Trace and antitrace maps for aperiodic sequences, their extensions and applications

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We study aperiodic systems based on substitution rules by means of a transfer-matrix approach. In addition to the well-known trace map, we investigate the so-called “antitrace” map, which is the corresponding map for the difference of the off-diagonal elements of the $2 \times 2$ transfer matrix. The antitrace maps are obtained for various binary, ternary, and quaternary aperiodic sequences, such as the Fibonacci, Thue-Morse, period-doubling, and Rudin-Shapiro sequences, and certain generalizations.

For arbitrary substitution rules, we show that not only trace maps, but also antitrace maps exist. Analogous maps for specific matrix elements of the transfer matrix can also be constructed, but the maps for the off-diagonal elements and for the difference of the diagonal elements coincide with the antitrace map. Thus, from the trace and antitrace map, we can determine any physical quantity related to the global transfer matrix of the system. As examples, we employ these dynamical maps to compute the transmission coefficients for optical multilayers, harmonic chains, and electronic systems.

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I. INTRODUCTION

The trace-map technique, first introduced in 1983, has proven to be a powerful tool to investigate the electronic spectrum of various aperiodic systems, such as the Fibonacci sequence (FS), the Thue-Morse sequence (TMS), and the period-doubling sequence. It has also been applied to investigate other physical systems, for instance, kicked two-level systems and classical and quantum spin systems. The technique was extended to study aperiodic systems in combination with the real-space renormalization-group technique. Recently, trace maps have been used to evaluate localization properties in a FS tight-binding model.

This technique was transferred to the field of optics in order to see the scaling of the light transmission coefficients through a Fibonacci dielectric multilayer. Now, we consider light that is vertically transmitted through a Fibonacci multilayer of two materials $a$ and $b$ which is sandwiched by two media of type $a$. The FS is constructed by the substitution rule $b \rightarrow a$, $a \rightarrow ab$. The corresponding transfer matrices $A_l$ are written as

\begin{align}
A_1 &= P_{ab}P_tP_{ba}, \\
A_2 &= P_a, \\
A_{l+1} &= A_lA_{l-1},
\end{align}

where $P_{ab}(P_{ba})$ stands for the propagation matrix from layer $a$ to $b$ ($b$ to $a$) and $P_a$ is the propagation matrix through the single layer $a$. They are given by

\begin{align}
P_{ab} &= P_{ba}^{-1} = \begin{pmatrix}
1 & 0 \\
0 & n_a/n_b
\end{pmatrix}, \\
P_a &= \begin{pmatrix}
\cos \delta_a & -\sin \delta_a \\
\sin \delta_a & \cos \delta_a
\end{pmatrix},
\end{align}

where $\delta_a = k n_a d_a$, $n_a$ is the refraction index of material $a$, $d_a$ denotes the thickness of the layers, and $k$ is the wave number in vacuum. The quantity $\delta_a$ is the phase difference between the ends of a layer. For material $b$, the quantities $P_b$, $\delta_b$, $n_b$, and $d_b$ are defined analogously.

The transmission coefficient is given by

\begin{equation}
t_l = \frac{4}{|A_l|^2 + 2},
\end{equation}

where $|A_l|^2$ is the sum of squares of the four elements of $A_l$. Since the transfer matrix is unimodular, we can express the transmission coefficient as

\begin{equation}
t_l = \frac{4}{x_l^2 + y_l^2},
\end{equation}

where $x_l$ and $y_l$ denote the trace and antitrace of the transfer matrix $A_l$, respectively. Here, the so-called “antitrace” of a $2 \times 2$ matrix

\begin{equation}
A = \begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\end{equation}

is defined as $y_A = A_{21} - A_{12}$, which follows the notion of Ref. From Eq. (1.4), we see that the transmission
the Wannier representation, 

\[ \phi \]

where

\[ 1 \]

matrix element between two neighboring sites.

monic chain composed of two kinds of masses, \( m_a \) and \( m_b \), which are arranged according to the FS, and are coupled by two kinds of springs, \( K_{aa} \) and \( K_{ab} = K_{ba} \). Making use of the transfer-matrix formalism, the equation of motion is

\[
\begin{pmatrix}
  a_{n+1} \\
  a_n \\
\end{pmatrix} = \begin{pmatrix}
  1 & -K_{n,n+1} \\
  K_{n,n+1} & 1 \\
\end{pmatrix} \begin{pmatrix}
  a_n \\
  a_{n-1} \\
\end{pmatrix}
\]

\[ = P_n \begin{pmatrix}
  a_n \\
  a_{n-1} \\
\end{pmatrix},
\]

(1.6)

where \( a_n \) is the displacement of the \( n \)th atom from its equilibrium position, \( K_{n,n \pm 1} \) denotes the strength of the harmonic coupling between neighboring atoms, \( a_n = K_{n,n-1} + K_{n,n+1} - m_n \omega^2 \), and \( \omega \) is the vibration frequency.

