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From Multi-Site to On-Site Transfer Matrix Models for Self-Similar Chains

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We show how transfer matrix models on chains that are self-similar (renormalizable) with respect to a substitution rule can be transformed from multi-site models in which transfer matrices depend on the nature of a finite number of neighboring sites, to on-site models in which transfer matrices depend on the nature of one site only. We present sufficient conditions and show that these conditions are satisfied in the case of quasiperiodic chains of two symbols that are renormalizable with respect to an invertible substitution rule. We illustrate the application of our results to tight-binding Schrödinger equations modeling the electronic behavior of self-similar chains of atoms and to models describing the transmission of light through self-similarly stacked multilayers.

KEY WORDS: Renormalization; quasicrystals; substitution rules; Schrödinger equation; trace maps.

1. INTRODUCTION AND OUTLINE

Since the late 1970's there has been an increasing interest in the physical properties of materials possessing a quasiperiodic or otherwise selfsimilar structure. For a recent survey see e.g. ref. 2. Models of physical systems possessing a quasiperiodic order, are usually studied through successive periodic approximations. In many cases, selfsimilar and quasiperiodic models can be considered as the fixed point of a renormalization operator.

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For instance, the celebrated quasiperiodic Fibonacci sequence of two letters a and b is a fixed point of the substitution rule $\sigma\colon (a, b) \mapsto (ab, a)$.

In the one-dimensional context of selfsimilar chains, many physical models can be formulated in terms of transfer matrices, cf. e.g. refs. 4, 11, 12. A classical example is the nearest neighbour tight binding model describing the electrons on a chain of atoms, with Hamiltonian

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

where $|i\rangle$ are on-site states forming an orthonormal basis of the Hilbert space containing the states for the entire chain. The $t_{i,j}$ are the hopping terms from site i to site j and V_i is the local potential at site i.

Let us consider chains of two types of atoms a and b, and let hopping terms $t_{i,j} \neq 0$ only if i and j are neighbours (nearest neighbour interactions). The hopping terms depend on which types of atoms appear at site i and j (throughout this paper, always $i, j \in \mathbb{Z}$). When the atom at site i is of type a and at site j of type b, we write $t_{i,j} = t_{a,b}$, and a similar convention will be used for the potential terms V_i. Thus we have $t_{i,i+1} \in \{t_{a,a}, t_{b,b}, t_{a,b}, t_{b,a}\}$ and $V_i \in \{V_a, V_b\}$ (a natural physical assumption will be that $t_{a,b} = t_{b,a}$). The energy spectrum can be found from solving the Schrödinger equation $H\Psi = E\Psi$ which, after identifying $\Psi = \sum_i \Psi_i |i\rangle$, gives rise to the difference equation

$$t_{i,i+1}\Psi_{i+1} + t_{i,i-1}\Psi_{i-1} + V_i\Psi_i = E\Psi_i \tag{2}$$

We may write the difference equation (2) as[4]

$$\Theta_{i-1} = T_{i-1,i,i+1}\Theta_i \tag{3}$$

with

$$T_{i-1,i,i+1} = \begin{pmatrix} (E - V_i)/T_{i,i-1} & -t_{i,i+1}/t_{i,i-1} \\ 1 & 0 \end{pmatrix} \tag{4}$$

and $\Theta_i = (\Psi_i, \Psi_{i+1})^T$.

This model has been studied with $t_{i,i+1} = 1$ for all i (diagonal model) and also with $V_i = 0$ and $t_{i,i+1} := t_{i+1}$ and $t_{i,i-1} := t_i$ with $t_j \in \{t_a, t_b\}$ (off-diagonal model) in which case one models a chain with a sequence of bonds of type a and b, rather than different sites (cf. also Section 3.1).

[4] In the literature, the usual convention is to write $\Theta_{i+1} = T\Theta_i$. We have chosen for another convention such that the order of the transfer matrices automatically will correspond to the order in which symbols occur in words.

The transfer matrix formulation of the Schrödinger equation is very useful in studying the eigenstates and the energy spectrum of H.

The diagonal model (with $t_{i,i+1} = 1$ for all i) leads to an *on-site* transfer matrix model in which each transfer matrix depends on the nature of one site only. Hence, the transfer matrix connecting Θ_{i-q} with Θ_i is $T_{i-q+1} \times \cdots \times T_i$, where $T_j = T_a$ if site j is of type a and $T_j = T_b$ if site j is of type b. The order in which the symbols occur in the chain thus corresponds precisely to the order in which the transfer matrices appear.

Let us now consider a substitution rule, e.g. the Fibonacci substitution rule a that is defined by $\sigma(a) = ab$ and $\sigma(b) = a$. Suppose we build a quasiperiodic chain using the Fibonacci substitution rule, then successive application of σ on the seed a leads to $a \mapsto ab \mapsto aba \mapsto abaab \mapsto \cdots$. Assuming periodic boundary conditions one finds that the periodic infinite chain with unit cell $\sigma^k(a)$ converges towards a quasiperiodic chain as k goes to infinity. This quasiperiodic chain is a fixed point of σ.

In the case of on-site models it is clear how an application of a substitution rule τ leads to an application of the substitution rule τ at the level of transfer matrices. Namely, the transfer matrices after the application of the substitution (inflation) rule are found by applying the substitution rule directly to the corresponding chain of transfer matrices, e.g. in the case of applying σ to the seed a we obtain on the level of transfer matrices $T_a \mapsto T_a \times T_b \mapsto T_a \times T_b \times T_a \mapsto T_a \times T_b \times T_a \times T_a \times T_b \mapsto \cdots$. In this context we will call an on-site transfer matrix model *renormalizable* when it admits a substitution rule on the transfer matrices that corresponds to the substitution rule on the chain (the substitution rules need not be identical).

In the case of multi-site transfer matrix models it is less obvious what the consequences of the renormalization procedure by substitution of a and b are on the level of the transfer matrices. Certainly, a substitution of a and b does no longer correspond to a straightforward similar substitution of transfer matrices t_a and t_b.

In studies of the off-diagonal model it was found that with appropriate choices of building blocks of transfer matrices one can transform the offdiagonal model into a diagonal one, cf. e.g. refs. 10, 12, 13. The present paper is partly motivated by these works and deals with transformations from multisite to renormalizable on-site transfer matrix models in a more general setting.

The main question we would like to address is:

> *Given a transfer matrix model on a selfsimilar chain that is renormalizable with respect to a substitution rule τ. Suppose the transfer matrix model is of multi-site type, i.e. the transfer matrices depend on the nature of more than one site. Then, under what circumstances can we transform the multi-site transfer matrix model into a renormalizable on-site transfer matrix model?*

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We will address this question in the general context of n-symbol alphabets and m-site transfer matrix models. We will pay attention in particular to the case of two-letter alphabets and two- and three-site transfer matrix models, such as those arising from the tight binding model (1). Because on-site models are easier to treat than multi-site models it is important to know whether one can transform one into the other. For instance, a transformation to an on-site model enables the use of trace maps (for further remarks and references see Section 4).

We will discuss our results in the context of electronic spectra of selfsimilar chains, as mentioned above, but also in the context of optical transmission properties of selfsimilarly stacked multilayers.

We will consider two types of transformations: alphabet transformations and transformations related to decomposition properties of transfer matrices.

Example 1.1 (Alphabet Transformation). Consider a two-site transfer matrix model with transfer matrices $T_{i,i+1}$, and a chain with two types of sites (atoms) a and b. Let the chain be renormalizable with respect to the Fibonacci substitution rule $\sigma(a, b) = (ab, a)$.

