the potential strength, but that the localization can be weaker than exponential. That the localization problem for this system is still under discussion can, for instance, be seen in Ref. 11.

With this somewhat detailed, but still rather selective introduction, we have wanted to show that the localization problem is a rather complex and in some parts rather nonintuitive issue, that is not completely understood yet. Since the Rudin-Shapiro sequence is suggested to be an extreme case, and there is still very few analytical result concerning this system, we present in Sec. II a new sequence with the same basic block structure and a very similar generating scheme as the Rudin-Shapiro sequence, but that is rigorously proven to generate a singular continuous spectrum for the tight-binding model.

We think it is of great interest to find a sequence as close as possible to the Rudin-Shapiro chain, concerning both building blocks and generating scheme, and compare some physical properties of this new chain with the Rudin-Shapiro chain. In Sec. III we study stationary electron transmission in a tight-binding model. Finally, optical transmission through multilayered materials is addressed in Sec. IV.

All systems are discrete and one dimensional and we would like to see if any fundamental differences in physical properties exist concerning the underlying sequence of these systems. If our result could also initiate some new successful

analytical attack on the old problem of the nature of the spectrum of the Rudin-Shapiro chain, it would be useful for a more complete understanding of the localization problem in low-dimensional systems.

II. SPECTRUM AND WAVE FUNCTIONS

The physical system studied first is a one-orbital tight-binding model with potentials V_n distributed aperiodically on a one-dimensional chain of atoms with unit spacing. The electron can hop between nearest-neighbor atoms according to the equation

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \begin{pmatrix} (E-V_n)t^{-1} & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}, \tag{1}$$

where ψ_n denotes the amplitude of the wave function on site n, E is the energy of the electron, and t is the hopping integral. We will consider binary aperiodic sequences of on-site potentials obtained from projections of fix points to substitution sequences. Here, a fix point is an invariant word of a substitution rule ξ which is defined on some finite set $\mathcal{A}$, called an alphabet. Truly infinite sequences, consistent with Eq. (1), are obtained as concatenation of these fix points.[12]

The above described deterministic aperiodic system has been extensively used to study the electronic properties in models for one-dimensional quasicrystals or aperiodic superlattices. It turns out that the poorly understood and somewhat exotic singular continuous electron spectrum is common among these models. If the on-site potentials is distributed according to the Fibonacci, Thue-Morse, and period-doubling sequences the spectrum is rigorously proven to be purely singular continuous regardless of the potential strength.[12] These results where obtained using the transfer matrix formalism. In this context, the transfer matrices are considered as operators $\mathcal{T}(\alpha)$, where $\alpha \in \mathcal{A}$, in the group of real unimodular matrices of order 2. When the map $\mathcal{T}$ is combined with the substitution rule ξ a dynamical system is formed, from which the properties of the spectrum in principle can be obtained. But it has turned out more useful to derive from this system a set of recursive equations for the traces of these transfer matrices, called the trace map. For a specific class of substitutions, meeting certain conditions of the substitution rule, and the corresponding trace map, Bovier and Ghez[13,14] have obtained sufficient conditions for the spectrum to be singular and purely singular continuous, respectively. The Rudin-Shapiro sequence is an example of a fix point to a substitution rule that does not belong to this class, and the nature of the spectrum for this model is still an open problem. In this context, it may be noted that the properties utilizing this class are not necessary in order to determine the spectral type. In the remaining part of this section, the Rudin-Shapiro system will be discussed and compared to an aperiodic chain having singular continuous spectrum.

A. The Rudin-Shapiro chain

In order to generate the Rudin-Shapiro sequence[5,6] from a substitution rule, a four-letter alphabet $\{a,b,c,d\}$ is needed followed by a final projection to give the binary sequence. The rule has the form

$$\xi(a)=ab, \quad \xi(b)=ac, \quad \xi(c)=db, \quad \xi(d)=dc. \tag{2}$$

If the letter a is used as the seed, the following word is found after four successive applications of the rule (2)

$$\xi^4(a)=abacabdbabacdcac, \tag{3}$$

and the Rudin-Shapiro sequence is obtained after identifying each a and b with A, and each c and d with B in the semi-infinite word $\xi^\infty(a)$. This fix point is actually easier to visualize if we apply the substitution rule (2) twice and then use the same projection as before. By defining the alphabet $\mathcal{A}=\{AA,AB,BA,BB\}$ consisting of two-letter words and the substitution rule acting on these words by

$$\xi(AA)=AAAB, \quad \xi(AB)=AABA,$$

$$\xi(BA)=BBAB, \quad \xi(BB)=BBBA, \tag{4}$$

the Rudin-Shapiro sequence is readily found as $\xi^\infty(AA)$. In practice we have to consider finite approximations of the sequence. The word AA is called the first generation of the sequence. The kth generation, containing 2^k elements, is found by applying the substitution rule (4) $(k-1)$ times. For example, the fourth generation Rudin-Shapiro chain reads

$$\xi^3(AA)=AAABAABAAAABBBAB. \tag{5}$$

Each element A (B) in the chain of atoms is assigned the value V $(-V)$, where we consider on-site potentials $V \geqslant 0$. From the substitution rule (2) an eight-dimensional trace map, with a six-dimensional invariant subspace, was derived.[15] The dynamics of this map can yield a lot of information about the spectral properties as well as the localization of wave functions. In all calculations made, we have set the hopping integral $t=-1$.

