Renormalization of aperiodic model lattices: spectral properties

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Abstract
Many of the published results for one-dimensional deterministic aperiodic
systems treat rather simplified electron models with either a constant site
energy or a constant hopping integral. Here we present some rigorous results
for more realistic mixed tight-binding systems with both the site energies
and the hopping integrals having an aperiodic spatial variation. It is shown
that the mixed Thue–Morse, period-doubling and Rudin–Shapiro lattices can
be transformed to on-site models on renormalized lattices maintaining the
individual order between the site energies. The character of the energy spectra
for these mixed models is therefore the same as for the corresponding on-site
models. Furthermore, since the study of electrons on a lattice governed by the
Schrödinger tight-binding equation maps onto the study of elastic vibrations
on a harmonic chain, we have proved that the vibrational spectra of aperiodic
harmonic chains with distributions of masses determined by the Thue–Morse
sequence and the period-doubling sequence are purely singular continuous.

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1. Introduction

Since the discovery of the quasicrystalline phase in Al–Mn alloys [1], a vast number of
investigations have been devoted to the physical properties of quasiperiodic or more general
aperiodic structures. Due to the complexity of such structures most theoretical studies are
confined to simple one-dimensional model lattices obtained from substitution sequences [2].
Several analytical as well as numerical methods have been developed for studying these
systems. In the pioneering works [3, 4] on the quasiperiodic Fibonacci lattice a trace map
technique was used. This method, which relies on the unimodularity of the transfer matrices,
has been applied to other well-known deterministic aperiodic systems, such as the Thue–Morse
model, the period-doubling model and the Rudin–Shapiro model (see e.g. [5] and references

therein). The transfer matrix approach is a very powerful tool for obtaining analytical results for the electronic, vibrational and optical properties of this class of systems. Many interesting new concepts such as, for example, the critical localization of wavefunctions and Cantor set energy spectra have emerged from the studies of these model systems.

In this paper, we study the electronic and vibrational properties of some one-dimensional aperiodic models that allow for a transfer matrix formulation. A classical example is the description of electrons on a lattice of atoms modelled by the tight-binding Hamiltonian

$$H = \sum_i \epsilon_i |i\rangle \langle i| + \sum_{i \neq j} t_{i,j} |i\rangle \langle j| \tag{1}$$

where ϵ_i is the site energy and $t_{i,j}$ is the hopping integral from site i to site j. In most of the so-far published work of one-dimensional aperiodically ordered systems either the site energy or the hopping integral is kept constant. We will consider lattices with two types of atoms A and B with site energies ϵ_A and ϵ_B, respectively, which are distributed according to some primitive substitution rules. When the atom at site i is of type A and at site j is of type B, we write $t_{i,j} = t_{A,B}$. With restriction on nearest-neighbour interaction, a more realistic mixed model, including four hopping matrix elements $t_{i,i+1} \in \{t_{A,A}, t_{A,B}, t_{B,A}, t_{B,B}\}$, is obtained. Expanding the total state vector $\Psi = \sum_i \psi_i |i\rangle$, the energy spectrum can be found from solving the Schrödinger equation $H\Psi = E\Psi$ which, after identifying $\Phi_i = (\psi_{i+1}, \psi_i)^T$, gives rise to the difference equation $\Phi_i = T_{i+1,i,i-1}\Phi_{i-1}$, with a transfer matrix $T_{i+1,i,i-1}$ of the form

$$T_{i+1,i,i-1} = \begin{pmatrix} 1/t_{i,i+1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} (E - \epsilon_i) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & t_{i,i-1} \end{pmatrix}. \tag{2}$$

If all hopping integrals $t_{i,i\pm1} = t$ (often normalized to -1) in (2), the well-known diagonal (on-site) tight-binding model is regained. In this case, the matrix (2) is unimodular and it depends on one site only, so there is a one-to-one correspondence between the substitution rule for the site energies and the string of transfer matrices. It has been rigorously proved that the spectrum is singular continuous and supported on a Cantor set of zero Lebesgue measure if the site energies are distributed according to the Fibonacci sequence [6], the Thue–Morse sequence [7] and the period-doubling sequences [7]; see also the results in [8, 9]. We refer to [10] for a review of recent results and the current status of the spectral theory of Schrödinger operators with substitution potentials.

However, the transfer matrix (2) is, in general, not unimodular and the trace map technique cannot be applied directly. Moreover, the one-to-one correspondence between the sequence of transfer matrices and the substitution sequence for the site energies is often destroyed. If it is possible to obtain such a correspondence, we say that the sequence of transfer matrices is *renormalizable* with respect to the substitution rule for the site energies. When these transfer matrices are unimodular, we refer to the lattice as a renormalizable on-site model for which the character of the energy spectrum is the same as for the corresponding diagonal model. We have borrowed this terminology from [11], where it was proved that a mixed Fibonacci model can be transformed to an on-site model on a renormalized lattice. This implies [5] that also the vibrational spectrum for the one-dimensional harmonic diatomic Fibonacci chain is purely singular continuous and all the generalized vibrational eigenstates are then neither localized nor extended in the ordinary sense. These states are often denoted as critical, a term that will be used here also. Another model based on substitution sequences that has enjoyed increasing popularity is one-dimensional quantum Ising chains [12]. The analytical treatment

of these models also involves renormalization procedures similar to what will be described in this paper.

The equation of motion for classical vibrations on a one-dimensional harmonic chain can be written as

$$m_i \omega^2 \xi_i = k_{i,i+1}(\xi_i - \xi_{i+1}) + k_{i,i-1}(\xi_i - \xi_{i-1}) \tag{3}$$

where m_i is the mass of atom i which is connected with spring constants $k_{i,i\pm1}$ to the neighbouring atoms and ξ_i is the displacement of the ith atom from its equilibrium position. We will only study the case of identical spring constants $k_{i,i\pm1} = 1$ for all i between two types of masses m_A and m_B which are aperiodically distributed on a chain. Equation (3) can then be rewritten in the transfer matrix formalism (see e.g. [13]), where the eigenvalue ω is multiplied with the masses which describe the aperiodic variation in the model. However, by introducing mass-dependent coordinates one obtains a transfer matrix that resembles the matrix (2) and the nature of the spectrum for this system is the same as for the above-described mixed electron model.