We propose to transform the alphabet $S = \{a, b\}$ into a new alphabet $\tilde{S} = \{A, B\}$ with $A := \sigma(a) = ab$ and $B := \sigma(b) = a$. Note that $\sigma(a)$ and $\sigma(b)$ both have the symbol a at the left. We try to construct new transfer matrices in terms of the new alphabet. We start with $\tilde{T}_B$. Because $\sigma(b) = a$ we propose $\tilde{T}_B = T_{a,?}$ where the question mark needs to contain a letter ensuring compatibility. We propose therefore that the question mark be an a such that $\tilde{T}_B = T_{a,a}$ and in writing out the product $\tilde{T}_B \times \tilde{T}_B$ the indices match up. Similarly, since $\sigma(a) = ab$, we can construct $\tilde{T}_A = T_{a,?} \times T_{b,?}$, which leads after filling in the question marks to $\tilde{T}_A = T_{a,b} \times T_{b,a}$.

One now easily checks that when $\sigma^n(w(a, b)) = w_n(a, b)$, with $w(a, b) \in S^*$, that $\sigma^n(w(A, B)) = w_n(A, B) = w_{n+1}(a, b)$, and that $\tilde{T}_{w_n(A,B)} = w_n(\tilde{T}_A, \tilde{T}_B)$ (keeping in mind periodic boundary conditions). For instance, $T_{\sigma^3(a)} = T_{abaab} = T_{a,b} \times T_{b,a} \times T_{a,a} \times T_{a,b} \times T_{b,a}$ and $\tilde{T}_{\sigma^2(A)} = \tilde{T}_A \times \tilde{T}_B \times \tilde{T}_A = T_{a,b} \times T_{b,a} \times T_{a,a} \times T_{a,b} \times T_{b,a}$.

Hence in terms the two-site transfer matrix model on the $a-b$ chain with transfer matrices T has been transformed to an on-site transfer matrix model on an $A-B$ chain with transfer matrices $\tilde{T}$, while preserving its renormalizability with respect to σ.

Remark 1.2. The transformations in Example 1.1 are precisely those used in refs. 10, 12, 13. In relation to these references, it should be noted that the juxtaposition rule $S_{i+1} = S_i S_{i-1}$ (with $S_0 = b$, $S_1 = a$) is equivalent to applying the Fibonacci substitution rule to the seed a.

In the context of alphabet transformations, our main (technical) result is a generalization of the procedure presented in Example 1.1, and presented in the following theorem:

Theorem 1.3. Let $S := \{s_1, ..., s_n\}$ be an n-symbol alphabet and let S^* denote the collection of all possible words (of finite length) with symbols from the alphabet S. Let $\tau: S \mapsto S^*$ be a substitution rule. Suppose we have an m-site transfer matrix model

$$\Theta_{i-1} = T_{i-q, ..., i-q+m-1} \Theta_i$$

with $\Theta_i := (\Psi_i, ..., \Psi_{i+p})^T$, on a chain that is selfsimilar (renormalizable) with respect to a substitution rule τ. Suppose that for some value of k the words $\tilde{s}_i = \tau^k(s_i)$ can be written as a concatenation of three words in $S^*: \tilde{s}_i = w_l w_i w_r$, where w_l and w_r are independent of i and of length l and r, such that $l + r = m - 1$. Then the m-site transfer matrix model can be transformed by an alphabet transformation into a renormalizable on-site transfer matrix model with the new alphabet $\tilde{S} := \{\tilde{s}_1, ..., \tilde{s}_n\}$ and the same substitution rule τ.

Remark 1.4. The above result implies that an m-site transfer matrix model on a renormalizable chain can be transformed into a renormalizable on-site model if firstly for all $i = 1, ..., n$ the $\tau(s_i)$'s have their right or leftmost symbol in common and secondly, for some k, τ^k applied to this symbol produces a word of length of at least $m - 1$. In fact, in that case it is clear that τ^{m-1} acting on this symbol gives rise to a word of length of at least $m - 1$ such that the conditions formulated in Theorem 1.3 are satisfied with $k = m - 1$.

In Section 2 we will prove Theorem 1.3 and illustrate its content with some examples in the context of two-symbol chains and two- and three-site transfer matrix models.

It should be noted that the conditions formulated in Theorem 1.3 and Remark 1.4 are sufficient but not claimed to be necessary. However, in case these conditions are not met it can often be shown that no alternative alphabet transformations can be found. As an illustration, in Appendix B it is proven that in the case of the Thue–Morse substitution $\tau(a, b) = (ab, ba)$ and a Fibonacci-squared substitution[5] $\tilde{\sigma}(a, b) = (aab, ba)$ no alphabet transformations exist that transform multi-site transfer matrix

[5] We call $\tilde{\sigma}$ a Fibonacci-squared substitution rule because the substitution matrix associated to $\tilde{\sigma}$ and the substitution matrix associated to σ^2 (square of the Fibonacci substitution rule σ) are identical, although $\sigma^2 \neq \tilde{\sigma}$. Note however, that $\tilde{\sigma}$ is not the only substitution with this property. We borrowed the terminology from ref. 14.

models on chains that are selfsimilar with respect to these substitution rules into renormalizable on-site transfer matrix models.

Invertible substitutions form an important class of substitutions. The n-symbols $s_1,..., s_n$ generating S^* may also be considered to generate a free group $\mathscr{F}_n$. This extension allows for words containing inverse symbols (e.g. s_1^{-1}). As S^* may be considered as a subset of $\mathscr{F}_n$, the action of $\tau: S \mapsto S^*$ can be extended in a natural way to $\tau: \mathscr{F}_n \mapsto \mathscr{F}_n$. τ is called *invertible* if τ is invertible in the latter context, i.e. if there exists a $\tau^{-1}: \mathscr{F}_n \mapsto \mathscr{F}_n$ such that $\tau \circ \tau^{-1} = \text{id}$. In that case $\tau \in \text{Aut}(\mathscr{F}_n)$, cf. ref. 16.

The Fibonacci substitution rule σ on $S = \{a, b\}$ is an example of an invertible substitution rule, with $\sigma^{-1}(a) = b$ and $\sigma^{-1}(b) = b^{-1}a$. In fact, (on-site transfer matrix models on) quasiperiodic two-symbol chains that are selfsimilar (renormalizable) with respect to invertible substitutions have many features in common, cf. ref. 22 and references therein. In this context we obtain the following theorem:

Theorem 1.5. Suppose we have an m-site transfer matrix model on a two-symbol chain that is renormalizable with respect to an *invertible* substitution rule τ, with $\tau^2(a) \neq a$ and $\tau^2(b) \neq b$. Then, this transfer matrix model can be transformed into a renormalizable on-site transfer matrix model smith the same substitution rule τ.

Importantly, Theorem 1.5 implies that the class of on-site transfer matrix models on quasiperiodic two-symbol chains that are renormalizable with respect to an invertible substitution include all multi-site transfer matrix models on such quasiperiodic chains as well.

It should be noted that the cases in which $\tau^2(a) = a$ or $\tau^2(b) = b$ are either permutations ($\tau = \text{id}$ or $\tau(a, b) = (b, a)$) or substitutions with $\tau(a) = a$ or $\tau(b) = b$. Substitutions of this form are not particularly interesting in the context of selfsimilar chains. In particular, when τ is a substitution associated with a renormalizable chain that is quasiperiodic (and not periodic), then necessarily $\tau^2(a) \neq a$ and $\tau^2(b) \neq b$.

Alternatively to alphabet transformations, in some models one may use decomposition properties of transfer matrices in order to go from a multi-site to an on-site model. Examples of such models are the off-diagonal tight binding model and a light transmission model. They will be discussed in Section 3. The constructions in these examples rely on the following result:

Theorem 1.6. Consider an m-site transfer matrix model with transfer matrices $T_{i-q,..., i-q+m-1}$. If these transfer matrices can be decomposed into two matrices

$$T_{i-q,..., i-q+m-1} = \hat{T}_{i-q,..., i-q+m-2} \times \hat{T}'_{i-q+1,..., i-q+m-1}$$

then by rearranging transfer matrices the m-site transfer matrix model can be transformed into an m'-site transfer matrix model with $m' = m - 1$.

