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Hidden dimers and their effect on the optical and electronic transmission in Thue–Morse aperiodic structures

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Abstract. We show that a Thue–Morse aperiodic structure presents a unique kind of positional correlation between its constituents, leading to an unattenuated transmission of light as well as electrons through it. The reason for this is a resonant tunnelling, whose origin can be traced back to the presence of certain 'dimers' which are not *explicitly displayed* in the structure. It is interesting to observe that under suitable conditions, two apparently uncorrelated constituents in a Thue–Morse sequence combine together to form a dimer and the entire system can be thought of as being composed of nested dimers only. This aspect has been analysed in terms of light propagation through a Thue–Morse multilayered system and its electronic counterpart.

1. Introduction

The problem of localization of electromagnetic waves in quasiperiodically ordered layered media has attracted considerable attention in the last decade (see [1–4, 7] and references therein). Due to recent advances in nanostructure technology, finite-size sequences of two different materials can now be grown in the laboratory [5]. Hence the results of such studies can be subjected to experimental investigation, as has already been done [6]. So far, the models considered have consisted of binary orderings of slabs of two different materials A and B, arranged following a typical inflation rule $A \rightarrow A^m B^n$, and $B \rightarrow A$. m and n are positive integers greater than zero, and $m = n = 1$ gives the well-known Fibonacci sequence of A and B [1]. The above inflation rule generates other quasiperiodic sequences for $n = 1$ and arbitrary values of m. However, it may be mentioned here that many more orderings, different from the one that we have referred to above, have been investigated (see [8, 9] and references therein), not only for studying optical properties, but as regards the electronic and related properties as well. We will name a few of them. Wen *et al* [9] proposed a class of substitution rules for generating various quasiperiodic chains and obtained relevant scaling properties of the corresponding energy spectrum. They also constructed explicit atomic surfaces for a subclass of these lattices. The nature of the atomic surfaces has also been studied by Luck *et al* [10] for different quasiperiodic self-similar structures. In addition to the electronic properties, phonon properties as well as diffusion characteristics of different quasiperiodic lattices were studied by Kohmoto and Banavar [11]. In fact, a wealth of literature has resulted from the extensive research on different properties of these systems over the past few years. As far as the problem of light propagation in binary quasiperiodic or aperiodic multilayers is concerned, the materials are characterized by different refractive indices n_A and n_B and layer thicknesses d_A and d_B. Results are available, in general, for normal incidence only, with the additional

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simplification $\delta_A = \delta_B$, where $\delta_{A\,(B)}$ stands for the phase acquired by light in travelling through a particular slab.

In general, owing to the nature of quasiperiodic ordering, the transmission coefficient (T) of light as a function of wavelength for transmission through a finite length of such multilayered media exhibits a rich multifractal character, as was first observed by Kohmoto *et al* [1]. It was shown that, for $\delta_A = \delta_B = (2n + 1)\pi/2$, the transfer matrices for crossing a multilayer at any generation j exhibit six-cycle behaviour; that is, $\mathbf{M}_j = \mathbf{M}_{j+6}$. Additionally, it is found that the entire multilayer turns out to be completely transparent to the incoming light for some special values of the wavelength that depend on the chosen sequence of A and B. In a Fibonacci sequence these values are obtained by looking at the zeros of the invariant of the 'trace map' [1].

The experimental realization of the localization of electromagnetic waves in aperiodically layered structures was achieved by Gellermann *et al* [6], who measured the optical transmission of a quasiperiodically ordered dielectric stack of SiO_2 (A type) and TiO_2 (B type). The experiment was done for a maximum of 55 layers (ninth-generation Fibonacci sequence) and the scaling of the transmission coefficient with increasing Fibonacci sequence at quarter-wavelength optical thickness was observed.