Sufficient conditions for which a mixed lattice can be transformed to an on-site model are given in [11], where it was proved that a mixed Thue–Morse lattice could not be transformed to an on-site model. We actually perform a renormalization of a mixed lattice with a Thue–Morse ordering to an on-site model in section 2. The idea is to introduce more degrees of freedom into the Thue–Morse sequence without changing the individual binary order between the elements in the sequence. This implies that also the vibrational spectrum for a harmonic diatomic Thue–Morse chain is purely singular continuous, a rigorous result that confirms the numerical evidence presented in [13]. A similar renormalization of the mixed period-doubling lattice is made in section 3, where the same conclusion is reached. This method applies to a series of binary aperiodic substitution sequences. In section 4, we show that the mixed Rudin–Shapiro lattice can be renormalized to an on-site model. Before turning the attention to these issues, we make the following remark.

Instead of varying the masses in equation (3) one can distribute two types of spring constants between identical atoms. Then, there is a correspondence between that system and the off-diagonal (transfer) electron model in which case one models a chain of bonds rather than different sites. The off-diagonal tight-binding model is the Hamiltonian (1) with site energies $\epsilon_i = 0$ and two kinds of bonds t_A and t_B distributed according to some aperiodic sequence. Upon multiplying a sequence of matrices given by (2) the factors can be grouped together resulting in a sequence of effective 'transfer' matrices, S_i, of the form [11]

$$S_i = \begin{pmatrix} E/t_{i-1,i} & -t_{i,i-1} \\ 1/t_{i-1,i} & 0 \end{pmatrix}. \tag{4}$$

By defining the hopping in the forward direction, i.e. $t_{i,i-1} \equiv t_i$ (and $t_{i,i+1} \equiv t_{i+1}$) where $t_i \in \{t_A, t_B\}$, the matrix S_i is unimodular and it depends on one index only. Hence, irrespective of the type of chain, the off-diagonal model is nothing but a disguised on-site model. As a consequence, all the dynamical relations obtained for the diagonal model apply to the off-diagonal model also, although the matrices entering these relations are different. Because of this analogue one might expect that the eigenstates for the off-diagonal model share the essential features of those for the diagonal model. As far as we know, this has only been rigorously confirmed [6] for the Fibonacci model. A study of the off-diagonal Rudin–Shapiro model is also presented in section 4. This is an interesting aperiodic model for which the nature of the spectrum, even for the diagonal case, is still unknown. Finally, we summarize our main results in section 5.

2. The Thue–Morse model

The on-site Thue–Morse model can be generated [2] from a repeated application of a substitution rule, acting on letters from the alphabet $\mathcal{A} = \{A, B\}$, defined by

$$A \rightarrow AB \qquad B \rightarrow BA \tag{5}$$

where the letters A and B represent the atoms on the lattice with site energies ϵ_A and ϵ_B. With the letter A as the seed, the first four generations of the sequence are AB, $ABBA$, $ABBABAAB$, $ABBABAABBAABABBA$, and the Thue–Morse sequence [14] is the semi-infinite invariant word (or fixed point) for the rule (5). This is a palindromic sequence [9], i.e. it contains arbitrary long palindromes, where a palindrome is a word that reads the same backwards as it does forwards. At each site i, we define the hopping from that site towards the neighbouring site to the left $t_{i,i-1} \equiv t_{i-1}$ and to the right $t_{i,i+1} \equiv t_{i+1}$. With this choice, we can label the different hopping integrals $t_{A,A}$, $t_{A,B}$, $t_{B,A}$ and $t_{B,B}$ with a letter A (B) if the neighbouring atom is of type A (B), respectively. With this labelling, the sequence of transfer matrices corresponding to the fourth generation Thue–Morse lattice can be written as

$$\Phi_{2^4} = T_{A,A,B} T_{A,B,B} T_{B,B,A} T_{B,A,B} T_{A,B,A} T_{B,A,A} T_{A,A,B} T_{A,B,B} T_{B,B,A}$$
$$\times T_{B,A,A} T_{A,A,B} T_{A,B,A} T_{B,A,B} T_{A,B,B} T_{B,B,A} T_{B,A,A} \Phi_0. \tag{6}$$

Note that the sequence of transfer matrices appears in opposite order compared to the letters in the original word. We have placed a letter A at the left-most position in the first transfer matrix in the string above indicating the hopping $t_{A,A}$ between the last and first atoms in the lattice. This is consistent with periodic boundary conditions. When this process is continued this letter will obviously be replaced by the letter B since the next atom in the sequence is a type B atom and the hopping element to this atom is $t_{A,B}$, in this order. Even with four different hopping matrix elements this string of transfer matrices appears as a palindrome and it is therefore unimodular. However, there is no direct correspondence between the letters in the word and the sequence of transfer matrices. The reason is that there are six different kinds of matrices, so the string of transfer matrices is not renormalizable with respect to the substitution rule. With a simple shift of one lattice site to the right adding the next transfer matrix in the sequence and removing the first one, we can find a simple recursion for the transfer matrices. Introducing the unimodular transfer matrices $\mathcal{T}_{BB}^{(1)} \equiv T_{A,B,B} T_{B,B,A}$, $\mathcal{T}_{BA}^{(1)} \equiv T_{A,B,A} T_{B,A,B}$, $\mathcal{T}_{AA}^{(1)} \equiv T_{B,A,A} T_{A,A,B}$ and $\mathcal{T}_{AB}^{(1)} \equiv T_{B,A,B} T_{A,B,A}$ the difference equation containing the sequence of transfer matrices can be written as $\Phi_{2^k+1} = \mathcal{T}_{BB}^{(k)} \Phi_1$, where the renormalized transfer matrices satisfy the recursion relations