This paper is outlined as follows. In Section 2 we deal with alphabet transformations and prove Theorem 1.3 and Theorem 1.5 and illustrate these results in the context of two- and three-site transfer matrix models. In Section 3 we will discuss how transfer matrix models can be transformed from multi-site to on-site model using decomposition properties of transfer matrices and prove Theorem 1.6. These results will be illustrated by the off-diagonal tight binding model and a model describing the optical transmission properties of stacked multilayers. The paper is concluded with a discussion of the applications of our results, in particular in relation to trace maps. Extended details on alphabet transformations are presented in the Appendices.

2. ALPHABET TRANSFORMATIONS

We consider the mechanism of transforming a multi-site transfer matrix model into an on-site model by choosing a new alphabet $\tilde{S}$ consisting of words in S^* such that in terms of the new alphabet $\tilde{S}$ the substitution rule τ acting on S induces a substitution rule $\tilde{\tau}$ on $\tilde{S}^*$. The new alphabet $\tilde{S}$ should furthermore be such that it allows a multi-site transfer matrix model on a τ-renormalizable chain in S to be formulated as an on-site transfer matrix model on a $\tilde{\tau}$-renormalizable chain in $\tilde{S}$.

We will focus on new alphabets $\tilde{S}$ of the form $\tilde{S} = \{\tau^k(s_1),..., \tau^k(s_n)\}$ for some value of k. In Appendix A more motivation is given for this choice. It is obvious that with this choice of new alphabet $\tilde{S}$ the action of τ on S induces an action on $\tilde{S}$ that is identical to that of τ, i.e. $\tilde{\tau} = \tau$.

We now have a way to change our alphabet while remaining renormalizable with respect to τ. The aim is now to use the new alphabet to construct on-site transfer matrices for the symbols in $\tilde{S}$. In order to be able to transform an m-site transfer matrix model into an on-site model in this way, we need the symbols in the new alphabet (which are words in S^*) to have at least $m-1$ S-symbols in common at their leftmost and/or rightmost ends. If this is the case, we have enough information on the neighbouring sites to be able to construct transfer matrices for symbols in $\tilde{S}$ that are effectively independent of the neighbouring sites. This is the content of Theorem 1.3, whose proof we will now discuss in more detail.

Proof of Theorem 1.3. The proof of Theorem 1.3 consists of the construction of the on-site transfer matrices. We start with an n-symbol alphabet $S = \{s_1,..., s_n\}$ and transfer matrices $T_{i-q,..., i-q+m-1}$ of an m-site model. We study this model on a chain that is renormalizable with respect to the substitution rule τ. One should note that when $\Theta_{i-1} = T_{i-q,\dots,i+m-1}\Theta_i$, we have

$$\Theta_{i-p} = T_{i-q-p+1,\dots,i-q-p+m} \times \cdots \times T_{i-q,\dots,i-q+m-1}\Theta_i$$

for all $p \geqslant 1$, where the product of transfer matrices is taken in such a way that the $m-1$ rightmost indices of one matrix correspond to the $m-1$ leftmost indices of the next one. The key point now is to realize that when we have an alphabet generated by words in S^* that have all together $m-1$ S-symbols in common at their leftmost and rightmost sides, that we then may construct transfer matrices for the symbols in the $\tilde{S}$ alphabet that are independent of the neighbouring sites, as the interactions always go through the $m-1$ outer S-symbols which all S-symbols have in common.

We will now construct the new transfer matrices. Let $\tau^k(s_i) = w_l w_i w_r$ for some positive integer value of k and all $i = 1,\dots, n$, with w_l and w_r words in S^* (independent of i) of length l and r such that $l + r = m - 1$. Let $\tilde{s}_i :=$ $\tau^k(s_i) = a_0^{(i)} \cdots a_{q_i-1}^{(i)}$ (with $a_j^{(i)} \in S$ and q_i is the number of S-symbols in the word $\tau(s_i)$) be the symbols in the new alphabet $\tilde{S}$. Note that all $\tilde{s}_i$ share their l leftmost S-symbols and r rightmost S-symbols. Now it is readily verified that the following transfer matrices $\tilde{T}_i$ represent the transfer matrices arising from the word $\tau^k(s_i)$:

$$\tilde{T}_i := T_{a_{-r}^{(i)} \cdots a_l^{(i)}} \times \cdots \times T_{a_{q_i-1-r}^{(i)} \cdots a_{q_i-1+l}^{(i)}}, \tag{5}$$

with the convention $a_j^{(i)} = a_{j \bmod q_i}^{(i)}$ (keeping in mind periodic boundary conditions).

This construction is rather straightforward and natural. Note that the construction needs nothing more than making a product of q_i transfer matrices in such a way that one can read the word $\tilde{s}_i$ at the $(r+1)$th indices of the consecutive transfer matrices. The rest of the indices then automatically follow.

With this definition of $\tilde{T}_i$ it is easily verified that the transfer matrices depend only on the $\tilde{S}$-symbol at site i, and that in products $\tilde{T}_i \times \tilde{T}_j$ the indices of the original transfer matrices match perfectly.

Thus we may associate with each symbol $\tilde{s}_i \in \tilde{S}$ the transfer matrix $\tilde{T}_i$. In this way we obtain an on-site renormalizable transfer matrix model with τ acting on the symbols in $\tilde{S}$. ∎

In the special case of two-symbol alphabets we obtain additional results. For the class of invertible two-symbol substitutions it can be shown that the procedure described in Theorem 1.3 and Remark 1.4 applies in all the interesting cases. This is the content of Theorem 1.5 of which we now present the proof.

Proof of Theorem 1.5. It is well-known[21] that the invertible substitutions on two-symbol alphabets are generated by the three substitutions α: $(a, b) \mapsto (b, a)$, β: $(a, b) \mapsto (ab, b)$, and δ: $(a, b) \mapsto (ba, b)$. The comment in Remark 1.4 concludes the proof. Namely, $\beta(a)$ and $\beta(b)$ have their rightmost symbol (b) in common and $\delta(a)$ and $\delta(b)$ have their leftmost symbol (b) in common. Note however that β and δ fix b. Hence, every substitution rule τ generated by concatenating a finite number of β's and δ's is such that $\tau(a)$ and $\tau(b)$ have their leftmost or rightmost symbol in common. As α is nothing more than a permutation of a and b, the same conclusion holds for concatenations of β's, δ's and α's (including at least one β or δ).

Finally, the lengths of the words $\tau^k(a)$ and $\tau^k(b)$ are not bounded (with growing k) if $\tau^2(a) \neq a$ and $\tau^2(b) \neq b$. Hence, in these cases there exists a value of $k \leqslant m-1$ such that $\tau^k(a)$ and $\tau^k(b)$ have $m-1$ leftmost and/or rightmost symbols in common. ∎

To illustrate our results, we will work out some examples of how the transformation is performed in the case of two- and three-site transfer matrix models and words in the two-symbol alphabet $S = \{a, b\}$. These are for instance the type of models arising in the context of the nearest-neighbour tight binding models with Hamiltonian (1).

2.1. Two-Site Models

We consider models of the form $\Theta_{i-1} = T_{i,i+1}\Theta_i$, with $\Theta_i = (\Psi_i, \Psi_{i+1})^T$, $S = \{a, b\}$ and substitution rule τ. We can transform to an on-site model in case $\tau(a)$ and $\tau(b)$ have their rightmost or leftmost symbol in common.