From the Schrödinger equation and the invariance of rule (4), with respect to the interchanging of all A's with B's, it follows that the spectrum is symmetric around the energy $E=0$, where the integrated density of states equals 1/2. Assuming that the atoms in a Rudin-Shapiro lattice contribute with one electron each, the Fermi energy is located at $E=0$. For the conduction properties, the existence of states with energy zero is therefore of special interest. Using the trace map, zero-energy states were found[16] for any periodic approximant corresponding to the even generations of the chain for certain values of the potential strength. We have made a similar numerical analysis of the trace map and found that the energy $E=0$ seems to be allowed also for any periodic approximant corresponding to the even generations of the Rudin-Shapiro chain if we choose the potential $V=2^{1/4}$. We show in Fig. 1 the eigenstate closest to the middle of the spectrum for a Rudin-Shapiro chain with 4096 sites calculated with rigid boundary conditions (note the logarithmic scale). The eigenstate shows some intricate self-similar pattern with an overall tendency towards localization. Due to the boundary conditions the eigenenergy is not exactly zero, but for larger even generations we get closer to the genuine zero-energy state. It may be noted that all results presented here are calculated in multiple precision in order to avoid divergence of transfer matrices multiplication, as well as the

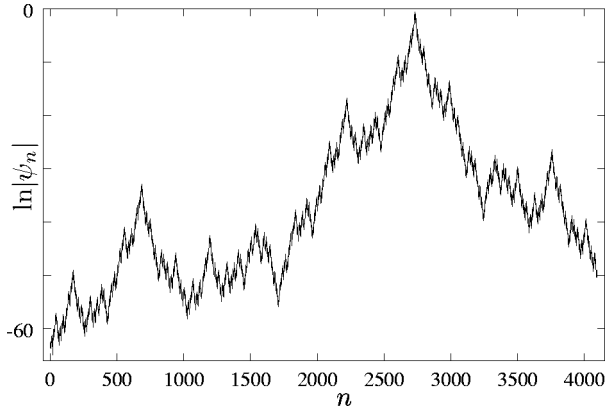

FIG. 1. The eigenstate closest to the center of the spectrum for the 12th generation Rudin-Shapiro chain with potential $V=2^{1/4}$, energy $E=-7.52755748\ldots\times10^{-33}$, using rigid boundary conditions. The logarithm of the absolute value of the wave function coefficient versus site index is shown.

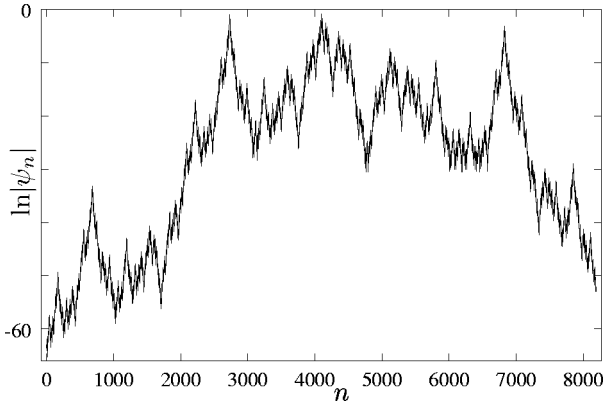

FIG. 2. ''Extendedlike'' state for a Rudin-Shapiro chain with 8192 sites, energy $E=-4.226165180\ldots\times10^{-23}$, and on-site potential $V=2^{1/4}$ using rigid boundary conditions. The absolute value of the wave function coefficient is plotted in logarithmic scale as a function of site index.

problem with near degeneracy of eigenvalues when determining the eigenstates. An exact zero-energy wave function, obtained from the transfer matrix multiplication (1) subjected to the initial conditions $\psi_0=0$ and $\psi_1=1$, will produce a non-normalized wave function with $E=0$ and a pattern almost impossible to distinguish from the state displayed in Fig. 1.

Other values of the energy, apart from $E=0$, for which the dynamics of the trace map is trapped into a six-dimensional invariant subspace are $E=\pm(2+V^2)^{1/2}$. The wave functions around these energivalues, where the integrated density of states equals 1/4 and 3/4, respectively, look sharply localized and they display a rich self-similar hierarchy of peaks. We conclude that, for this potential strength and every even generation of the Rudin-Shapiro chain, all states show an overall tendency towards localization. However, numerical investigations indicate that the Lyapunov exponent vanishes, so that the localization is weaker than exponential. Especially, this holds true for the state shown in Fig. 1.

A different feature is found for the odd generations, keeping the value $V=2^{1/4}$ for the potential strength. The energy $E=0$ seems to never occur for these generations. This trend of nonrecurrence of zero energy with respect to generation number is already known.[15,16] It turns out that for odd generations there exist, what we call, ''extendedlike'' states. In Fig. 2 we show an example of this behavior for one of the states closest to the central gap. This kind of state is not only confined around the center of the spectrum but are also found in, for example, the vicinity of the energies $E=\pm(2+\sqrt{2})^{1/2}$. It is hard to believe that, in the limit of large chains, this kind of state is consistent with a pure point spectrum. In Ref. 10 it is argued that the spectrum for the Rudin-Shapiro model should be pure point for potentials $V\geqslant1$. But Fig. 2 indicates that this may not be the case, and that there exist values of the potential, e.g., $V=2^{1/4}$, such that the states are ''extendedlike'' and that the spectrum probably contains a continuous part. In Ref. 12 it is intuitively conjectured that any primitive substitution sequence should have singular continuous spectrum, although with a number of open questions yet to be closed before reaching such a conclusion. The Rudin-Shapiro sequence is a primitive substitution, which means that there exists an integer k such that for any two letters $\alpha,\beta\in\mathcal{A}$ the word $\xi^k(\alpha)$ contains the letter β. However, our result does not rule out the possibility of a mixed spectrum for $V\geqslant1$ or possibly even a pure point spectrum for strong enough potentials. It would indeed be very interesting if there exists a perfectly ordered substitutional sequence with a pure point spectrum.