$$\begin{aligned}
\mathcal{T}_{BB}^{(k+1)} &= \mathcal{T}_{BA}^{(k)} \mathcal{T}_{BB}^{(k)} & \mathcal{T}_{BA}^{(k+1)} &= \mathcal{T}_{BB}^{(k)} \mathcal{T}_{AA}^{(k)} \\
\mathcal{T}_{AA}^{(k+1)} &= \mathcal{T}_{AB}^{(k)} \mathcal{T}_{AA}^{(k)} & \mathcal{T}_{AB}^{(k+1)} &= \mathcal{T}_{AA}^{(k)} \mathcal{T}_{BB}^{(k)}
\end{aligned} \tag{7}$$

for any integer $k \geqslant 1$. The dynamical system (7) is then a renormalizable on-site model with respect to the substitution rule

$$\begin{aligned}
BB &\rightarrow BBAB & AB &\rightarrow AABB \\
AA &\rightarrow AABA & BA &\rightarrow BBAA
\end{aligned} \tag{8}$$

where the elements should be viewed as two-letter words. Using this new substitution rule we get the corresponding first four generations BB, $BBAB$, $BBABAABB$, $BBABAABBAABABBAB$. Note that these are just the generations for the original Thue–Morse sequence but shifted one letter to the right removing the first letter. This means that if we distribute the site energies according to this 'Thue–Morse-like' substitution sequence, the

mixed model is a renormalizable on-site model and its spectrum has the same character as that of the corresponding diagonal model. This primitive substitution sequence contains arbitrarily long palindromes even when viewed as built from these two-letter words. The first $2^{(k-1)} - 1$ two-letter words in every even generation of the sequence (8) of length 2^k is a palindrome of length $2^k - 2$, simply because the corresponding generation for the original Thue–Morse sequence is a palindrome itself. The infinite sequence contains therefore palindromes of arbitrary length implying that the spectrum is purely singular continuous for arbitrary but different values of the site energies [9, 15]. It is, in fact, sufficient to consider the sequence as composed by the single elements A and B in some $\mathcal{A}^*$, which is the set of all finitely long words that can be written using an alphabet $\mathcal{A}$. This can be accomplished by defining the alphabet $\mathcal{A} = \{a, b, c, d\}$ and the substitution rule acting on it as

$$a \rightarrow ab \qquad b \rightarrow ca \qquad c \rightarrow cd \qquad d \rightarrow ac \qquad (9)$$

followed by a projection that sends each a and b to a B and each c and d to an A. Then every word in the sequence can always be written as a product of palindromes of the elements A and B with diverging lengths and centre positions. The substitution rule (9) might be viewed as a generalization of the Thue–Morse sequence since the original substitution rule (5) is regained by the identification $d = a$ and $c = b$ in (9). From a stringent point of view, we cannot say that the fixed point of the substitution rule (8) is the Thue–Morse sequence, but it is a fixed point with the same order between the elements A and B as for the Thue–Morse sequence. One may also note that the spectra for the periodic approximants in the two descriptions not necessarily coincide which perhaps could be the case also for the infinite systems, although both their spectra are purely singular continuous. Hence, the electronic spectrum for a mixed lattice having a Thue–Morse ordering does not change its character compared to the diagonal case. This also proves that the vibrational spectrum for an infinite chain of two masses m_A and m_B (connected with a uniform spring constant) with a Thue–Morse ordering is purely singular continuous. The actual appearance of the spectrum in the vibrational case is qualitatively different from the electronic case, but the generalized eigenstates are all extended (critical) for both models. We show an example of the displacement pattern for a Thue–Morse chain in figure 1. The normalized eigenstate, found from numerically solving equation (3), corresponds to an eigenfrequency for which the transfer matrices commute [13] producing a lattice-like displacement pattern. This particular frequency belongs to a countable dense subset of energies in the spectrum whose associated wavefunctions are extended and satisfy the Born–von Karman boundary conditions [13].

For an explicit study of wavefunctions in the mixed model it is useful to derive a trace map for the system (7), which now is a straightforward procedure following the lines in [16]. We will not pursue this matter here, but instead comment on another mixed model obtained from generalizing the off-diagonal tight-binding model [17]. To distinguish this generalization from our mixed model, we denote the two types of bonds by the letters L (S) instead of A (B). Then, one can identify four distinct local environments denoted as α, β, γ and δ corresponding to lattice points flanked by $L - L$, $L - S$, $S - L$ and $S - S$ bonds, respectively. When distributing the bonds according to the Thue–Morse sequence, one can replace every right-most index with the middle index in every transfer matrix in equation (6). For example, the last matrix $T_{B,A,A}$ should be replaced by $T_{S,\beta,L}$ in the string corresponding to the first two bonds LS in the sequence. Doing so, one finds that the string of transfer matrices is renormalizable with respect to the substitution rule $\beta \rightarrow \beta\delta$, $\delta \rightarrow \gamma\beta$, $\gamma \rightarrow \gamma\alpha$ and $\alpha \rightarrow \beta\gamma$ for the lattice points, which represent different site energies. However, the corresponding matrices are not all unimodular and the trace map technique cannot be applied directly. In spite of the non-unimodularity of the transfer matrices a trace map for this system was found [17] using a
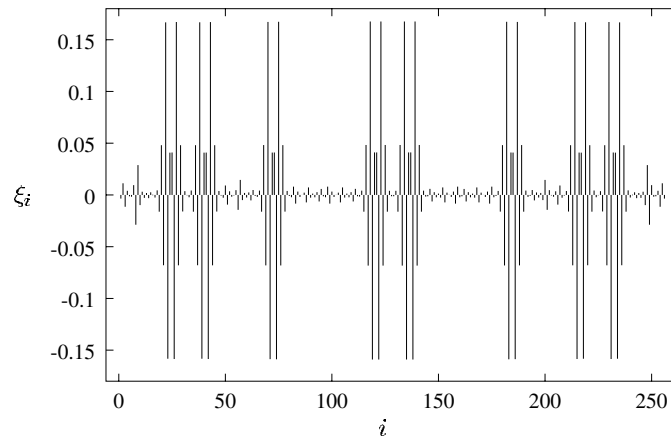
Figure 1. A normalized vibrational eigenstate with frequency $\omega = 1.799\,081\cdots$ for a harmonic chain containing 256 masses $m_A = 2$ and $m_B = 1$ arranged according to the Thue–Morse sequence. Rigid boundary conditions are used. Note the corresponding subsequence $ABBABAABBAABABBA$ of length $2^4 = 16$.

real-space renormalization-group method [18]. This system was reconsidered in [19] where a trace map was derived by grouping the matrices together in a certain way obtaining a recursion of unimodular matrices. However, we would like to stress that this substitution rule is in fact identical to the substitution rule (9). With four distinct elements this rule does not generate a palindromic sequence and from this point of view one cannot draw any general conclusions about the spectral properties of the model from the substitution itself. In this aspect, the mixed model considered in this paper has the advantage of making these predictions possible.