In case $\tau(a)$ and $\tau(b)$ have their leftmost symbol in common, we may construct new transfer matrices

$$\tilde{T}_i := T_{a_0^{(i)} a_1^{(i)}} \times \cdots \times T_{a_{q_i-1}^{(i)} a_0^{(i)}} \tag{6}$$

where it should be noted that we read the word $\tau(s_i)$ in the leftmost symbols in the indices of the consecutive transfer matrices. In case they have their rightmost symbol in common we read $\tau(s_i)$ in the rightmost symbols:

$$\tilde{T}_i := T_{a_{q_i-1}^{(i)} a_0^{(i)}} \times \cdots \times T_{a_{q_i-2}^{(i)} a_{q_i-1}^{(i)}} \tag{7}$$

One example of an alphabet transformation from a one-site to a two-site transfer matrix model was presented in Example 1.1 on an ad-hoc basis. In the following example we illustrate the procedure following the lines of Theorem 1.3.

Example 2.1. Consider $\tau(a, b) = (ab, abbaab)$. $\tau(a)$ and $\tau(b)$ both have the symbol a at the left, and the symbol b at the right. Hence we have two ways to construct the matrices $\tilde{T}_A$ and $\tilde{T}_B$, where we take $A := \tau(a) = ab$ and $B := \tau(b) = abbaab$.

Method 1. Using that $\tau(a)$ and $\tau(b)$ both have an a at the left, we arrive at the transfer matrices

$$\tilde{T}_A = T_{a,b} \times T_{b,a}, \qquad \tilde{T}_B = T_{a,b} \times T_{b,b} \times T_{b,a} \times T_{a,a} \times T_{a,b} \times T_{b,a} \tag{8}$$

where the words ab and $abbaab$ are read in the leftmost indices of consecutive transfer matrices.

Method 2. Using that $\tau(a)$ and $\tau(b)$ both have a b at the right, we may define the new transfer matrices in such a way that one reads the words in the rightmost indices;

$$\tilde{T}_A = T_{b,a} \times T_{a,b}, \qquad \tilde{T}_B = T_{b,a} \times T_{a,b} \times T_{b,b} \times T_{b,a} \times T_{a,a} \times T_{a,b} \tag{9}$$

One should note that the constructions in both cases are equivalent (taking into account periodic boundary conditions). Namely, the transfer matrices obtained from method 1 can be obtained from those obtained from method 2 by moving the leftmost transfer matrix $T_{b,a}$ into the rightmost position.

It is furthermore interesting to note that in contrast to the Fibonacci substitution rule σ, the substitution rule $\tau(a, b) = (ab, abbaab)$ is not invertible (it is the composition $\tau_1 \circ \tau_2$ of the invertible substitution rule $\tau_1(a, b) = (a, aba)$ with the noninvertible Thue–Morse substitution rule $\tau_2(a, b) = (ab, ba)$). This example illustrates the fact that the invertibility condition as stated in Theorem 1.5 is a sufficient condition rather than a necessary condition for the existence of an alphabet transformation from multi-site into on-site transfer matrix models.

2.2. Three-Site Models

We consider three-site transfer matrix models of the form

$$\Theta_{i-1} = T_{i-1,i,i+1} \Theta_i \tag{10}$$

As $m = 3$, we need all together $m - 1 = 2$ common symbols in $\tau(a)$ and $\tau(b)$ at the right- and/or leftmost sides. We therefore consider three cases: $\tau^k(a)$ and $\tau^k(b)$ share (I) the two leftmost symbols, (II) the leftmost and the rightmost symbol, or (III) the two rightmost symbols.

It should be noted that in the case of m-site models a necessary condition for the words $\tau^k(s_i)$ having a leftmost or rightmost symbol in common, is that the words $\tau(s_i)$ have a leftmost or rightmost symbol in common. Namely, if $\tau(s_i)$ and $\tau(s_j)$ do not have their left-or rightmost symbol in common, then neither have $\tau^k(s_i)$ and $\tau^k(s_j)$. In order to have $m-1$ symbols in common it suffices to consider only values $k \leqslant m-1$, cf. also Remark 1.4. In the case of two-site models it suffices to consider only $k=1$, but in the case of three-site models we may need to consider $k=2$ as well.

Our rules lead to the following constructions:

$$\text{(I)} \quad \tilde{T}_i := T_{a_0^{(i)}, a_1^{(i)}, a_2^{(i)}} \times \cdots \times T_{a_{q_i-1}^{(i)} a_0^{(i)}, a_1^{(i)}} \tag{11}$$

$$\text{(II)} \quad \tilde{T}_i := T_{a_{q_i-1}^{(i)}, a_0^{(i)}, a_1^{(i)}} \times \cdots \times T_{a_{q_i-2}^{(i)}, a_{q_i-1}^{(i)}, a_0^{(i)}} \tag{12}$$

$$\text{(III)} \quad \tilde{T}_i := T_{a_{q_i-2}^{(i)}, a_{q_i-1}^{(i)}, a_0^{(i)}} \times \cdots \times T_{a_{q_i-3}^{(i)} a_{q_i-2}^{(i)}, a_{q_i-1}^{(i)}} \tag{13}$$

In the cases (I), (II) and (III) we read the words $\tau(s_i)$ respectively at the first, second and third indices of the consecutive transfer matrices.

We illustrate these constructions with some explicit examples.

Example 2.2. Consider the noninvertible substitution rule $\tau(a, b) = (ab, abbaab)$. Note that $\tau(a)$ and $\tau(b)$ have a common ab at the right. Following the construction in case (III) above we arrive at

$$\begin{aligned} \tilde{T}_A &= T_{a,b,a} \times T_{b,a,b}, \\ \tilde{T}_B &= T_{a,b,a} \times T_{b,a,b} \times T_{a,b,b} \times T_{b,b,a} \times T_{b,a,a} \times T_{a,a,b}. \end{aligned} \tag{14}$$

Note that we read the words ab and $abbaab$ in the rightmost indices of the transfer matrices.

Alternatively, we may use the fact that $\tau(a)$ and $\tau(b)$ have a common a at the left and a common b at the right. Following (II); one obtains

$$\begin{aligned} \tilde{T}_A &= T_{b,a,b} \times T_{a,b,a}, \\ \tilde{T}_B &= T_{b,a,b} \times T_{a,b,b} \times T_{b,b,a} \times T_{b,a,a} \times T_{a,a,b} \times T_{a,b,a}, \end{aligned} \tag{15}$$

and we read the words ab and $abbaab$ in the second (middle) indices of the consecutive transfer matrices. Note again that the choices in (14) and (15) differ only in the position of an outer $T_{a,b,a}$.

Example 2.3. Consider the invertible Fibonacci substitution rule $\sigma(a, b) = (ab, a)$. Because the length of $\sigma(b)$ is smaller than $m-1=2$ we cannot directly apply our general procedure. Thus we need to apply σ to arrive at more appropriate words $\sigma^k(a)$ and $\sigma^k(b)$. Because $\sigma(a)$ and $\sigma(b)$ have their leftmost symbol a in common and $\sigma^2(a) \neq a$ it follows that for some finite value of $k \leqslant m-1$ we will arrive at suitable words (cf. Remark 1.4 and Theorem 1.5). As we consider $m=3$ here, $k=2$ will suffice. And indeed, $\sigma^2(a, b)=(aba, ab)$, such that $\sigma^2(a)$ and $\sigma^2(b)$ have ab in common at the left. This leads us to follow (I) and construct

$$\tilde{T}_A = T_{a,b,a} \times T_{b,a,a} \times T_{a,a,b}, \qquad \tilde{T}_B = T_{a,b,a} \times T_{b,a,b} \tag{16}$$

with $A=\sigma^2(a)=aba$ and $B=\sigma^2(b)=ab$ which can be read from the leftmost indices in the consecutive transfer matrices.