Coming back to the 'perfect-transmission' situation, we find that it also occurs for some other quasiperiodic sequences [2–4]. The reasons are, however, different. For example, Dulea *et al* [3] reported that for a sequence with $m = 1$, and arbitrary n, one gets $T = 1$ for $\delta_A = \delta_B = \delta = k\pi/n$, k being an integer. This happens irrespective of the ratio of the refractive indices of the two constituent materials of the multilayer. The complete transparency in this case is due to the elements B always occurring in clusters of size n. For the specific choice of the phase $\delta = k\pi/n$, the transfer matrix for crossing these clusters turns out to be the identity, leaving behind an array of elements A only. For the same choice of phase, the matrix product for the whole chain of A elements also becomes the identity, which makes the overall transmission coefficient unity.

The corresponding problems in the electronic case, namely the possibility of getting extended electronic eigenstates and perfect transmission across arbitrarily large aperiodic chains, have also been studied for the past few years [12, 13]. The reason for the occurrence of perfect transmission in some of these lattices has been traced to the presence of correlations in the atomic positions. For example, in the so-called 'random-dimer model' [12] there are a finite number of extended (perfectly transmitting) states, whereas in some of the infinite quasiperiodic chains the positional correlation persists at all scales of length. This results in an infinite number of energies supporting extended Bloch-like eigenstates and, hence, complete transmission in these lattices [13].

In this communication, we re-examine the problem of transmission of light and electrons through a Thue–Morse (TM) aperiodic structure. The TM lattice [14] is already known to sustain extended electronic states [15] in spite of its aperiodicity. At the same time, unit transmission of light waves through a TM heterostructure has also been reported [7]. However, there still remains scope for obtaining a microscopic view of the basic mechanism responsible for such phenomena. This is because the TM lattice is not known to possess an 'invariant' as in the classical case of a quasiperiodic Fibonacci chain [1]; neither can one locate any obvious 'dimer'-like positional correlations as in the cases reported in references [12] and [13]. Most interestingly, we find that the cause of the unattenuated transmission in the TM case is once again the presence of dimers. However, the dimers are 'hidden' in the sense that two very widely separated building blocks of a TM sequence can form dimers in very special situations, and their presence cannot be revealed otherwise. This situation is in contrast to what we already know regarding the canonical cases discussed in references [12] and [13]. Normally, on a technical level the optical problem has to be dealt with quite differently from the electronic

case, because of the presence of additional interfacial matrices in the former case. Of course, Lamb and Wijnands [8] have shown that one can avoid the explicit appearance of the interface matrices by a suitable change of basis. For the present study we choose to discuss two different cases. First, we address the problem of light propagation in the Thue–Morse arrangement. There is a possibility of getting an infinite number of transmission windows, in view of our previous experience with the electronic case [13], and we look into that aspect. Second, we show that the known results for the electronic case are restored if we recognize the proper dimers embedded in any finite TM chain. The basic reason for the unit electronic transmission then becomes obvious. In addition, we report a model-dependent situation in which once again resonance occurs at a special value of the energy of the electron. This energy could not be obtained in the earlier analyses.

2. Light wave propagation in a Thue–Morse multilayer

A Thue–Morse (TM) sequence is generated following the growth rule A $\rightarrow$ AB and B $\rightarrow$ BA [14]. Our basic aim is to examine the conditions under which a multilayer grown in this sequence yields full transmission of light. Our investigations show that a special positional correlation among the two kinds of block in the multilayer is responsible for the full transmission of light in these multilayers. Again, because of the self-similarity inherent to the structure of the Thue–Morse sequence, it is possible to extract, in a renormalization group sense, a whole hierarchy of conditions for attaining complete transparency of light across arbitrarily large multilayer stacks. As far as we are aware, this feature does not seem to have been emphasized in the literature so far.

Let us now consider a binary system with A and B representing the two different blocks in the layered system that is grown by placing A and B blocks sequentially following the TM generation rule. Let the thicknesses and the refractive indices of the materials be d_{A}, n_{A} and d_{B}, n_{B} respectively. The phases of the light waves, when they propagate through the two media, are $\delta_{\mathrm{A}} = n_{\mathrm{A}} k d_{\mathrm{A}}/\cos(\theta_{\mathrm{A}})$ and $\delta_{\mathrm{B}} = n_{\mathrm{B}} k d_{\mathrm{B}}/\cos(\theta_{\mathrm{B}})$ respectively. k is the wave vector of the incident light and θ_i is the angle of incidence. For our analysis we need not restrict ourselves to normal incidence, and we work in the general case where δ_{A} is not equal to δ_{B}.