We end this section by a comparison of the substitution rules (5) and (8) for the Thue–Morse ordering applied to the off-diagonal tight-binding model, where all the site energies $\epsilon_i = 0$. The spectrum is then obviously symmetric around the value $E = 0$ for a distribution of two bonds t_A and t_B following the Thue–Morse sequence (5). As pointed out in the introduction, one can use the trace map [13] for the diagonal model to obtain the allowed energy values. The value $E = 0$ is actually in the spectrum, and it is easy to evaluate the corresponding wavefunction using the matrix (4) together with the substitution rule. By viewing the Thue–Morse sequence as built up from the two-letter words AB and BA, the corresponding matrices are $\mathcal{S}_{BA}^{(1)} \equiv S_B S_A$ and $\mathcal{S}_{AB}^{(1)} \equiv S_A S_B$, respectively. These two matrices are the inverses of each other and they can be written as

$$\mathcal{S}_{BA}^{(1)} = \begin{pmatrix} -R & 0 \\ 0 & -1/R \end{pmatrix} \qquad \mathcal{S}_{AB}^{(1)} = \begin{pmatrix} -1/R & 0 \\ 0 & -R \end{pmatrix} \qquad (10)$$

where $R = t_B/t_A$ denotes the ratio of the bonds. From the substitution rule and (10), we have $\mathcal{S}_{BA}^{(k+1)} = \mathcal{S}_{AB}^{(k)} \mathcal{S}_{BA}^{(k)} = I$, where I denotes the unit matrix, for all integers $k \geqslant 1$. This means in particular that $E = 0$ is an eigenvalue for every finite generation beyond the first one of the sequence, implying that this value is in the spectrum for the infinite Thue–Morse chain. There are two linearly independent solutions for this energy and the corresponding generalized eigenstate is not normalizable and it is thereby critical. This means that $E = 0$ belongs to the singular continuous part of the spectrum for all $R \neq \pm 1$. One may note that for $R = -1$ the matrices (10) will be unit matrices and the corresponding eigenstate is periodic [20]. We show in figure 2 one of the two linearly independent solutions at $E = 0$ obtained from the recursion $\Phi_{2^8} = \mathcal{S}_{BA}^{(8)} \Phi_0$, where $\Phi_0 = (1, 0)^T$. In this case, the sequence of wavefunction coefficients ψ_i
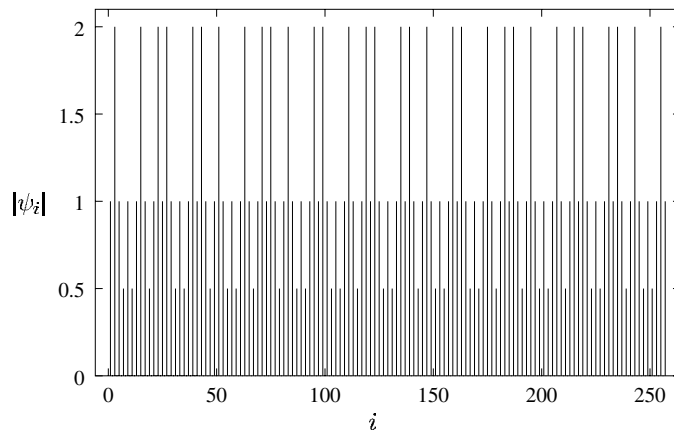
Figure 2. A lattice-like electronic wavefunction at $E = 0$ for $R = t_B/t_A = 2$, where 256 bonds t_A and t_B are arranged according to the Thue–Morse sequence. The absolute value of the wavefunction coefficient versus the site number is shown.

can be thought of as being composed of three subsequences, two of which are periodic and one that follows the Thue–Morse sequence. The wavefunction coefficient is trivially (due to the initial condition) zero at every even (0, 2, 4, etc) site and has the value 1 at every fourth (1, 5, 9, etc) site, which constitute the periodic subsequences. The remaining sites ($j = 4i + 3$, $i \geqslant 0$) form a subsequence of coefficients $\{\psi_j\} = \{-2, -1/2, -1/2, -2, \ldots\}$ which follows the Thue–Morse sequence exactly, reflecting the structural nature of the supporting lattice. This lattice-like eigenstate originates from the fact that the matrices $\mathcal{S}_{BA}^{(k)}$ and $\mathcal{S}_{AB}^{(k)}$ commute at every length scale, i.e. for every generation number $k \geqslant 1$. The value $E = 0$ is in the spectrum also for the sequence generated from the substitution rule (8), but it is not an eigenvalue for the different finite generations of the sequence. In this case we have two more matrices corresponding to the words AA and BB, which are $\mathcal{S}_{AA}^{(1)} \equiv S_A S_A = -I$ and $\mathcal{S}_{BB}^{(1)} \equiv S_B S_B = -I$, where I is the unit matrix. If these two matrices appear with an equal density and if also the number of matrices in (10) is equal for the infinite string then $\mathcal{S}_{BB}^{(\infty)} \equiv \lim_{k \to \infty} \mathcal{S}_{BB}^{(k)} = I$ and $E = 0$ belongs to (the singular continuous part of) the spectrum. This problem is equivalent to the problem of determining the density of the two-letter words in the alphabet $\mathcal{A} = \{BB, AB, AA, BA\}$ for the infinite sequence, which is given by the eigenvector corresponding to the largest eigenvalue of the substitution matrix [2]. The substitution matrix M is defined from the relation $n^{(l+1)} = M n^{(l)}$, where $n^{(l)}$ is a vector whose components are the number of different two-letter words in the sequence when the substitution rule has been applied l times. The substitution matrix for the substitution rule (8) can be written as

$$M = \begin{pmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{11}$$

The eigenvalues of M are 2, 0, 1 and -1. Note that the eigenvalues (2 and 0) of the substitution matrix corresponding to the substitution rule (5) are contained in this description. A positive eigenvector, corresponding to the largest eigenvalue 2, is $(2, 1, 2, 1)^T$ from which the desired result follows. Hence, even if the eigenvalues of the periodic approximants for the two

descriptions of the Thue–Morse ordering are not equal it still might well be the case that the spectra actually coincide.