One again easily verifies that when $\sigma^n(w(a, b))=w_n(a, b)$, that $\sigma^n(w(A, B))=w_n(A, B)=w_{n+2}(a, b)$, and that $\tilde{T}_{w_n(A,B)}=w_n(\tilde{T}_A, \tilde{T}_B)$ (taking into account periodic boundary conditions). For instance, $T_{\sigma^3(a)}=T_{abaab}=T_{a,b,a} \times T_{b,a,a} \times T_{a,a,b} \times T_{a,b,a} \times T_{b,a,b}$ and $\tilde{T}_{\sigma(A)}=\tilde{T}_A \times \tilde{T}_B=T_{a,b,a} \times T_{b,a,a} \times T_{a,a,b} \times T_{a,b,a} \times T_{b,a,b}$.

3. DECOMPOSITION PROPERTIES

Occasionally there may be other methods for transforming multi-site models into on-site models that do not rely on alphabet transformations but use more model specific decomposition properties of the transfer matrices instead.

It is important to recognize alternative methods to transform multi-site into on-site models, in particular in the case of chains for which no alphabet transformations exist with this property, e.g. in the case of Thue–Morse and square-Fibonacci chains (cf. Appendix B).

In this section we describe two models for which such alternative methods exist: the off-diagonal tight binding model and a model for light transmission through stacked multilayers. These methods are based on decomposition properties of transfer matrices. A more abstract treatment will be presented in Section 3.3. We first consider some examples.

3.1. Off-Diagonal Tight Binding Model

The off-diagonal tight binding model, is the model (1) with $V_i=0$ and $t_{i,i+1}:=t_{i+1}$ and $t_{i,i-1}:=t_i$ with $t_j \in \{t_a, t_b\}$ leading to the discrete Schrödinger equation

$$t_{i+1}\Psi_{i+1} + t_i \Psi_{i-1} = E\Psi_i \tag{17}$$

It gives rise to transfer matrices of the form

$$T_{i,i+1} = \begin{pmatrix} E/t_i & -t_{i+1}/t_i \\ 1 & 0 \end{pmatrix} \tag{18}$$

from which one sees that the off-diagonal tight binding model is a two-site model. This model was studied on a Fibonacci chain in refs. 10, 12, 13 and in these references alphabet transformations were used to transform the two-site model into an on-site one, cf. Remark 1.2. If one studies this model on a Thue–Morse chain such an alphabet transformation does not exist, which raises the question whether there exist other methods for making the model on-site.

We will show that the transfer matrices of the off-diagonal tight binding model possess a decomposition property which enables a transformation to an on-site model, irrespectively of the type of chain. Namely, we may decompose $T_{i,i+1}$ into a product of two matrices

$$T_{i,i+1} = \begin{pmatrix} 1/t_i & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} E & -t_{i+1} \\ 1 & 0 \end{pmatrix} \tag{19}$$

As a result of this decomposition property, we may construct new transfer matrices depending on the nature of one site only.

$$T'_i = \begin{pmatrix} E & -t_i \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1/t_i & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} E/t_i & -t_i \\ 1/t_i & 0 \end{pmatrix} \tag{20}$$

It is clear that products of transfer matrices $T_{i,i+1}$ can be written in terms of T'_i's, e.g.

$$\begin{aligned} &\cdots T_{a,b} \times T_{b,a} \times T_{a,a} \times T_{a,b} \times T_{b,a} \times T_{a,a} \cdots \\ &= \cdots T'_a \times T'_b \times T'_a \times T'_a \times T'_b \times T'_a \cdots. \end{aligned} \tag{21}$$

We thus find that the off-diagonal model is a disguised on-site model, rather than a truly multi-site transfer matrix model.[6]

3.2. Light Transmission Through Multilayers

Optical transmission properties in multilayers selfsimilarly stacked according to various substitution rules, among which are the Fibonacci and Thue–Morse rule, have been studied both theoretically[12,17] and experimentally.[6,3,9]

We will present two different approaches towards studying the optical transmission properties in multilayers. One approach[12] gives rise to a

[6] It should be noted that by following a similar procedure, the three-site transfer matrix model derived from (1) can be identified as a disguised two-site transfer matrix model.

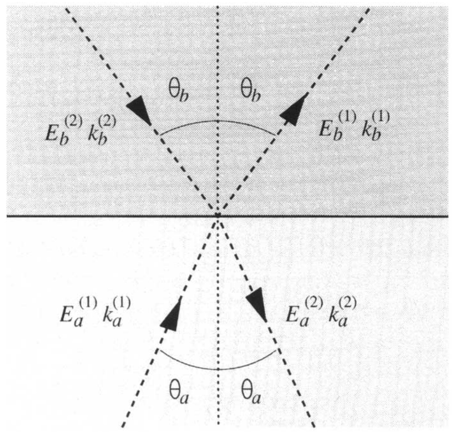

Fig. 1. Electromagnetic wave propagation across interface of two layers.

multi-site transfer matrix model and the other approach[6] gives rise to an on-site transfer matrix model. Both approaches are physically equivalent, and thus these models provide a link between a multi-site model and an on-site model irrespectively of the substitution rule. The physical problem is illustrated in Fig. 1. In layer a there is an electric field,

$$\mathbf{E}_a = \mathbf{E}_a^{(1)} \exp(i(\mathbf{k}_a^{(1)} \cdot \mathbf{r} - \omega t)) + \mathbf{E}_a^{(2)} \exp(i(\mathbf{k}_a^{(2)} \cdot \mathbf{r} - \omega t)) \tag{22}$$

Choosing the direction of $\mathbf{z}$ to be the direction of the interface normal, $\mathbf{k}_a^{(1)}, \mathbf{k}_a^{(2)}$ denote the wavevector in layer a going in the $+z$, $-z$ direction respectively. The expressions for layer b are analogous.

Let layer a have thickness d_a and refractive index n_a, and let Θ_a be the angle with the interface normal, and analogous definitions for layer b, see Fig. 1. Let k_0 be the free space wavenumber. We assume TE-polarization. Hence $\mathbf{E}$ and $\partial \mathbf{E}/\partial z$ are continuous at the interface.

In ref. 12, Kohmoto *et al.* choose as a basis,

$$E_+ = E^{(1)} + E^{(2)}, \qquad E_- = \frac{E^{(1)} - E^{(2)}}{i} \tag{23}$$

in terms of which the values of E at either side of the interface are related as,

$$\begin{pmatrix} E_+ \\ E_- \end{pmatrix}_b = T_{b,a} \begin{pmatrix} E_+ \\ E_- \end{pmatrix}_a \qquad \text{with} \quad T_{b,a} := \begin{pmatrix} 1 & 0 \\ 0 & \dfrac{n_a \cos(\Theta_a)}{n_b \cos(\Theta_b)} \end{pmatrix}. \tag{24}$$

Analogous expressions hold for light passing the interface from layer b to a.

The transmission within layer a is described by a transfer matrix,

$$T_a = \begin{pmatrix} \cos(\delta_a) & -\sin(\delta_a) \\ \sin(\delta_a) & \cos(\delta_a) \end{pmatrix}, \qquad \delta_a = \frac{n_a k_0 d_a}{\cos(\Theta_a)} \tag{25}$$

and analogously for layer b. It should be noted that we assume the light to be propagating through the entire sample, i.e. $0 \leqslant \Theta_a, \Theta_b < \pi/2$.