B. A chain with singular continuous spectrum

We introduce an aperiodic sequence by letting the primitive substitution rule

$$\xi(a)=ab,\quad \xi(b)=ad,\quad \xi(c)=fe,$$

$$\xi(d)=dc,\quad \xi(e)=ad,\quad \xi(f)=fe, \tag{6}$$

defined on the alphabet $\{a,b,c,d,e,f\}$, act on the seed a an infinite number of times. Due to the regularity of these relations it suffices to consider the two-letter words alphabet $\mathcal{A}=\{ab,ad,dc,fe\}$. Starting from the first generation of the substitution (6), the rule can be expressed as concatenation of different generations of words by

$$\omega^{(k+1)}=\omega^{(k)}\eta^{(k)},\quad \eta^{(k+1)}=\omega^{(k)}\sigma^{(k)},$$

$$\sigma^{(k+1)}=\sigma^{(k)}\tau^{(k)},\quad \tau^{(k+1)}=\tau^{(k)}\eta^{(k)}. \tag{7}$$

Here $\omega^{(k)}=\xi^k(a)$ stands for the kth generation of the sequence, containing 2^k elements, where the initial conditions are $\omega^{(1)}=ab$, $\eta^{(1)}=ad$, $\sigma^{(1)}=dc$, and $\tau^{(1)}=fe$. The combination of the substitution rule with the transfer matrix is accomplished by introducing the initial transfer matrices $\mathcal{M}_1=\mathcal{T}(b)\mathcal{T}(a)$, $\mathcal{N}_1=\mathcal{T}(d)\mathcal{T}(a)$, $\mathcal{O}_1=\mathcal{T}(c)\mathcal{T}(d)$, and $\mathcal{P}_1=\mathcal{T}(e)\mathcal{T}(f)$. Then, it follows from the relations (7) that the recursion of the transfer matrices can be written as

$$\mathcal{M}_{k+1}=\mathcal{N}_k\mathcal{M}_k, \quad \mathcal{N}_{k+1}=\mathcal{O}_k\mathcal{M}_k, \tag{8}$$

$$\mathcal{O}_{k+1}=\mathcal{P}_k\mathcal{O}_k, \quad \mathcal{P}_{k+1}=\mathcal{N}_k\mathcal{P}_k,$$

where $\mathcal{M}_k$ is the corresponding kth generation transfer matrix. In the Appendix we derive a trace map for this system and prove analytically that the corresponding electron spectrum is purely singular continuous regardless of the potential strength.

Given the substitution sequence $\xi^{\infty}(ab)$ a variety of binary sequences can be obtained using different projections. As long as they are aperiodic sequences, they will all share the property of having purely singular continuous spectra. From now on each *a*, *b*, and *c* is identified with an *A*, and each *d*, *e*, and *f* is projected onto the element *B* in the sequence $\xi^{\infty}(ab)$. Starting from the second iteration of the rule (6) this procedure is equivalent to let the binary substitution act on the alphabet $\mathcal{A}=\{AA,AB,BA,BB\}$ according to

$$\xi(AA)=AAAB, \quad \xi(AB)=AABA, \tag{9}$$

$$\xi(BA)=BABB, \quad \xi(BB)=BBAB,$$

producing the binary aperiodic sequence $\xi^{\infty}(AA)$. As an example, the fourth generation is given by [see. Eq. (5)]

$$\xi^3(AA)=AAABAABAAAABBABB. \tag{10}$$

This sequence is to be compared to the Rudin-Shapiro sequence described by the rule (4). In this notation both sequences are defined by primitive substitutions acting on the same alphabet. Inspection of the relations (4) and (9) reveals that the infinite sequences contain strings of the elements *A* and *B* of length 1–4. Using the substitution matrix[17] we conclude that the density of the elements in the alphabet appear with equal weight, implying that the elements *A* and *B* are equally common for both sequences. The substitution matrix for the rule (9) reads

$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \tag{11}$$

with eigenvalues $0,0,1$, and 2. A matrix with integer coefficients is said to possess the Pisot property[18–20] if the leading eigenvalue of the matrix has modulus greater than unity and all other eigenvalues are less than unity in modulus. Here the second largest eigenvalue is exactly one and the matrix is said to belong to a marginal case. For the Rudin-Shapiro sequence the corresponding matrix belongs to the non-Pisot case, in agreement with the nonexistence of Bragg peaks in the Fourier spectrum.[17]

In order to compare the electronic eigenstates for finite generations of this chain with the states found for the Rudin-Shapiro chain in Sec. II A, we choose the same parameter values for the hopping integral and the potential strength used there. First, we mention that for this chain states with zero energy for potential strength seem to exist both larger and less than one. Here, they are not of the same interest because the spectrum for this chain is not symmetric around zero, which is easily seen from the substitution rule (9). The really interesting part is that for almost any value of the potential strength and for large, but finite lattices, the eigenstates show localization properties similar to the states found for the Rudin-Shapiro chain, despite the fact that the spectrum is purely singular continuous. That is, all states are extended in the sense that they are non-normalizable for the infinite chain. As for the Rudin-Shapiro model,[21] there exist values of the on-site potential such that the wave functions also appear extendedlike for this chain. However, the generic property seems to be an overall tendency towards localization for finite approximations of the chain. The special value $V=2^{1/4}$ gives even stronger localization of the states than the states found for the Rudin-Shapiro chain. This characteristic feature is shown in Fig. 3 for an arbitrary state near the middle of the spectrum for the sequence (9) with 2048 sites. This example clearly demonstrates that aperiodic chains with singular continuous spectra can show strong localization properties, regarding the electronic wave functions, for large but finite approximations of the chains. Consequently, this puts earlier arguments and conjectures about the spectral properties for the Rudin-Shapiro model in a partly different perspective.