The matrices required for studying propagation through the layers are [1]

$$\mathbf{M}_{\mathrm{BA}} = \begin{pmatrix} 1 & 0 \\ 0 & n_{\mathrm{A}} \cos\theta_{\mathrm{A}}/n_{\mathrm{B}} \cos\theta_{\mathrm{B}} \end{pmatrix}.$$

We also define $\mathbf{M}_{\mathrm{AB}} = \mathbf{M}_{\mathrm{BA}}^{-1}$. The matrices $\mathbf{M}_{\mathrm{BA}}$ and $\mathbf{M}_{\mathrm{AB}}$ represent the light propagation across the interfaces B $\leftarrow$ A and A $\leftarrow$ B respectively. The propagation within the layer A is represented by the matrix

$$\mathbf{M}_{\mathrm{A}} = \begin{pmatrix} \cos\delta_{\mathrm{A}} & -\sin\delta_{\mathrm{A}} \\ \sin\delta_{\mathrm{A}} & \cos\delta_{\mathrm{A}} \end{pmatrix}.$$

There is a similar matrix corresponding to the propagation through layer B. The transmission coefficient for crossing a finite length of the layered structure—say, the lth-generation segment—is given by [1]

$$T_l = 4/(M_l^2 + 2). \tag{1}$$

Here, $\mathbf{M}_l$ is the product of the matrices $\mathbf{M}_{\mathrm{AB}}$, $\mathbf{M}_{\mathrm{BA}}$, $\mathbf{M}_{\mathrm{A}}$ and $\mathbf{M}_{\mathrm{B}}$ according to the Thue–Morse sequence in any generation l, and M_l^2 denotes the sum of the squares of the four elements of $\mathbf{M}_l$. For example, in the second generation the sequence is ABBA and the corresponding string of transfer matrices will be $\mathbf{M}_{\mathrm{A}}\mathbf{M}_{\mathrm{BA}}\mathbf{M}_{\mathrm{B}}\mathbf{M}_{\mathrm{B}}\mathbf{M}_{\mathrm{AB}}\mathbf{M}_{\mathrm{A}}$. We assume that at any generation, the entire

slab is sandwiched between two A-type layers on both sides. For the sake of convenience, we investigate the problem of full transmission through layers of arbitrarily large systems in two categories.

(i) *The r-independent case:* Let us define $r = n_A \cos\theta_A / n_B \cos\theta_B$. The first five generations are

$$S_0 = A$$
$$S_1 = AB$$
$$S_2 = ABBA$$
$$S_3 = AB\,\underbrace{BA}\,\underbrace{BA}\,AB$$
$$S_4 = ABBA\,\underbrace{BAAB}\,\underbrace{BAAB}\,ABBA.$$

It is interesting to observe that in all the strings beyond S_1 there is a central cluster of identical elements or an identical pair of blocks. For example, in S_2 there is a paired cluster BB at the centre, while in S_3 we have a pair of BA blocks (underbraced) occurring side by side. In each of these strings the identical pair of blocks are flanked by the same combinations of A and B. Thus, in S_4, for example, the central pair is formed by BAAB (underbraced) and in both the wings we have ABBA. Let us talk specifically about S_2, which has the first flavour of a TM sequence. The string of transfer matrices controlling the transmission through this block is $\mathbf{M}_2 = [\mathbf{M}_A\mathbf{M}_{BA}\mathbf{M}_B\mathbf{M}_B\mathbf{M}_{AB}\mathbf{M}_A]$. $\mathbf{M}_2$ is unimodular. Now, if we set $\delta_B = \pi/2$, the central pair of matrices $\mathbf{M}_B\mathbf{M}_B$ turns out to be the identity with a negative sign. Also, $\mathbf{M}_{AB}$ being equal to $\mathbf{M}_{BA}^{-1}$, we are finally left with an A–A pair. As we have sandwiched the whole block between two A-type materials, the overall transmission coefficient will be determined by the matrix

$$\mathbf{M}_A^4 = \begin{pmatrix} \cos(4\delta_A) & -\sin(4\delta_A) \\ \sin(4\delta_A) & \cos(4\delta_A) \end{pmatrix}.$$