To each layer one thus must assign two transfer matrices: one transmission matrix and one interface matrix. In terms of these matrices, the transfer matrix model is a two-site model (as the interface matrix depends on two consecutive layers). For the Fibonacci ordering of multilayers, an alphabet transformation may be used to transform this two-site model into an on-site one, cf. Remark 1.2. Namely, choosing the new alphabet $A := \sigma(a) = ab$ and $B := a(b) = a$ one obtains corresponding transfer matrices

$$M_A := T_a \times T_{a,b} \times T_b \times T_{b,a}, \qquad M_B := T_a \times T_{a,a} = T_a \tag{26}$$

An alternative approach was suggested recently by Bertolotti *et al.*[6] Following Born and Wolf,[7] they choose as basis,

$$E'_+ = E^{(1)} + E^{(2)}, \qquad E'_- = \frac{\partial}{\partial z}(E^{(1)} + E^{(2)}) = ik_z(E^{(1)} - E^{(2)}) \tag{27}$$

Since $\mathbf{E}$ and $\partial\mathbf{E}/\partial z$ are continuous at the interface for TE-polarization, with this basis choice one obtains the transfer matrices

$$T'_{b,a} = T'_{a,b} = \mathbb{1}_2, \qquad T'_a = \begin{pmatrix} \cos(\delta_a) & \dfrac{\sin(\delta_a)}{k_0 n_0 \cos(\Theta_a)} \\ -k_0 n_a \cos(\Theta_a)\sin(\delta_a) & \cos(\delta_a) \end{pmatrix}, \tag{28}$$

with an analogous definition for T'_b. Importantly, the transfer matrix model thus obtained is an on-site model! Hence, in this particular physical context, by changing the basis on which to describe the problem, one can go from a multi-site to an on-site transfer matrix model.

Let us now consider this transformation in more detail. Let S_a be a matrix

$$S_a := \begin{pmatrix} 1 & 0 \\ 0 & -k_0 n_a \cos(\Theta_a) \end{pmatrix} \tag{29}$$

and let S_b be a similar matrix with indices a replaced by b. Then one easily verifies that[7]

$$T_{a,b} = S_a^{-1} \times S_b \tag{30}$$

$$T_{b,a} = S_b^{-1} \times S_a \tag{31}$$

$$T_a = S_a^{-1} \times T'_a \times S_a \tag{32}$$

$$T_b = S_b^{-1} \times T'_b \times S_b \tag{33}$$

Hence, when M is a product of transfer matrices T_a, T_b, $T_{a,b}$, $T_{b,a}$ (with basis choice (23)) connecting a layer of type a to another layer of type a separated by an arbitrary sequence of layers, and M' represents the same layers in terms of T'_a and T'_b (with basis choice (27)), then

$$M' = S_a \times M \times S_a^{-1} \tag{34}$$

Analogously, when M connects two layers of type b then

$$M' = S_b \times M \times S_b^{-1} \tag{35}$$

Taking into account periodic boundary conditions one immediately finds that both bases (23) and (27) lead to essentially the same transfer matrices (as one is allowed to transfer a rightmost matrix to the leftmost position), e.g.

$$\begin{aligned} &\cdots T_a \times T_{a,b} \times T_b \times T_{b,a} \times T_a \times T_a \times T_{a,b} \times T_b \times T_{b,a} \times T_a \cdots \\ &= \cdots T'_a \times T'_b \times T'_a \times T'_a \times T'_b \times T'_a \cdots \end{aligned} \tag{36}$$

3.3. Proof of Theorem 1.6

Consider a transfer matrix model with transfer matrices $T_{i-q,\dots,i-q+m-1}$ which can be decomposed as

$$T_{i-q,\dots,i-q+m-1} = \hat{T}_{i-q+l_1,\dots,i-q+p_1-1} \times \hat{T}'_{i-q+l_2,\dots,i-q+p_2-1} \tag{37}$$

with $\min(l_1, l_2) = 0$ and $\max(p_1, p_2) = m$. Using this decomposition property we may construct new transfer matrices of the form

$$T'_{i+q',\dots,i-q'+m-1} := \hat{T}'_{i-q+l_2,\dots,i-q+p_2-1} \times \hat{T}_{i-q+l_1+1,\dots,i-q+p_1} \tag{38}$$

[7] Note that we assume propagation through the whole sample, i.e. $0 \leqslant \Theta_a, \Theta_b < \pi/2$.

where $q' := q - \min(l_1 + 1, l_2)$ and $m' := \max(p_1 + 1, p_2) - \min(l_1 + 1, l_2)$. Hence, $m' \in \{m-1, m, m+1\}$, and $m' < m$ if and only if $l_1 = 0$, $l_2 > 0$, $p_1 < m$, and $p_2 = m$. In that case $m' = m - 1$ and $q' = q - 1$. This case is described in Theorem 1.6. ∎

The construction in Section 3.1 and Section 3.2 are examples of the above construction. In the light transmission model we encountered transfer matrices occurring in pairs of the form $T_i \times T_{i,i+1} = S_i^{-1} \times T'_i \times S_{i+1}$, leading to new transfer matrices $S_i \times S_i^{-1} \times T'_i = T'_i$. For the construction in the case of the off-diagonal tight binding model see Eqs. (19)–(20).

4. DISCUSSION

In this last section we will discuss some implications of the results we have obtained above, that illustrate the importance of recognizing the existence of transformations from multi-site to on-site models.

We will focus on the use of trace maps in the context of the tight binding transfer matrix models with Hamiltonian (1) on two-symbol chains.[8]

When the transfer matrices in a model are elements of $SL(2, \mathbb{C})$ (such as those arising in the context of (1)), then by application of the Cayley–Hamilton theorem one obtains trace maps $F: \mathbb{R}^3 \mapsto \mathbb{R}^3$ mapping $(\mathrm{Tr}(T_a), \mathrm{Tr}(T_b), \mathrm{Tr}(T_{ab}))$ to $(\mathrm{Tr}(T_{\tau(a)}), \mathrm{Tr}(T_{\tau(b)}), \mathrm{Tr}(T_{\tau(ab)}))$. These maps are polynomial maps with integer coefficients.[1] For instance, the trace map associated to the Fibonacci substitution rule $\sigma(a, b) = (ab, a)$ is given by

$$F: (x, y, z) \mapsto (z, x, xz - y) \tag{39}$$

The trace of $T_{\tau^k(a)}$ is thus the x-coordinate of $F^k(\mathrm{Tr}(T_a), \mathrm{Tr}(T_b), \mathrm{Tr}(T_{ab}))$. (For more background on trace maps see the review by Peyrière[16] and references therein.)

In on-site models, trace maps are a useful tool in determining properties of physical models.[4, 8, 10–13, 19, 22] For instance, the energy spectrum of the tight binding Schrödinger equation (2) can be found as the intersection of the nonwandering set (points that do not escape to infinity) of the trace map with a line (of initial conditions) parameterized by the energy value E.[11, 19][9]

[8] For discussions on the application of trace maps in other models see e.g. refs. 4, 12.

[9] Also in the optical transmission model, the intersection of a line of initial conditions (parameterized by the free wave number) with the nonwandering set of the trace map corresponds to wavenumbers satisfying a (quasi-) nonresonance condition implying a nonzero transmission coefficient, cf. ref. 12.

Hence the energy spectra of Fibonacci chains with different variations of the tight binding model (1) are all related to the same trace map (39). The only difference between the various models are their initial conditions (i.e. the line parameterized with E that intersects the nonwandering set of F). For instance, the diagonal model ($t_{i,i+1}=1$) has initial condition $(E-V_a, E-V_b, (E-V_a)(E-V_b)-2)$. In the case of the off-diagonal model (17) using transfer matrices (20) is terms of which the transfer matrix model is on-site, one obtains the initial conditions $(E/t_a, E/t_b, (E^2-t_a^2-t_b^2)/(t_at_b)^2)$. In the case of the three-site model with transfer matrices (4) more complicated initial conditions are found.

Importantly, many aspects of the energy spectrum of Fibonacci chains are consequences of the nature of the nonwandering set of the trace map F, and do not depend so much on the details of the line of initial conditions. In particular, the multifractal and scaling properties of the spectrum are closely related to the structure of the nonwandering set, and hence shared by a large class of transfer matrix models.[10] Recently, it has been recognized that an important property of the Fibonacci substitution rule is its invertibility, and that aperiodic two-symbol chains that are renormalizable with respect to invertible substitutions share many important properties with the Fibonacci chain, cf. ref. 22 and references therein. Theorem 1.5 implies that multi-site models on two-symbol chains that are selfsimilar with respect to invertible substitutions naturally belong to the class of on-site models on such chains, and hence share many properties.