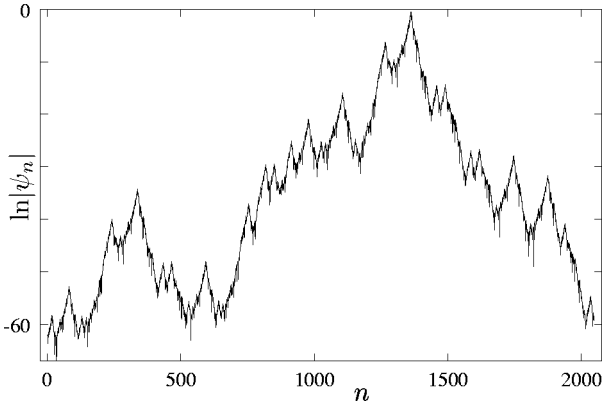

FIG. 3. The natural logarithm of the absolute value of the wave function amplitude plotted as a function of site index for the chain (9) with 2048 sites, potential $V=2^{1/4}$, and energy $E=0.087064038\cdots$ using rigid boundary conditions.

III. ELECTRON TRANSMISSION

In this section we will study stationary transmission through a finite, aperiodic chain described by the discrete time-independent Schrödinger equation, which is equivalent to the ordinary tight-binding Eq. (1), with the hopping integral normalized to -1,

$$V_n\psi_n-\psi_{n+1}-\psi_{n-1}=E\psi_n, \tag{12}$$

for $1\leqslant n\leqslant N$. The finite chain is embedded in an infinite, periodic chain, where the wave functions are taken as single Bloch waves specified by a wave vector k

$$\psi_n = R_0 e^{ikn} + R_1 e^{-ikn}, \quad n \leqslant 1,$$

$$\psi_n = T e^{ikn}, \quad n \geqslant N, \tag{13}$$

with R_0, R_1, and T defining the incident, reflected, and transmitted wave amplitudes, respectively. For the periodic chain [also described by Eq. (12) with $V_n \equiv 0$], the energy E is related to the Bloch wave vector k through $E = -2\cos k$. Motivated by the semi-infinite extension of the periodic chain to the left and to the right, we use this relation for the energy also in the finite aperiodic sample. Hence, we are restricted to the energy interval $-2 \leqslant E \leqslant 2$.

The transmission coefficient t is defined as the fraction of the transmitted intensity $|T|^2$ to the incident intensity $|R_0|^2$. Inferring the quantities defined by

$$x_n = |\psi_n|^2/|T|^2, \quad y_n = \mathrm{Re}(\psi_n \psi_{n-1}^*)/|T|^2, \tag{14}$$

the four-dimensional Eq. (12) in real domain can, by the use of current conservation [$J \equiv \mathrm{Im}(\psi_n \psi_{n-1}^*)$], be reduced to a two-dimensional mapping[22–24]

$$x_{n-1} = x_n^{-1}(y_n^2 + \sin^2 k), \quad \forall n,$$

$$y_{n-1} = -y_n + x_{n-1}(V_{n-1} - E), \quad 2 \leqslant n \leqslant N+1, \tag{15}$$

where the initial conditions are $x_{N+1} = 1$, $y_{N+1} = \cos k$. Iteration of Eq. (15) from the output end to the input end of the finite, aperiodic chain gives, using Eqs. (13) and (14), the transmission coefficient

$$t = \frac{4\sin^2 k}{x_1 + x_0 - 2y_1 \cos k + 2\sin^2 k}. \tag{16}$$

The transmission problem is directly related to the wave functions for the chains described by Eq. (12), with on-site potentials V_n distributed according to the sequences studied in Sec. II. Therefore, the strength of the on-site potential is again chosen as $V = 2^{1/4}$. In all calculations made, we have normalized the transmitted intensity $|T|^2 = 1$. In Figs. 4(a) and 4(b) we show the transmission spectrum in an energy interval around $E = 0$ for two generations of the Rudin-Shapiro chain with length $N = 256$ and $N = 512$, respectively. The transmission coefficient in the gaps is roughly squared when doubling the chain length and the transmission in these regions is practically zero. By choosing the wave vector $k = \arccos(-E/2)$, the current density will cause the transmission peaks to shift a small amount in energy compared with the energy spectra of the corresponding chains. For the even generation of the Rudin-Shapiro chain, we find a single peak with transmission coefficient $t \approx 0.63 \times 10^{-2}$ at approximately zero energy, while for the odd generation a gap at the center of the spectrum appears surrounded by peaks with $t \approx 0.40$. The field intensities $x_n = |\psi_n|^2$ as a function of site index n for these peaks look similar in structure as the corresponding wave functions studied in Sec. II. The existence of ''extendedlike'' states for the even generations of the Rudin-Shapiro sequence results in peaks with better transmission through these chains than through the chains corresponding to the odd generations of the sequence. Despite the overall tendency towards localization of the wave functions for the odd generations of the sequence, we find peaks with good transmission [the peak at $E = -0.055583429\cdots$ in Fig. 4(a) has $t \approx 0.86$], which is explained by the self-similarity of the corresponding field intensities. For this value of the potential strength, we do not find perfect transmission anywhere and the field intensities (or the corresponding wave functions) cannot be strictly self-similar.