3. The period-doubling model

The site energies of the period-doubling model can also be generated by two symbols A and B, where the period-doubling sequence [21] is the invariant word of the substitution rule

$$A \to AB \qquad B \to AA. \tag{12}$$

Using this rule, with the letter A as the seed, the generations of the sequence are $AB, ABAA, ABAAABAB, ABAAABABABAAABAA, \ldots$. With the same labelling of the hopping integrals as in the mixed Thue–Morse model the sequence of transfer matrices corresponding to the fourth generation period-doubling lattice reads

$$
\begin{aligned}
\Phi_{2^4} = {} & T_{A,A,A}T_{A,A,B}T_{A,B,A}T_{B,A,A}T_{A,A,A}T_{A,A,B}T_{A,B,A}T_{B,A,B}T_{A,B,A} \\
& \times T_{B,A,B}T_{A,B,A}T_{B,A,A}T_{A,A,A}T_{A,A,B}T_{A,B,A}T_{B,A,A}\Phi_0
\end{aligned}
\tag{13}
$$

where periodic boundary conditions are used. There is no direct correspondence between the letters in the word and the sequence of transfer matrices in this case either. However, with a similar shift of one lattice site to the right as in the Thue–Morse model, we find that the difference equation containing the sequence of transfer matrices can be written as $\Phi_{2^k+1} = \mathcal{T}_{AAAB}^{(k)}\Phi_1$ for any integer (generation number) $k \geqslant 2$. In this case the renormalized transfer matrices satisfy the recursion relations

$$\mathcal{T}_{AAAB}^{(k+1)} = \mathcal{T}_{ABAB}^{(k)}\mathcal{T}_{AAAB}^{(k)} \qquad \mathcal{T}_{ABAB}^{(k+1)} = \mathcal{T}_{AAAB}^{(k)}\mathcal{T}_{AAAB}^{(k)} \tag{14}$$

where the initial unimodular transfer matrices have been defined by $\mathcal{T}_{AAAB}^{(2)} \equiv T_{B,A,A}T_{A,A,A}T_{A,A,B}T_{A,B,A}$ and $\mathcal{T}_{ABAB}^{(2)} \equiv T_{B,A,B}T_{A,B,A}T_{B,A,B}T_{A,B,A}$. We find that the system (14) is a renormalizable on-site model with respect to the substitution rule

$$BAAA \to BAAABABA \qquad BABA \to BAAABAAA \tag{15}$$

where the elements should be viewed as four-letter words. Using this new rule, we get the corresponding generations $BAAA, BAAABABA, BAAABABABAAABAAA, \ldots$. Once again these are just the generations for the original period-doubling sequence but shifted one lattice site to the right. For the diagonal model these two descriptions have identical spectra for the different periodic approximants. This is because the trace is invariant under a cyclic permutation of the matrices in the string, so one can move the last letter to the first position in any generation without changing the spectrum. Indeed, following the lines in [5], one can show that the latter description has purely singular continuous spectrum. If we define the trace coordinates $x_k \equiv \mathrm{Tr}\,\mathcal{T}_{AAAB}^{(k)}$ and $y_k \equiv \mathrm{Tr}\,\mathcal{T}_{ABAB}^{(k)}$ the trace map can, using the relations (14), be written as

$$x_{k+2} = x_{k+1}(x_k^2 - 2) - 2 \qquad k \geqslant 2 \tag{16}$$

where the invariant $\mathcal{J} \equiv x_{k+1} - x_k y_k = -2$, for all $k \geqslant 2$, has been used. These relations for the mixed model are in perfect agreement with those for the diagonal model [22]. By adding the inverses of the words, extending the structure to a free group, the result follows from noting that the induced substitution corresponding to the reduced trace map of (16) is semi-primitive [8] and that the beginning of the sequence can be written as the square of the word $BAAA$ followed by the element $(BAAA)^{-1}BABA$, which remains invariant under a two-fold application of the substitution rule. This result is, of course, quite natural since the substitution rule (15) again generates a period-doubling sequence. We arrive at the
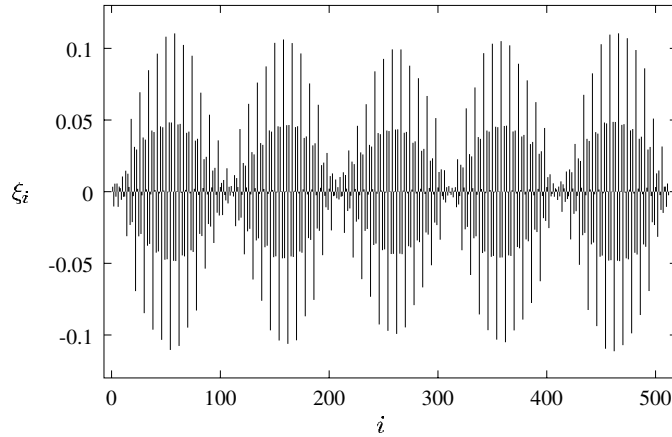
Figure 3. The normalized vibrational eigenstate corresponding to the eigenvalue number 390 for a harmonic chain containing 512 masses $m_A = 2$ and $m_B = 1$ arranged according to the period-doubling sequence. Free boundary conditions are used.

conclusion that the mixed period-doubling lattice is a renormalizable on-site model with the same character for the vibrational and electronic spectra, namely purely singular continuous. An example of a vibrational eigenstate for a diatomic period-doubling chain is shown in figure 3. The displacement pattern exhibits an almost periodic-like feature which could be a consequence of the fact that the period-doubling sequence is a limit-periodic sequence.