Interestingly, we have shown in Appendix B that in the case of the Thue–Morse sequence and a Fibonacci-squared sequence, multi-site models cannot be transformed into on-site models by alphabet transformations. For instance, when studying the general three-site (disguised two-site, cf. footnote 3) tight binding model (1) the trace map formalism cannot be applied. It would be interesting to further study the properties of such multi-site models and compare them to the properties of on-site models. In this respect it should also be noted that in the case of multi-site models derived from models with neighbor interactions reaching further than nearest neighbors, the transfer matrices will in general no longer be 2×2. For recent work in the context of trace maps of $n\times n$ matrices with $n>2$, see [5,20].

[10] For more references on the spectral properties of quasiperiodic Schrödinger equations and trace maps see e.g. refs. 2, 8, 16, 18, 22.

APPENDICES

A. Alphabet Transformations that Are Compatible with Renormalization

In this appendix we discuss how an alphabet S can be transformed into an alphabet $\tilde{S}$ such that the action of a substitution rule τ on S naturally leads to a substitution rule $\tilde{\tau}$ on S.

Let us consider an n-symbol alphabet $S := \{s_1, ..., s_n\}$. We are interested in writing a word $w \in S^*$ in terms of a word $\tilde{w}$ in a different n-symbol alphabet $\tilde{S}$, where each symbol in the alphabet $\tilde{S}$ is a word in S^*.

The fact that the elements of $\tilde{S}$ correspond to elements of S^*, can be interpreted as the existence of a morphism μ from $\tilde{S}^*$ to S^* so that for any word $\tilde{w}$ in $\tilde{S}^*$, $\mu(\tilde{w})$ is a word in S^*.

Let us briefly illustrate this notation with an example. Let $S = \{a, b\}$ and $\tilde{S} = \{\tilde{a}, \tilde{b}\}$, such that $\mu: (\tilde{a}, \tilde{b}) \mapsto (abb, a)$. Consider the word $w = abba$ in S^*. This word can also be expressed as a word $\tilde{w} = \tilde{a}\tilde{b}$ in $\tilde{S}^*$, namely $\mu(\tilde{w}) = w$.

We now consider the action of a substitution rule τ on words w in S^* that are equal to $\mu(\tilde{w})$ for some $\tilde{w}$ in $\tilde{S}^*$:

$$\tau(w) = \tau \circ \mu(\tilde{w}) \tag{40}$$

Now suppose there exists a substitution $\tilde{\tau}$ on these words $\tilde{w}$ in $\tilde{S}^*$ that is equivalent to the substitution τ on the words w, then

$$\mu \circ \tilde{\tau}(\tilde{w}) = \tau(w) = \tau \circ \mu(\tilde{w}) \tag{41}$$

Thus if the action of a substitution rule τ on words w in S^* corresponds to the action of a substitution rule $\tilde{\tau}$ on words $\tilde{w}$ in $\tilde{S}^*$, then (40) and (41) imply that the transformation $\mu: \tilde{S}^* \mapsto S^*$ must be such that

$$\mu \circ \tilde{\tau} = \tau \circ \mu \tag{42}$$

It is immediate from (42) that whenever we choose $\mu(\tilde{s}_j) = \tau^k(s_j)$ for some integer $k > 0$ and all $s_j \in S, \tilde{s}_j \in \tilde{S}$, the morphism μ is compatible with the renormalization scheme and $\tilde{\tau} = \tau$ (as a substitution rule on an n-symbol alphabet). This is the underlying reason for choosing this morphism in Theorem 1.3. It is the most straightforward solution to (42).

In Appendix B we will make further use of (42).

B. Nonexistence of Alphabet Transformations from Multisite to On-Site Models

In this appendix we will demonstrate the fact that in the case of the Thue–Morse substitution rule $\sigma(a, b) = (ab, ba)$ and the Fibonacci-squared substitution rule $a(a, b) = (aab, ba)$ no alphabet transformations exist that transform a multi-site transfer matrix model on these chains into a renormalizable on-site transfer matrix model.

Importantly, the words $\tau(a)$ and $\tau(b)$ do not have their leftmost or rightmost symbol in common, and neither do $\tilde{\sigma}(a)$ and $\tilde{\sigma}(b)$. A necessary condition for the existence of such a transformation is that we find a μ and $\tilde{\tau}$ such that $\mu \circ \tilde{\tau} = \tau \circ \mu$ or $\mu \circ \tilde{\tau} = \tilde{\sigma} \circ \mu$ respectively (cf. (42)), where $\tilde{\tau}(a)$ and $\tilde{\tau}(b)$ have their leftmost or rightmost symbol in common (otherwise the indices in of the transfer matrices will never be able to match). See also Appendix A and Section 2.

We will prove the impossibility of finding such μ and $\tilde{\tau}$ in the case of the Thue–Morse and of a Fibonacci-squared substitution rule. We have chosen these cases as prototypical examples of aperiodic selfsimilar two-symbol chains generated by noninvertible substitutions τ for which $\tau(a)$ and $\tau(b)$ do not share their leftmost and/or rightmost symbol, with the Thue–Morse chain being almost periodic (but not quasiperiodic) and our Fibonacci-squared chain being quasiperiodic.

It is tempting to conjecture that whenever τ fixes an aperiodic chain, $b \in \tau^2(a)$ and $a \in \tau^2(b)$, and the words $\tau(a)$ and $\tau(b)$ do not have their leftmost or rightmost symbol in common, such μ and $\tilde{\tau}$ can never be found. However, a general result in this direction is beyond the scope of the present paper.

B.1. Thue–Morse. In our analysis, we will give a slightly (but equivalent) interpretation to (42). Namely, in this equation we may view μ, τ, and $\tilde{\tau}$ all as substitutions on n-letter alphabets $S \mapsto S^*$, acting on words $w(S) = w(a, b)$ in a natural way as $\mu(w(S)) := w(\mu(S)) = w(\mu(a), \mu(b))$, etc. By this we circumvent complications in notation due to the difference between the alphabets S and $\tilde{S}$. With this convention, we write out (42):

$$\tau\mu_1(a, b) = \mu_1(\tau(a), \tau(b)) = \tilde{\tau}_1(\mu_1(a, b), \mu_2(a, b)) \tag{43}$$

$$\tau\mu_2(a, b) = \mu_2(\tau(a), \tau(b)) = \tilde{\tau}_2(\mu_1(a, b), \mu_2(a, b)) \tag{44}$$

where $\mu_1(a, b) := \mu(a)$, $\mu_2(a, b) := \mu(b)$, $\tilde{\tau}_1(a, b) := \tilde{\tau}(a)$, $\tilde{\tau}_2(a, b) := \tilde{\tau}(b)$.

Suppose $\tilde{\tau}(a)$ and $\tilde{\tau}(b)$ both start with the symbol a. We will show that there exists no substitution rule μ that solves (42) when τ is the Thue–Morse substitution rule $\tau(a, b) = (ab, ba)$.

We write out (43):

$$\tau\mu_1(a, b) = \mu_1(a, b)\, w(\mu_1(a, b), \mu_2(a, b)) \tag{45}$$

It is not difficult to show that the word $\mu_1(a, b)$ must hence consist of the first p symbols of the word $\tau^k(a)$ or $\tau^k(b)$ for some k such that $|\tau^k(a)| \geqslant p$ or $|\tau^k(b)| \geqslant p$. We use the notation $|w|$ to denote the length of the word w, which is in turn a shorthand notation for $w(a, b)$.

We now use the fact that in the case of Thue–Morse $|\tau w| = 2\,|w|$. Hence $2\,|\mu_2| = |\tau\mu_2| \geqslant |\mu_1|$. Because $\tau\mu_1 \neq \mu_1\mu_1$ (no periodic word is fixed under the Thue–Morse substitution), we hence have either $|\mu_1| = |\mu_2|$ or $|\mu_1| = 2\,|\mu_2|$.