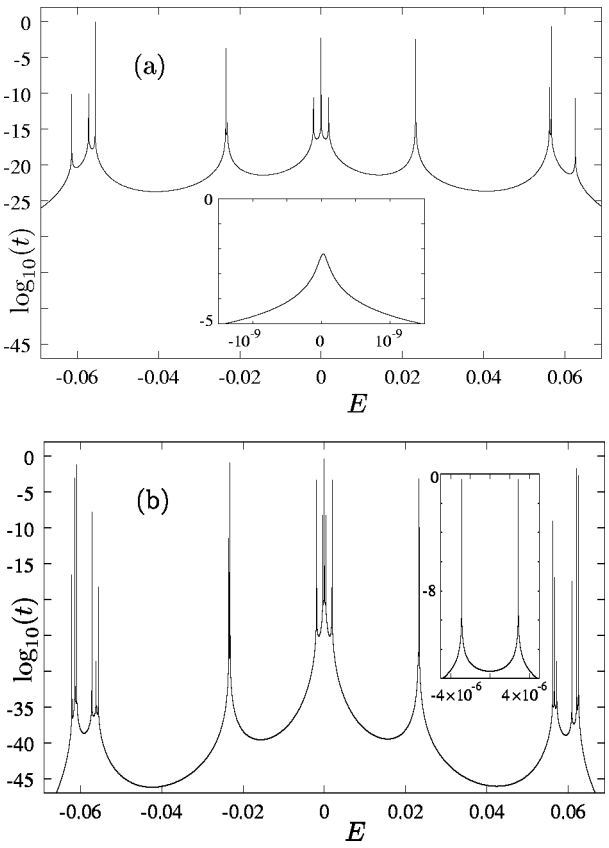

FIG. 4. The logarithm of the transmission coefficient t as a function of energy E for a Rudin-Shapiro chain with on-site potential $V = 2^{1/4}$ and length N using the same scale. (a) $N = 256$. (b) $N = 512$. The insets show magnifications of the regions around the center of the spectra.

The transmission through a sequence of on-site potentials generated by the substitution rule (9) essentially share the properties described above for the Rudin-Shapiro model. We show in Fig. 5 the transmission coefficient as a function of energy around a region of the middle of the spectrum for the chain (9) with $N = 256$. The transmission peaks for this model are even more narrow than the peaks in Fig. 4(a) and the corresponding field intensities appear more localized than for the Rudin-Shapiro chain. As an example, we show in the inset of Fig. 5 the field intensities as a function of position for one of the peaks in Fig. 5 with high transmission. Note that, when plotted in linear scale, only the dominating peaks of the distribution of the field intensities can be seen.

IV. OPTICAL TRANSMISSION THROUGH MULTILAYERS

To further compare some physical properties of the lattice presented in this paper and the Rudin-Shapiro lattice, we

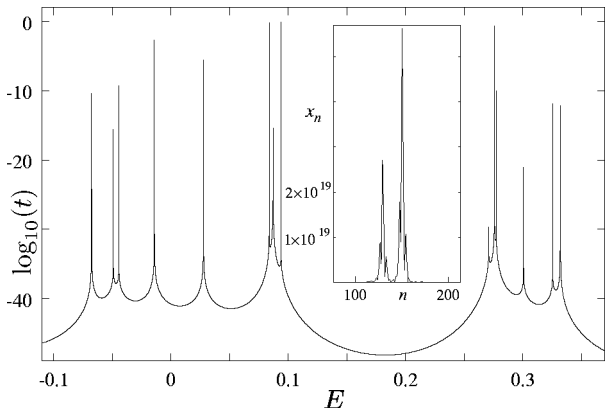

FIG. 5. The logarithm of the transmission coefficient t as a function of energy E for the chain (9) with $N=256$, and potential strength $V=2^{1/4}$. The inset shows the field intensities x_n versus position n corresponding to the peak with $E=0.083741813\cdots$ and $t\approx0.70$ in the main figure.

present numerical calculations of optical transmission through two different multilayers, based on the two sequences. Since the formalism used has been described earlier in several other places,[25–27,21,28] the presentation here will be rather short. The system which we analyze in this section consists of a finite dielectric multilayer constructed of two components A and B characterized by wavelength-independent refractive indices n_A and n_B, and thicknesses d_A and d_B, respectively. The multilayer is inserted between two semi-infinite media of type A. The wave polarization is parallel to the layer surfaces and for simplicity the thicknesses are assumed to be adjusted such that the variation of the phase is the same in both types of layers A and B (i.e., $\delta_A=k_Ad_A=k_Bd_B=\delta_B=\delta$), where k_A and k_B are the wave vectors within the two different types of layers. The values of the electric field and its first derivative at the interface of two successive layers are components of some vector given by the unimodular transfer matrix associated with the layer n,

$$M_n=\begin{pmatrix}1 & 0\\ 0 & k_{n+1}/k_n\end{pmatrix}\begin{pmatrix}\cos\delta & -\sin\delta\\ \sin\delta & \cos\delta\end{pmatrix}, \tag{17}$$

which means that

$$M_n=\begin{pmatrix}\cos\delta & -r_n^{-1}\sin\delta\\ r_n\sin\delta & \cos\delta\end{pmatrix}, \tag{18}$$