Obviously a choice of $\delta_A = \pi/4$ (or $\pi/2$) will make the entire matrix product equal to either an identity matrix (with a plus or a minus sign) or $-i\boldsymbol{\sigma}_y$, $\boldsymbol{\sigma}_y$ being a Pauli matrix. In either case, the transmission coefficient T_2 is one, as is evident from equation (1). In fact, it is interesting to note that for $\delta_B = \pi/2$, the transmission coefficient for the second-generation segment (ABBA) is unity *irrespective of the choice* of δ_A. For $\delta_A = \pi/4$ one gets $T = 1$ for all generations, even or odd, except S_3. However, when $\delta_A = \pi/2$, for all generations, we will have $T = 1$ as long as $\delta_B = \pi/2$. Thus, the set of parameters $\delta_A = k\pi/4$, $\delta_B = m\pi/2$ will give rise to unit transmission for any generation, k and m being integers. The choices of k and m really do not depend on which generation we are interested in. The above analysis reveals an additional interesting fact that has so far been overlooked for a TM chain. It is the mechanism by which one attains such unit transmission. In generation S_2, as the central BB pair contributes an identity matrix, the interface matrices $\mathbf{M}_{BA}$ and $\mathbf{M}_{AB}$ 'cancel' each other and the remaining A matrices that formed the flanks (and were initially separated from each other) automatically form an AA doublet. So, we actually have a 'nested' pairing effect in the arrangement of the elements that is revealed only for a specific choice of the phases. The effect is more striking if we go over to the fourth-generation sequence S_4. In this chain we have only two *isolated* Bs which occupy the fifth positions both from the left and the right ends of the chain. At the centre there is a BB pair flanked by AA blocks on either side. As soon as the central pair of matrices $\mathbf{M}_B\mathbf{M}_B$ becomes identity, the AA blocks at the flanks form a quadruplet with the interface matrices nicely taking care of each other. A choice of $\delta_A = \pi/4$ then reduces $\mathbf{M}_A^4$ to minus the identity and the isolated Bs automatically form a doublet. Once

again the interface matrices nullify each other. This process goes on and ultimately the whole string of transfer matrices corresponding to the bulk system turns out to be the identity. The matrix $\mathbf{M}_4$ is now composed of the product $\mathbf{M}_A\mathbf{M}_A$ due to the outer A-type layers. Clearly, $\mathbf{M}_A^2 = -i\boldsymbol{\sigma}_y$ and, hence, $T_4 = 1$. Thus under suitable conditions even the isolated As and Bs in the same string form doublets and quadruplets, bringing out the underlying positional correlation between the constituents. The TM sequence has not been emphasized so far either in the electronic case or in the case of optical transmission in this sequence.

(ii) *Other cases:* Let us now look into other possibilities for getting complete transmission through a TM layered structure. We start with the fourth-generation chain S_4. We will use the well-known Cayley–Hamilton theorem for 2×2 unimodular matrices, namely,

$$\mathbf{M}^2 = \mathrm{tr}(\mathbf{M})\mathbf{M} - \mathbf{I}. \tag{2}$$

$\mathbf{I}$ is the identity matrix. We see that if $\mathrm{tr}(\mathbf{M})$ can be made equal to zero, then the product of two identical matrices becomes equal to $-\mathbf{I}$. Considering the string S_4 as a specific example, we note that, as it is unimodular, we can make the product matrix corresponding to the central block BAABBAAB equal to $-\mathbf{I}$ by forcing the trace of $\mathbf{M}_c = \mathbf{M}_B\mathbf{M}_{AB}\mathbf{M}_A\mathbf{M}_A\mathbf{M}_{BA}\mathbf{M}_B$ to assume the value zero. This leads to the equation