In case $|\mu_1| = |\mu_2|$ we have $\tau\mu_1 = \mu_1\mu_2$. If also $\tau\mu_2 = \mu_1\mu_2$ then it follows that $\mu_1 = \mu_2$ which leads to $\tau\mu_1 = \mu_1\mu_1$ which has no solution. Alternatively, we have $\tau u_2 = \mu_1\mu_1$ that we may combine with $\tau\mu_1 = \mu_1\mu_2$ to give

$$\tau^2\mu_1 = \tau\mu_1\mu_1\mu_1 \tag{46}$$

In case $|\mu_1| = 2\,|\mu_2|$ we are immediately led to $\tau\mu_1 = \mu_1\mu_2\mu_2$ and $\tau\mu_2 = \mu_1$. This also gives rise to (46).

In order to prove that no solution exist, we are left to show that (46) has no solution for μ_1.

Suppose $\mu_1(a, b)$ is a solution of (46). When μ_1 is a solution $\tau\mu_1$ is automatically also a solution, and hence then there must be at least one solution μ_1 that is not the image of a word w under τ (such that $\mu_1 \neq \tau w$ for all w). Without loss of generality we will assume μ_1 is such a word.

We now aim to reconstruct the preimage of $\tau^2\mu_1$. Note that $\tau^2\mu_1$ ends with $\mu_1\mu_1$. Because μ_1 itself is not the image of a word and $\tau^2\mu_1$ ends with μ_1, $|\mu_1|$ must be odd. Hence, since the last $\tau^2\mu_1$ ends with $\mu_1\mu_1$ the last symbol of μ_1 and the first symbol of μ_1 must form the word $\tau(a) = ab$ or $\tau(b) = ba$. However, if we know the first symbol of μ_1 we also know the second symbol (because μ_1 consists of the first p symbols of $\tau^k(a)$ or $\tau^k(b)$). Suppose that $|\mu_1| \geqslant 3$. In that case $\mu_1 = abb\cdots$ or $\mu_1(a, b) = baa\cdots$. Because the preimage of μ_1 is not the image of a word under τ we find that the last and first symbol of μ_1 must form the word $\tau(a)$ or $\tau(b)$ and so must the second and third symbol. However, aa and bb are not such words. We are left to show that also $|\mu_1| \nleqslant 2$. $|\mu_1| \neq 1$ because μ_1 must not begin and end with the same symbol. If $|\mu_1| = 2$ it is forced to be $\tau(a)$ or $\tau(b)$ which is in a contradiction with the assumption.

We thus proved that $\tau\mu_1$ and $\tau\mu_2$ cannot start with μ_1. Thus $\tilde{\tau}(a)$ and $\tilde{\tau}(b)$ cannot start with the same symbol.

We are left to show that $\tilde{\tau}(a)$ and $\tilde{\tau}(b)$ also cannot end with the same symbol. Let us suppose that they both end with μ_1. In that case one has to consider the extra possibilities $\tau\mu_1 = \mu_2\mu_2\mu_1$, $\tau\mu_2 = \mu_1$, and $\tau\mu_1 = \mu_2\mu_1$, $\tau\mu_2 = \mu_1\mu_1$ which leads to

$$\tau^2\mu_1 = \mu_1\mu_1\tau\mu_1 \tag{47}$$

The demonstration that this equation has no solutions for μ_1 is analogous to that of (46).)

In this way we prove that there do not exist substitution rules $\tilde{\tau}$ and μ, with $\tilde{\tau}(a)$ and $\tilde{\tau}(b)$ sharing a rightmost or leftmost symbol, that solve (42) with τ being the Thue–Morse substitution rule. Hence there exist no alphabet transformations that transform a multi-site model on a Thue–Morse chain to a renormalizable on-site model.

B.2. Fibonacci-Squared. We now perform a similar analysis for the case of a Fibonacci-squared substitution rule $\tilde{\sigma}(a, b) = (aab, ba)$.

In contrast to the Thue–Morse substitution, the ratio between the length of a word and the length of its image under $\tilde{\sigma}$ is not constant. This will complicate the analysis slightly. We find

$$2\,|\mu_1| \leqslant |\tilde{\sigma}\mu_1| \leqslant 3\,|\mu_1|, \qquad 2\,|\mu_2| \leqslant |\tilde{\sigma}\mu_2| \leqslant 3\,|\mu_2| \tag{48}$$

Let us focus on the case that $\tilde{\sigma}\mu_1$ and $\tilde{\sigma}\mu_2$ start with the same symbol in $\mu(S)$. Suppose they both start with μ_1. In that case we find that $|\mu_1| \leqslant |\tilde{\sigma}\mu_2|$.

Note that we may restrict to $2\,|\mu_1| < |\tilde{\sigma}\mu_1| < 3\,|\mu_1|$ and $2\,|\mu_2| < |\tilde{\sigma}\mu_2| < 3\,|\mu_2|$, leaving out the equality signs. Namely, the equality sign applies only when μ_1 or μ_2 are words of only a's or only b's. It is not difficult to show that such solutions cannot arise.

We will eliminate the remaining possibilities step by step. Instead of providing proofs at every step, to reduce the length of this section we will sketch the flow of the argument and leave some (easy) details to the reader.

Using arguments analogous to those used in Section B.1, one can show that

$$\tilde{\sigma} \neq \mu_1\mu_1 \ldots, \qquad \tilde{\sigma}\mu_1 \neq \mu_1 \cdots \mu_1 \tag{49}$$

These restrictions eliminate a lot of possibilities. The remaining cases are all of the form $\tilde{\sigma}\mu_1 = \mu_1\mu_2 \ldots$.

When $\tilde{\sigma}\mu_1 = \mu_1\mu_2\mu_1\mu_2$ then length requirements enforce $\tilde{\sigma}\mu_2 = \mu_1$, giving rise to $\tilde{\sigma}^2\mu_1 = \tilde{\sigma}\mu_1\mu_1\tilde{\sigma}\mu_1\mu_1$ which is not allowed. Namely, since $\tilde{\sigma}\mu_1$ starts with μ_1, one then obtains $\tilde{\sigma}^2\mu_1 = \mu_1 \cdots \mu_1$ which can be ruled out using similar arguments that establish (49).

When $\tilde{\sigma}\mu_1 = \mu_1\mu_2$ it follows that $|\mu_1| < |\mu_2| < 2\,|\mu_1|$, leaving still many possibilities. However, it is not difficult to show that $\tilde{\sigma}\mu_2 \neq \mu_1 \cdots \mu_1$ because that would imply that $\tilde{\sigma}^2\mu_1 = \mu_1 \cdots \mu_1$, and that $\tilde{\sigma}\mu_2 \neq \cdots \mu_1\mu_2$ because that would imply that $\mu_2 = \cdots \mu_1$ giving $\tilde{\sigma}\mu_1 = \mu_1 \cdots \mu_1$. There is only one $\tilde{\sigma}\mu_2$ possibility left to check, namely $\tilde{\sigma}\mu_2 = \mu_1\mu_2\mu_2$. In this last case, it would follow that $\mu_2 = \mu_1 ...$ which would imply that $\tilde{\sigma}\mu_1 = \mu_1\mu_1 ...$ which is ruled out in (49).

Finally, when $\tilde{\sigma}\mu_1 = \mu_1\mu_2\mu_2$ length requirement enforce $\tilde{\sigma}\mu_2 = \mu_1$ giving rise to $\tilde{\sigma}^2\mu_1 = \mu_1 \cdots \mu_1$.

Now we exhausted all possibilities of $\tilde{\sigma}\mu_1$ and $\tilde{\sigma}\mu_2$ starting with μ_1. The rest of the proof consists of verifying that they also cannot both start with μ_2 or both end with μ_1 or μ_2. This verification follows similar arguments as presented above and will be omitted.

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