where r_n equals 1 if the nth layer is of type A, or n_A/n_B if it is of type B. The propagation of light through N layers is now represented by a total transfer matrix $M_N(\delta)$ which is a suitable product of transfer matrices of the type just described above associated which each layer n. For a multilayer sandwiched between two layers of type A the transmission coefficient $T_N(\delta)$ is then given by

$$T_N(\delta)=[(m_{11}+m_{22})^2+(m_{21}-m_{12})^2]/4, \tag{19}$$

where the m_{ij} are the matrix elements of the total transfer matrix $M_N(\delta)$. We present the result by plotting the transmission coefficient $T_N(\delta)$ as function of the phase δ in the interval π to 2π. The same values of the two refractive indices ($n_A=2.0$ and $n_B=2.75$, respectively) are used in all cases studied here. Since the result depends strongly on the length N of the multilayer we display the result for both $N=256$ and $N=512$. In Fig. 6 panels (a) and (b) concern sequence (9), and panels (c) and (d) concern the Rudin-Shapiro sequence. The sequence (9) gives a ''band'' of very

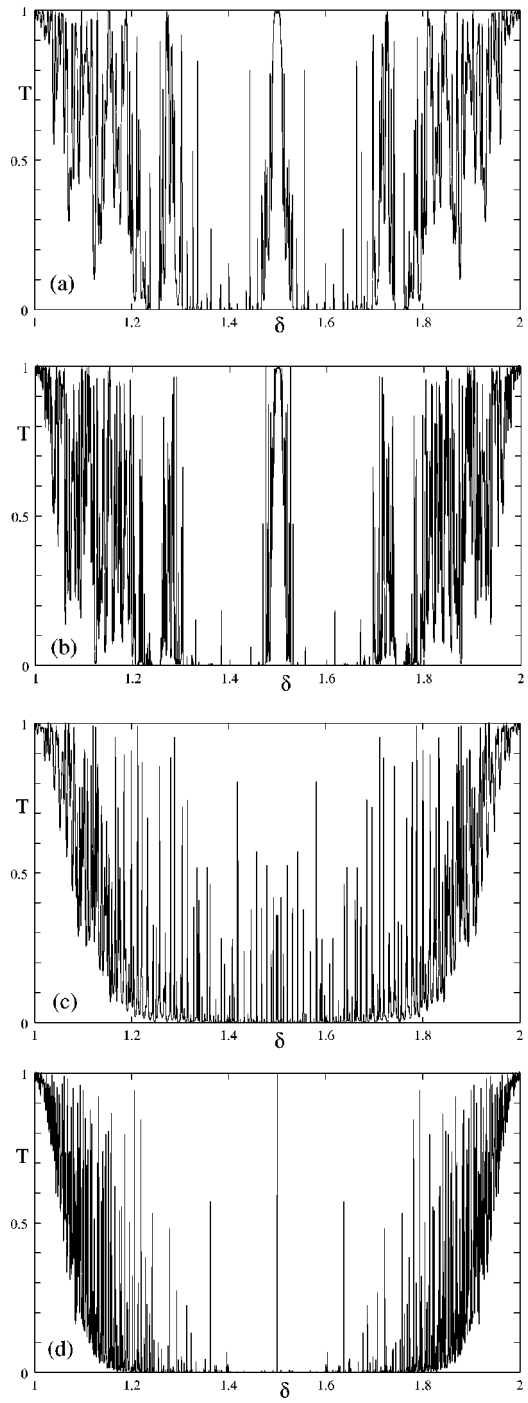

FIG. 6. The transmission coefficient T as a function of the phase δ in units of π for a multi-layer given by (a) the sequence (9) with $N=256$, (b) the sequence (9) with $N=512$, (c) the Rudin-Shapiro sequence with $N=256$, and (d) the Rudin-Shapiro sequence with $N=512$.

high transmission in the middle of the spectrum (with a local maximum exactly in the middle) and the width of this ''band'' decreases as N is increasing. The transmission through the Rudin-Shapiro multilayers show a much more evenly spread out variation (with a minimum at the absolute middle point for the short sample with $N=256$). Note the very drastic shrinking of the center region as N is doubled and that the transmission at $\delta=3\pi/2$ now instead has a maximum (perfect transmission). Since the Rudin-Shapiro sequence has some properties in common with a disordered sequence, we have also studied the transmission through various disordered multilayers having the same lengths and identical optical parameters. It turns out that the development of certain peaks (as well as gaps) in the transmission spectra agree for the Rudin-Shapiro case and the random cases. The random cases also showed a more evenly spread out variation similar to the Rudin-Shapiro case. Peaks with perfect transmission at $\delta=3\pi/2$ were never found for the different random multilayers.

V. SUMMARY

The localization properties for deterministic aperiodic chains were investigated in the on-site tight-binding model. The Rudin-Shapiro chain was considered in some detail. The existence of a zero-energy state for any periodic approximant corresponding to the even generations of this chain was numerically indicated. For these generations of the chain, we also pointed out the overall tendency towards localization of the eigenstates. The wave functions for finite chains corresponding to the odd generations of the Rudin-Shapiro sequence gave a different picture. Here, we found ''extended-like'' states, even for amplitudes of the on-site potential $V>1$ in units of the hopping integral, a result which is in contradiction with earlier arguments about the generic property of localization for finite Rudin-Shapiro lattices.