4. The Rudin–Shapiro model

The Rudin–Shapiro sequence [23] has an absolutely continuous Fourier transform [2], a property it has in common with random sequences. This binary sequence is usually generated from a substitution rule [2] with four different letters $a \rightarrow ab, b \rightarrow ac, c \rightarrow db$ and $d \rightarrow dc$, followed by a final projection that sends each a and b to an A and each c and d to a B. One can also consider the binary Rudin–Shapiro sequence as built from an alphabet of two-letter words $\mathcal{A} = \{AA, AB, BA, BB\}$ subjected to an infinite application of the substitution rule [24]

$$AA \rightarrow AAAB \qquad AB \rightarrow AABA \qquad BA \rightarrow BBAB \qquad BB \rightarrow BBBA \qquad (17)$$

where we refer to the seed AA as the first generation of the sequence. The different generations of the Rudin–Shapiro sequence thus read $AA, AAAB, AAABAABA, AAABAABAAAABBBAB, \ldots$. There are very few rigorous results concerning the electronic spectrum and the associated wavefunctions already for the diagonal Rudin–Shapiro model. This sequence is neither palindromic [15, 28] nor does it meet the requirements in [8] for a possible exclusion of eigenvalues in the spectrum. Numerical results indicate [25] that for finite approximations of the sequence all eigenstates are localized, for almost any value of the potential strength, but that the localization can be weaker than exponential.

Analytical results for the spectral properties at the centre of the spectrum in the corresponding off-diagonal model can be obtained without too much difficulty. When distributing two bonds t_A and t_B the spectrum for the off-diagonal Rudin–Shapiro chain is symmetric around the value $E = 0$. To show that this value really belongs to the spectrum one can use the trace map for the corresponding diagonal model [16] applied to the relevant matrices (4), but we make use of the substitution matrix [2], M, instead. We note that every four-letter word in (17) begins with either of the words AA or BB. Using (4) the effective
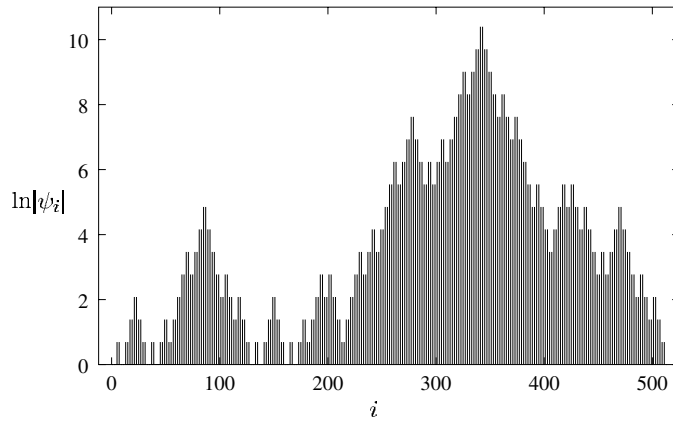
Figure 4. Non-normalized electronic wavefunction at $E = 0$ for an arrangement of 512 bonds t_A and t_B following the Rudin–Shapiro sequence for $R = t_B/t_A = 2$. The natural logarithm of the absolute value of the wavefunction coefficient ψ_i versus site number i is shown.

transfer matrices $\mathcal{S}_{AA}^{(1)} = \mathcal{S}_{BB}^{(1)} = -I$, where I is the unit matrix, correspond to these words. The other two matrices present are those in (10) corresponding to the words AB and BA, respectively. Since all of these four matrices commute, we only have to count the number of appearances of the latter two-letter words in the sequence. If they appear with an equal weight in some generation of the sequence, then $E = 0$ is an eigenvalue since the entire matrix will be a unit matrix. Iteration of the relation for the substitution matrix starting with the word AA gives $\boldsymbol{n}^{(l+1)} = M^l \boldsymbol{n}^{(1)}$, where the initial condition is $\boldsymbol{n}^{(1)} = (1, 0, 0, 0)^T$. The relation between the number of two-letter words in any generation of the Rudin–Shapiro sequence can be found by a diagonalization of M. This information can be extracted from [26] where this has been explicitly worked out. We find that for every *odd* generation $k = 2l + 1$, where $l \geqslant 1$, the number of words of the types AB and BA is equal, implying that $E = 0$ is an eigenvalue. For the *even* generations $m = 2l$, where $l \geqslant 1$, of the sequence, the energy $E = 0$ is in general not an eigenvalue since the difference between the number of words AB and the number of words BA is equal to $2^{(l-1)} \neq 0$. From the substitution rule (17), without explicit calculations, the matrix relations for the different generations satisfy

$$\mathcal{S}_{AA}^{(2l+1)} = \mathcal{S}_{BA}^{(2l)} \mathcal{S}_{AA}^{(2l)} = I \tag{18}$$

$$\mathcal{S}_{AA}^{(2l+2)} = \mathcal{S}_{BA}^{(2l+1)} \mathcal{S}_{AA}^{(2l+1)} = \mathcal{S}_{BA}^{(2l+1)} = \left(\mathcal{S}_{BA}^{(1)}\right)^{2l} \tag{19}$$