$$\tan(2\delta_A)\tan(2\delta_B) = 2r/(1+r^2). \tag{3}$$

It is therefore obvious that for a particular choice of r, one can tune the phases δ_A and δ_B so as to satisfy equation (3). Under these conditions, the transfer matrix for crossing the central pair of clusters becomes an identity matrix with a negative sign. Now, the trace of the sequence ABBA is same as that of BAAB. Therefore, as soon as the central pair of BAAB clusters offers an identity contribution (barring a phase factor), the ABBA clusters at the two wings form a doublet and, under the same conditions as the above, their product matrix becomes identity. If we start out with an arbitrarily long string of As and Bs, the geometry of S_4 will occur locally everywhere, and the conditions obtained from equation (3) will give rise to an unattenuated transmission through the entire segment. It can be seen that though there is a dimer consisting of BA–BA in the central portion of the earlier string S_3, the presence of the interface matrix $\mathbf{M}_{AB}$ prevents this pair from contributing an identity matrix and therefore one has to exclude these odd-numbered generations. One can, however, start with a bigger (even) generation. Because of the inherent self-similarity, bigger *central* clusters will always be found which occur in pairs. It is not difficult to check that for all even-numbered generations, the product matrices will have their determinants equal to one, so an application of the Cayley–Hamilton theorem can be made without any difficulty. Such bigger strings of interest are generated by applying the TM inflation rules twice in succession, i.e. by replacing B by BAAB and A by ABBA. It is to be noted that using the same kind of idea in the case of a larger string, one can end up with more and more involved equations. A legitimate question in this regard is that of whether the solutions of these equations can be obtained in every case. An exact answer is always difficult (if not impossible) to find as the renormalization process can, in principle, go on indefinitely. However, one can make a check by means of explicit numerical calculations up to several generations. For example, if we choose to discuss a specific case—e.g., that for normal incidence with $\delta_A = \delta_B = \delta$ and $r = 2$—it can be worked out in detail that the trace of the transfer matrix $\mathbf{M}_c$ corresponding to one block belonging to the central pair forming the dimer (the dimer is, of course, $\cdots\mathbf{M}_c\mathbf{M}_c\cdots$), at any even generation from S_4 onwards, is of the form

$$\mathrm{tr}(\mathbf{M}_c) = \sum_{n=0}^{N/2} a_n \cos(2n\delta)$$

where N is the number of elements A and B in the block which forms half the dimer. It is difficult to ensure that the above form, when put equal to zero, will always generate non-trivial values for δ. However, at the same time, the form itself suggests that it will not be unnatural to expect multiple zeros of $\mathrm{tr}(\mathbf{M}_c)$ and, hence, a set of values for δ. For example, in figure 1 we show results for generations S_4 and S_6 with each member of the dimer in the two situations comprising of 4 and 16 elements respectively. The new values of δ in the second case (dashed lines) are clearly seen. For the general case, we have checked our prediction for different combinations of r and δ_B, and in each case we have been able to get different values of δ_A for a fixed δ_B up to the eighth generation. This gives us confidence, and we conclude this section by saying that the self-similarity of the structure leads to an intuitive understanding that one should get more and more different values of the wavelength that propagates unattenuated through the structure.

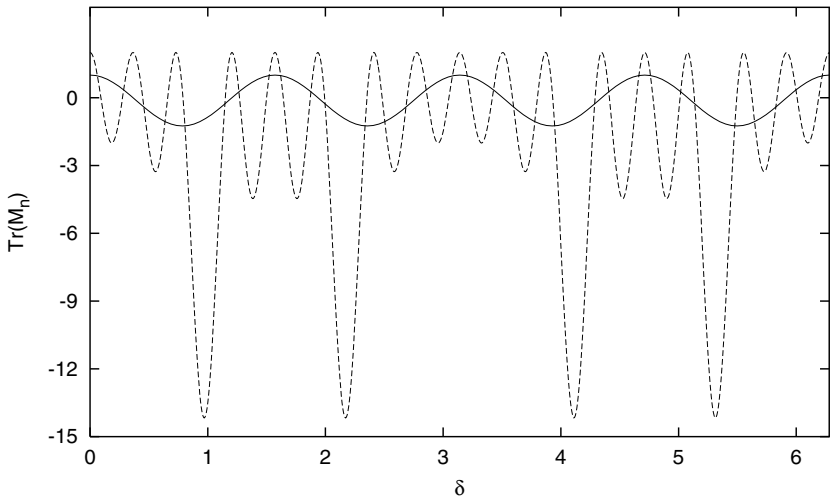

Figure 1. Values of the phase δ for which the central pair of matrices becomes an identity (with a minus sign). The solid line and the dashed line correspond to the fourth- and sixth-generation structures respectively.