A step towards the question of localization in more general aperiodic chains was taken by introduction of an aperiodic substitution sequence which has several features in common with the Rudin-Shapiro sequence. A trace map for this system was derived and we proved analytically that the electron spectrum is singular continuous. However, it turned out that for almost any value of the potential strength the wave functions for finite approximations showed localization properties similar to the states found for the Rudin-Shapiro lattice, despite the fact that the spectrum is singular continuous. We came to the conclusion that aperiodic chains with singular continuous spectra can show strong localization properties regarding the electronic wave functions, for large but finite approximants. This result points in the direction that singular continuous spectra could be a universal property for tight-binding systems with on-site potentials generated from primitive substitutions. Consequently this result also puts earlier arguments and conjectures about the spectral properties for the Rudin-Shapiro model in a partly different perspective.

Stationary electron transmission through finite chains based on the two discussed sequences was numerically investigated by the use of a dynamical map. The transmission properties were found to be in accordance with the localization of the electronic wave functions, i.e., mostly low transmission coefficients, for both models. Despite the rather strong localization, we found peaks with high transmission which is traced to the self-similarity of the field intensities, or equivalently to the self-similarity of the corresponding wave functions.

Finally, we considered optical transmission through dielectric multilayers ordered according to these sequences, and an arbitrary disordered multilayer. We showed that the two aperiodically ordered multilayers can have perfect transmission in the center, with a ''bandlike'' structure for the sequence introduced in this article. In the global structure, the Rudin-Shapiro multilayer showed more in common with the representative for the disordered multilayers.

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APPENDIX A

For an arbitrary substitution rule, Kolář and Nori[15] have shown the existence of a finite subset $\mathcal{B}\subset\mathcal{A}^*$ and polynomial maps F_β for each $\beta\in\mathcal{B}$, such that

$$x_{k+1}(\beta)=F_\beta[x_k(\beta_1),\ldots,x_k(\beta_{|\mathcal{B}|})], \tag{A1}$$

where the trace coordinate $x_k(\beta)\equiv\mathrm{tr}\,\mathcal{T}^k(\beta)$ is defined as the trace of the corresponding kth generation transfer matrix. Here, the set $\mathcal{A}^*$ consists of all finitely long words that can be written using the alphabet $\mathcal{A}$. In order to obtain an explicit expression for the trace map, corresponding to the system (8), we can use the formula[15]

$$\mathrm{tr}(\Theta\Lambda\Theta\Xi)=\mathrm{tr}(\Theta\Lambda)\mathrm{tr}(\Theta\Xi)+\mathrm{tr}(\Lambda\Xi)-\mathrm{tr}(\Lambda)\mathrm{tr}(\Xi), \tag{A2}$$

which is easily derived from the Cayley-Hamilton theorem and applies to all unimodular matrices of order two. Introducing the trace coordinates defined by

$$\begin{gathered}
k_k=\mathrm{tr}(\mathcal{O}_{k+1}\mathcal{M}_{k+1}),\quad s_k=\mathrm{tr}(\mathcal{P}_k\mathcal{O}_k),\\
l_k=\mathrm{tr}(\mathcal{N}_{k+1}\mathcal{P}_{k+1}),\quad t_k=\mathrm{tr}(\mathcal{N}_k\mathcal{P}_k),\\
m_k=\mathrm{tr}(\mathcal{M}_k),\quad u_k=\mathrm{tr}(\mathcal{O}_k\mathcal{N}_k),\\
n_k=\mathrm{tr}(\mathcal{N}_k),\quad v_k=\mathrm{tr}(\mathcal{M}_k\mathcal{P}_k)-\mathrm{tr}(\mathcal{M}_k)\mathrm{tr}(\mathcal{P}_k),\\
o_k=\mathrm{tr}(\mathcal{O}_k),\quad w_k=\mathrm{tr}(\mathcal{P}_k\mathcal{O}_k\mathcal{N}_k),\\
p_k=\mathrm{tr}(\mathcal{P}_k),\quad x_k=\mathrm{tr}(\mathcal{P}_k\mathcal{O}_k\mathcal{M}_k)\\
q_k=\mathrm{tr}(\mathcal{N}_k\mathcal{M}_k),\quad y_k=\mathrm{tr}(\mathcal{M}_k\mathcal{N}_k\mathcal{P}_k),\\
r_k=\mathrm{tr}(\mathcal{O}_k\mathcal{M}_k),\quad z_k=\mathrm{tr}(\mathcal{M}_k\mathcal{N}_k\mathcal{O}_k)
\end{gathered} \tag{A3}$$

and making use of the relations (8), Eq. (A2), and the invariance of the trace with respect to cyclic permutation of the matrices, we get the trace map

$$
\begin{aligned}
k_{k+1} &= m_{k+1}w_{k+1} - o_k p_k s_k + p_k^2 + o_k^2 - 2,\\
l_{k+1} &= s_{k+1}q_{k+1} + o_k p_k s_k - p_k^2 - o_k^2 + 2\\
&\quad + n_{k+1}(x_{k+1} - m_{k+1}s_{k+1}),\\
m_{k+1} &= q_k,\\
n_{k+1} &= r_k,\\
o_{k+1} &= s_k,\\
p_{k+1} &= t_k,\\
q_{k+1} &= q_k r_k + u_k - n_k o_k,\\
r_{k+1} &= k_k,\\
s_{k+1} &= p_k w_k - u_k,\\
t_{k+1} &= l_k,\\
u_{k+1} &= o_k x_k - v_1 - m_k p_k,\\
v_{k+1} &= v_1 (= v_k),\\
w_{k+1} &= p_k(o_k l_k - y_k) - o_k z_k + q_k,\\
x_{k+1} &= q_k(p_k w_k - u_k) + p_k(x_k - m_k s_k) + m_k o_k - r_k,\\
y_{k+1} &= p_{k+1}q_{k+1} + n_{k+1}v_1 + o_{k+1},\\
z_{k+1} &= k_k r_k + s_k u_k - o_k w_k - n_k p_k + t_k.
\end{aligned}
\tag{A4}
$$