for all integers $l \geqslant 1$, where I is the unit matrix and $\mathcal{S}_{BA}^{(1)}$ is the matrix in (10). Depending on the value of the ratio $R = t_B/t_A$ of the bonds, relation (19) determines the growth or decay of the wavefunction at the end of each even generation. However, for the infinite sequence all two-letter words are in fact equally common, since the largest eigenvalue of the substitution matrix M is 2 with the corresponding eigenvector $(1, 1, 1, 1)^T$, which gives the density of the words. This shows not only that the spectrum is symmetric about the energy $E = 0$, but also that this value is in the spectrum for the Rudin–Shapiro sequence. In other words, we have $\mathcal{S}_{AA}^{(\infty)} \equiv \lim_{k \to \infty} \mathcal{S}_{AA}^{(k)} = I$. Like for the Thue–Morse model the corresponding generalized eigenstates are critical for all $R \neq \pm 1$, and this value of the energy belongs to the singular continuous component of the spectrum. We show in figure 4 one of the two linearly independent solutions at $E = 0$ for $R = 2$ obtained from the recursion $\Phi_{2^9} = \mathcal{S}_{AA}^{(9)} \Phi_0$, where $\Phi_0 = (1, 0)^T$, plotted in logarithmic scale. If this state were to be plotted in linear scale only the dominating wavefunction coefficients would be seen, and it could easily had been referred

to as a typically localized state. Due to the initial condition the wavefunction coefficients are zero at every even site which are not shown in the figure. It is worthwhile to note that a similar type of non-recurrence of zero energy, as expressed by relations (18) and (19), with respect to generation number has been encountered [24, 27] also for the diagonal Rudin–Shapiro model, but in these studies the role of even and odd generations is interchanged with respect to the energy $E = 0$.

From the relation (19), we see that it requires ever longer strings of matrices before an identity matrix is formed explaining the self-similarity as well as the rather strong localization property of the wavefunction in figure 4. We suggest that *hidden squares* of arbitrary lengths in the sequence are responsible for this generic localization property in the Rudin–Shapiro chain. There are squares of ever growing lengths of the four 'elements' $ABAA$, $BAAA$, $ABBB$ and $BABB$ which are not words in the sequence, i.e. they are not the image of any word under the substitution rule (17), although they belong to the set $\mathcal{A}^*$. Furthermore, these squares all intersect each other and they cross over the different generation breaks in an intricate way. We can write, using the substitution rule (17), the fifth generation matrix as

$$\mathcal{S}_{AA}^{(5)} = \mathcal{S}_{BA}^{(2)}\mathcal{S}_{AB}^{(1)}\mathcal{S}_{BB}^{(1)}\mathcal{S}_{AB}^{(1)}\left[\mathcal{S}_{AA}^{(1)}\mathcal{S}_{BA}^{(1)}\right]^2\mathcal{S}_{BB}^{(1)}\mathcal{S}_{AA}^{(2)}\mathcal{S}_{BA}^{(2)}\mathcal{S}_{AA}^{(2)} \tag{20}$$

where the matrix $\left[\mathcal{S}_{AA}^{(1)}\mathcal{S}_{BA}^{(1)}\right]^2$ corresponds to the element $(ABAA)^2 \in \mathcal{A}^*$. Upon iterating (20) one step, we find from (17) that $(ABAA)^2 \to (AABAAAAB)^2$ with the corresponding matrix $\left[\mathcal{S}_{AA}^{(2)}\mathcal{S}_{BA}^{(2)}\right]^2$, i.e. the following six matrices in the sequence $\mathcal{S}_{AA}^{(2)}\mathcal{S}_{BA}^{(2)}\mathcal{S}_{AA}^{(2)}$ couple to the first one in the string (20), building the square. In this way squares of ever growing length are formed, a procedure that applies to the other three elements as well. For example, the first three matrices $\mathcal{S}_{BA}^{(2)}\mathcal{S}_{AB}^{(1)}$ in the string (20) combine with the last matrix $\mathcal{S}_{AA}^{(1)}$ upon iteration forming a square corresponding to the square of $BAAA$. We have not made any assumptions about the matrices in (20), so this applies to the diagonal model as well as to the original formulation of the substitution rule [2] with four different single letters. This purely combinatorial property of squares on any length scale of the Rudin–Shapiro chain should imply results on the spectrum. It certainly governs the recurrence and the self-similarity of the wavefunctions and under certain additional conditions it should imply the absence of eigenvalues in the spectrum. Unfortunately, we could not quite put this on a solid mathematical foundation, especially the exclusion of exponentially decaying solutions. However, we believe that if a deterministic aperiodic chain, generated from a primitive substitution rule, contains arbitrarily long squares of an 'element', not necessarily a word from the substitution rule, the corresponding spectrum should be purely singular continuous. If this conjecture can be proved, it would cover the Rudin–Shapiro chain. An example of a sequence containing arbitrarily long squares was recently constructed in [24] showing a similar localization property as the Rudin–Shapiro chain does, but was proved to have only a singular continuous component in the spectrum.

Finally, in the off-diagonal model there is a *dual* wavefunction with respect to a periodic system, obtained when letting the bond ratio change according to $R \to 1/R$. We show in figure 5 the dual wavefunction of the one displayed in figure 4, although plotted in linear scale. The actual appearance of this eigenstate is different from that of figure 4, but in view of equation (19) they express exactly the same type of localization property. Actually, in a logarithmic plot it could have been represented as the mirror of the unshaded area in figure 4, since the change in bond ratio is equivalent to the change of wavefunction coefficients as $\psi_n \to 1/\psi_n$. It is clearly seen in figure 5 how the formation of squares in the sequence, upon iterating the relation (20), influences the wavefunction. Of course, there is a dual wavefunction also in the off-diagonal Thue–Morse model, with the property that only the wavefunction
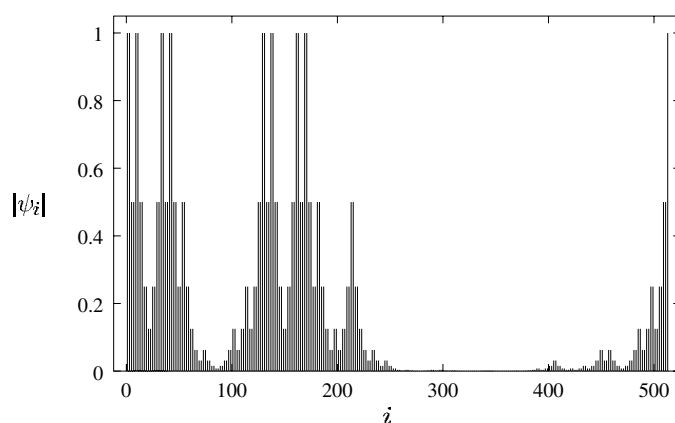
Figure 5. Electronic wavefunction at $E = 0$ for an arrangement of bonds t_A and t_B following the Rudin–Shapiro sequence for $R = t_B/t_A = 1/2$. The dual wavefunction of the one shown in figure 4. Here the absolute value of the wavefunction coefficient is plotted as a function of site index.

coefficients following the Thue–Morse sequence itself will be mutually interchanged in figure 2.