3. The electronic case

The electronic case is less complicated than the earlier part, the simple reason for this being the absence of interface matrices. Here, we deal with the standard tight-binding Hamiltonian

$$H = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{\langle ij\rangle} \left[t_{ij} |i\rangle\langle j| + t_{ji} |j\rangle\langle i| \right] \tag{4}$$

where ϵ_i is the on-site potential which can assume two values ϵ_A and ϵ_B depending on the type of the site and t is the nearest-neighbour hopping integral, taken to be unity in this work. The transfer matrix now assumes the form

$$\mathbf{M}_i = \begin{pmatrix} E - \epsilon_i & -1 \\ 1 & 0 \end{pmatrix}.$$

E is the energy of the electron. The first non-trivial dimer appears in the generation S_3, and resonance occurs whenever the trace of the total transfer matrix for crossing a BA pair vanishes.

The corresponding energy is given by

$$E = [\epsilon_A + \epsilon_B \pm \sqrt{(\epsilon_A - \epsilon_B)^2 + 8}]/2.$$

Once this correlation is appreciated, it is not unnatural, following the arguments given in the previous section, that a (countable) infinity of extended eigenstates can be traced in the thermodynamic limit. Obviously, it is difficult to prove mathematically that solutions to the polynomial equations in E will exist in all the cases. Once again, we have worked out numerically the results for several generations and checked that our expectations are correct. Obviously, bigger and bigger clusters will now be forming dimers, and each bigger cluster can be looked upon as a renormalized version of the original pair BA. It can easily be checked that the eigenvalues for these extended states are identical to those already reported in the literature [15]. It is important to appreciate that the nature of the positional correlation between the constituents in this particular lattice is different from that for the standard dimer models, either random or quasiperiodic, in the sense that, here, the dimer correlation is not transparent.

This approach also unveils a very specific set of extended eigenstates. By looking at the fourth-generation chain we find that the transfer matrix for crossing the central BB pair becomes the identity for $E = \epsilon_B$. Simultaneously, if we choose $\epsilon_B = \epsilon_A \pm \sqrt{2}$, then a resonant tunnelling occurs in the S_4 string and in all subsequent generations. This of course, holds for a specific model. Thus in addition to the previous correlations, we get another one leading to an extended eigenstate. The resonance occurs sharply only at the specified energy $E = \epsilon_B$ for all generations $l \geqslant 4$, as can be seen from figure 2, where, for this latter model, we show how the bandwidth of resonance shrinks with increasing generation index, indicating that a delta-function-like peak will show up for the infinite lattice at the special value of the energy. The situation is the same for all of the other cases as well.

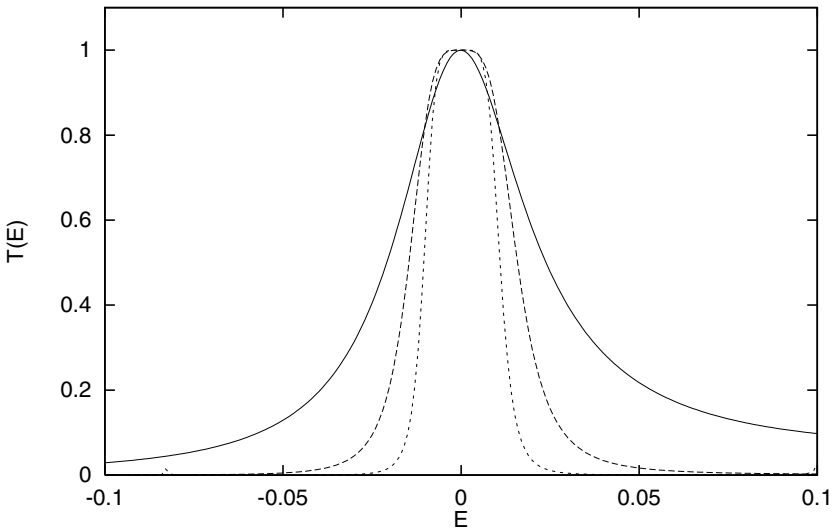

Figure 2. Transmission coefficients for the electronic cases with $\epsilon_B = 0$ and $\epsilon_A = \sqrt{2}$ around the resonance energy $E = 0$ for three successive generations S_4 (solid line), S_5 (dashed line) and S_6 (dotted line). The decay of the bandwidth of the resonance is evident from the behaviour of $T(E)$.