It is straightforward to expand the right-hand sides of all these relations in terms of the defined trace map coordinates (A3) for index $k \geqslant 1$. When the initial conditions are specified the coordinate $v_k = v_1$ is a constant and will be dropped from Eq. (A4) leaving 15 trace coordinates. This number can actually be reduced further, but the reduction of the number of trace coordinates is not relevant for our purpose since there is in fact nothing unique about this specific trace map. In view of Eq. (A1) this trace map represents a new dynamical system based on the traces of the transfer matrices and the elements of the finite set $\mathcal{B}$ are chosen as the words corresponding to the initial trace maps coordinates (A3). For example, the coordinate $q_1 = \mathrm{tr}\mathcal{T}(abad)$, corresponds to the word $\omega^{(2)} = abad$, which is included in set $\mathcal{B}$. The other elements are found in a similar fashion.

To every given trace map, there always exists a unique reduced trace map,[13] i.e., the mapping obtained when only the monomial of highest degree are kept in the full trace map. Here, degree simply refers to the number of elements associated with each variable. With the trace map defined by Eq. (A4), with v_k eliminated, we get the corresponding unique reduced trace map

$$
\begin{aligned}
k_{k+1} &= l_k o_k p_k q_k, \quad l_{k+1} = p_k q_k r_k w_k,\\
m_{k+1} &= q_k, \quad n_{k+1} = r_k,\\
o_{k+1} &= s_k, \quad p_{k+1} = t_k,\\
q_{k+1} &= q_k r_k, \quad r_{k+1} = k_k,\\
s_{k+1} &= p_k w_k, \quad t_{k+1} = l_k,\\
u_{k+1} &= o_k x_k,\\
w_{k+1} &= l_k o_k p_k, \quad x_{k+1} = p_k q_k w_k,\\
y_{k+1} &= q_k r_k t_k, \quad z_{k+1} = k_k r_k.
\end{aligned}
\tag{A5}
$$

To proceed from here we suppress all subscripts in the reduced trace map (A5) and redefine the finite set $\mathcal{B}$ according to $\mathcal{B} = \{k,l,m,n,o,p,q,r,s,t,u,w,x,y,z\}$. Now the reduced trace map (A5) can be considered as a mapping $\phi: \mathcal{B} \to \mathcal{B}^*$. Here, the order of the elements is not specified so this mapping is not unique. More importantly the mapping ϕ, in this particular case, belongs to the class of *semiprimitive*[13] substitutions. A substitution ϕ on an alphabet $\mathcal{B}$ is called semiprimitive if there exists a subset $\mathcal{C} \subset \mathcal{B}$ such that ϕ maps $\mathcal{C}$ into $\mathcal{C}^*$, and the restriction of ϕ to $\mathcal{C}$ is a primitive substitution, and in addition $\phi^k(\beta)$, for some positive integer k, contains at least one letter from $\mathcal{C}$ for each letter $\beta \in \mathcal{B}$. Using Eq. (A5), it follows that the choice $\mathcal{C} = \{k,l,o,p,q,r,s,t,w\}$ meets all of these conditions, and hence ensures that our reduced trace map is semiprimitive.

When the substitution ϕ, associated with the trace map (corresponding to a primitive substitution ξ), is semiprimitive as described above, and if there also exists a finite integer k_0 such that $\xi^{k_0}(\alpha_0)$, where $\alpha_0 \in \mathcal{A}$, contains the word $\beta\beta$ for some $\beta \in \mathcal{B}$, the spectrum is singular.[13] From the substitution rule (6), we have

$$
\xi^4(ab) = \xi^3(ab)\xi^2(ab)dcfefead. \tag{A6}
$$

Since $fe \in \mathcal{B}$ [remember that $p_1 = \mathrm{tr}\mathcal{T}(fe)$] and $\xi^4(ab)$ contains the square of the element fe the spectrum is singular, i.e., supported on a set of zero Lebesgue measure.

In order to establish the absence of eigenvalues in the spectrum, the structure $\mathcal{A}^*$ is extended to a free group $\hat{\mathcal{A}}^*$ by adding the formal inverses of the letters in $\mathcal{A}$ as generators. When the spectrum is singular as described above, and if in addition there exist finite integers n_0, m_0 such that $\xi^{n_0}(\alpha_0) = \xi^{m_0}(\gamma_0)\xi^{m_0}(\gamma_0)\delta\omega$, where $\gamma_0 \in \mathcal{C}$, $\omega \in \hat{\mathcal{A}}^*$, and $\delta \in \hat{\mathcal{A}}^*$ has the property that there exists a finite integer k_0 such that $\xi^{k_0}(\delta) = \delta$. Then the spectrum is purely singular continuous

and supported on a generalized Cantor set (i.e., a perfect nowhere dense set) of zero Lebesgue measure.[13,14] Using this extension, we may write

$$\xi^2(ab)=(abad)^2\delta\delta^{-1}(ad)^{-1}dc, \tag{A7}$$

where $\xi(\delta)=\delta$ is satisfied with $\delta=fe(ab)^{-1}\in\hat{\mathcal{A}}^*$. Hence, with $\omega=\delta^{-1}(ad)^{-1}dc\in\hat{\mathcal{A}}^*$ and $\gamma_0=abad\in\mathcal{C}$ (more correctly, $q\in\mathcal{C}$) the conclusion of a purely singular continuous electron spectrum is reached.

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