The mixed Rudin–Shapiro model can also be transformed to an on-site model on a renormalized chain, but the substitution rule (17) turns out to have too few degrees of freedom. If we move the first letter A to the last position in any generation of the Rudin–Shapiro sequence, i.e. the new generations become AA, $AABA$, $AABAABAA$, $AABAABAAAABBBABA, \ldots$, this new sequence will then have the same individual order between the basic elements A and B, and the spectra agree for the two descriptions for any finite generation. In order to generate the sequence from a substitution rule we need to consider building blocks or words of length four

$$
\begin{aligned}
AABA &\rightarrow AABAABAA & ABAA &\rightarrow AABBBABA \\
AABB &\rightarrow AABAABAB & ABAB &\rightarrow AABBBABB \\
BBAA &\rightarrow BBABBABA & BABA &\rightarrow BBAAABAA \\
BBAB &\rightarrow BBABBABB & BABB &\rightarrow BBAAABAB
\end{aligned}
\tag{21}
$$

where we choose the word $AABA$ to be the seed. Of course, we could equally well have defined a substitution rule acting on eight single letters and used a final projection to obtain the binary sequence. Doing so, one finds that the original Rudin–Shapiro sequence defined as a substitution on four single elements is contained in this description using another projection. By rigorous deduction it is easily verified that the mixed Rudin–Shapiro model is a renormalizable on-site model with respect to the substitution rule (21), when the site energies and the four hopping integrals are distributed as before. One actually needs to consider strings of transfer matrices of length 16 in order to obtain unimodular matrices, which corresponds to the words obtained from applying the rule (21) once more, a procedure analogous to the one used for the mixed period-doubling model. Thus, the vibrational spectrum and the spectrum for the mixed electron model have the same type as that of the conventional diagonal model. The vibrational modes for the eigenfrequencies in the lower part of the vibrational spectrum have obviously more extended-like character. An example is shown in figure 6, where the displacements ξ_i seem to take values along two smooth curves. In the upper part of the spectrum the vibrational eigenstates show localization properties very similar to the eigenstates of the electron models.
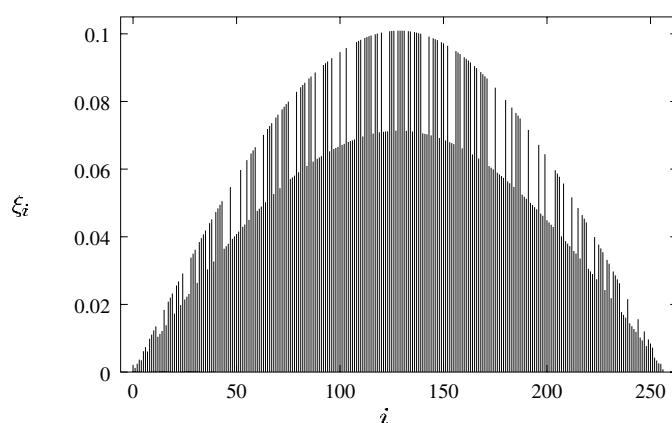
Figure 6. The normalized vibrational eigenstate with lowest frequency ($\omega = 0.009840\cdots$) for a harmonic chain containing 256 masses $m_A = 2$ and $m_B = 1$ arranged according to the Rudin–Shapiro sequence. Rigid boundary conditions are used.

This renormalization method indeed applies to a number of binary aperiodic substitution sequences but there are also examples for which it does not work. Another primitive substitution sequence for which the absence of eigenvalues in the spectrum has not been rigorously proved is the paperfolding sequence [29]. It can be generated by the substitution rule $a \to ab, b \to cb, c \to ad$ and $d \to cd$ followed by a final projection that sends each element a and b to an A and each c and d to a B. Like for the Rudin–Shapiro sequence this procedure is equivalent to the substitution rule $AA \to AABA$, $BA \to ABBA$, $AB \to AABB$ and $BB \to ABBB$ acting on two-letter words. It turns out that there are not enough degrees of freedom in this sequence for transforming such a mixed lattice to an on-site model, at least not with the method described in this paper.

5. Conclusions

We have studied the spectral properties of more realistic mixed tight-binding models with an aperiodic distribution of both site energies and hopping integrals. It is shown that the mixed Thue–Morse model, the mixed period-doubling model and the mixed Rudin–Shapiro model can all be transformed to conventional on-site models on renormalized chains maintaining the individual binary order of the site energies. From these results it rigorously follows that the electronic spectra for these mixed models have the same character as those of the corresponding on-site models. That is, the introduction of correlated nearest-neighbour hopping for the on-site Thue–Morse and period-doubling models leaves the singular continuous nature of their spectra unchanged. The study of electrons on such mixed lattices naturally maps onto the study of elastic vibrations on harmonic chains from which we have proved that the vibrational spectra for harmonic chains with distribution of masses determined by the Thue–Morse sequence and the period-doubling sequence are purely singular continuous. A similar result has earlier only been rigorously proved for the Fibonacci model. We have also explored the nature of vibrational and electronic eigenstates for these systems. The Thue–Morse model was shown to support lattice-like eigenstates whereas the period-doubling model showed eigenstates that in some way reflected the limit-periodic property of the sequence. Finally, a study of the off-diagonal Rudin–Shapiro model led to the conclusion that hidden squares in the sequence are

likely to be responsible for its apparent localization properties. At the same time the existence of these ever growing squares should imply the absence of eigenvalues in the spectrum.

Acknowledgments

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