In figure 3 we display the absolute values of the amplitudes of this special wave function for a tenth-generation lattice with $E = \epsilon_B = 0$ and $\epsilon_A = -\sqrt{2}$. We exhibit the amplitudes only for 256 lattice sites to prevent the figure from becoming unclear. The extended nature of the

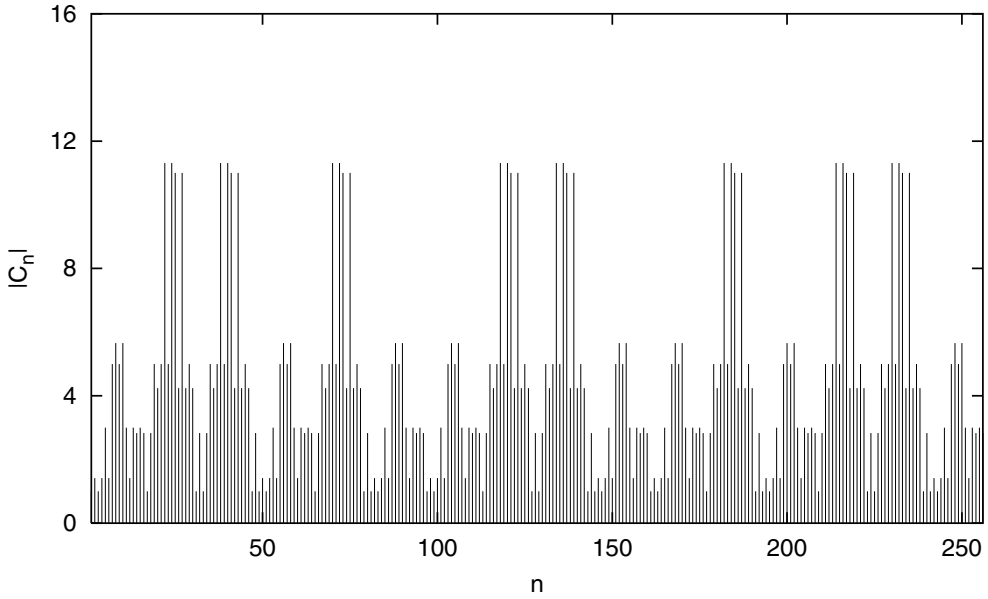

Figure 3. Absolute values of the amplitudes of an extended wave function in a particular model discussed in the text. Here, $\epsilon_A = -\sqrt{2}$, $\epsilon_B = 0$ and $E = 0$. The hopping integral t is set equal to one. Clusters of amplitudes follow a TM sequence, as can be seen.

wave function is clear. An additional interesting feature shows up here. It can be checked that the values of the amplitudes at 16 successive sites, starting from the first site, group together in two different ways. The pattern of distribution for the first 16 sites is different from that for the second 16 sites. These two different patterns then repeat themselves following the TM substitution rule. In figure 3, these two different branches can be easily identified.

4. Concluding remarks

In short, we have shown that the Thue–Morse sequence presents a unique example of an aperiodic lattice which has dimer-like positional correlations between the constituent elements. The dimers are not transparently displayed in the structure, as they are for other classical examples, but their presence is revealed under some special conditions. Apparently, very widely separated elements in the original chain can then be looked upon as the elements of a dimer at a different scale of length. The transfer matrices for crossing these elements then collapse to form identity matrices giving rise to unattenuated light transmission or electron transmission. The microscopic reason for the existence of extended Bloch-like electronic states can thus be analysed from this viewpoint.

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