From the corresponding global transfer matrix \( A_l = \prod_{n=N_l}^1 P_n \), the transmission coefficient \( t_l \) and the Lyapunov exponent \( \Gamma_l \) are given by

\[
t_l = \frac{4 \sin^2 k}{(z_l \cos k - y_l)^2 + x_l^2 \sin^2 k},
\]

(1.7)

\[
\Gamma_l = \frac{1}{N_l} \ln(|A_l|^2) = \frac{1}{N_l} \ln(x_l^2 + y_l^2 - 2),
\]

(1.8)

where \( z_l = (A_l)_{11} - (A_l)_{22} \), \( N_l \) denotes the number of atoms in the chain, and \( \cos k = m_a/(2K_{aa}) \).

As our third example of physical systems based on aperiodic substitution sequences, we consider the transmission in electronic systems. This is closely related to the harmonic chain considered above. The Schrödinger equation for a one-dimensional tight-binding model with nearest-neighbor hopping can be written in matrix form as follows:

\[
\begin{pmatrix}
  \phi_{n+1} \\
  \phi_n \\
\end{pmatrix} = \begin{pmatrix}
  E - \epsilon_n & -\epsilon_{n+1} \\
  \epsilon_{n+1} & E - \epsilon_n \\
\end{pmatrix} \begin{pmatrix}
  \phi_n \\
  \phi_{n-1} \\
\end{pmatrix}
\]

(1.9)

where \( \phi_n \) denotes the amplitude of the wave function in the Wannier representation, \( E \) the corresponding energy, \( \epsilon_n \) the on-site energy at site \( n \), and \( t_{n,n \pm 1} \) the hopping matrix element between two neighboring sites. \( M_n \) is the local transfer matrix associated with site \( n \). The transmission coefficient is given by

\[
t_l = \frac{4 - E^2}{(z_l E/2 - y_l)^2 + x_l^2 (1 - E^2/4)},
\]

(1.10)

where the quantities \( x_l \), \( y_l \), and \( z_l \) are again related to the global transfer matrix of the chain, i.e., the product \( A_l = \prod_{n=N_l}^1 M_n \) of the local transfer matrices along the chain. Note the similarity to Eq. (1.7). The corresponding Lyapunov exponent \( \Gamma_l \) is given by the same expression (1.8).

For the latter two systems, the Lyapunov exponent is completely determined by the trace and the antitrace; however, we need to know \( z_l \) to calculate the transmission coefficient. Fortunately, it turns out that the maps for \( z_l \) and \( y_l \) are the same, as will be shown in Sec. IV. Therefore, the trace and antitrace map are sufficient to determine the transmission coefficient and the Lyapunov exponent. Thus it is desirable to construct antitrace maps for various aperiodic sequences, which is the motivation of the work presented here.

The paper is organized as follows. In Sec. II, we give the antitrace maps for various classes of aperiodic sequences, including the FS, the TMS, the period-doubling sequence, and certain generalizations. The extension to arbitrary substitution rules and to maps for matrix elements are discussed in Sec. III and in Sec. V, respectively. It is shown that the antitrace maps and the maps for matrix elements exist for arbitrary substitution rules and that the maps for non-diagonal elements and for the difference of the diagonal elements coincide with the antitrace maps. Applications to the computation of transmission coefficients and Lyapunov exponents in different aperiodic systems are investigated in Sec. VI. Finally, in Sec. VII, we conclude.

II. TRACE AND ANTITRACE MAPS FOR TWO-LETTER SEQUENCES

We now proceed with the derivation of the antitrace maps of various classes of aperiodic sequences. We also include the corresponding trace maps for reasons which will become clear later. In this part, we make ample use of several relations for unimodular matrices. Therefore, we append a compilation of these relations in Appendix A.

A. Generalized Fibonacci sequences

There are many kinds of generalized FSs. Here, we study two-letter sequences \( FS(m,n) \) that can be generated by the inflation scheme

\[
S_0 = b, \quad S_1 = a, \quad S_{l+1} = S_l^m S_l^n
\]

(2.1)

with arbitrary positive integers \( m \) and \( n \), where \( FS(1,1) \) corresponds to the well-known standard FS. Equivalently, they can also be generated by the substitution rule

\[
b \rightarrow a, \quad a \rightarrow a^m b^n.
\]

(2.2)

The total number of letters \( a \) and \( b \) in the word \( S_l \) is denoted by \( F_l \) and satisfies the recursion relation

\[
F_{l+1} = m F_l + n F_{l-1}, \quad F_0 = F_1 = 1.
\]

(2.3)
In the limit of an infinite sequence, the ratio of word lengths for subsequent inflation steps is given by

$$\sigma = \lim_{i \to \infty} \frac{F_{i+1}}{F_i} = \frac{m + \sqrt{m^2 + 4n}}{2}. \quad (2.4)$$

Some values of \(\sigma\) and commonly used terms for special cases of so-called “metallic means” are:

- FS(1, 1): \(\sigma_g = \frac{1 + \sqrt{5}}{2}\) golden mean,
- FS(2, 1): \(\sigma_s = 1 + \sqrt{2}\) silver mean,
- FS(3, 1): \(\sigma_b = \frac{3 + \sqrt{13}}{2}\) bronze mean,
- FS(1, 2): \(\sigma_c = 2\) copper mean,
- FS(1, 3): \(\sigma_n = \frac{1 + \sqrt{13}}{2}\) nickel mean.

It is known that the sequences FS\((m, n)\) with \(n = 1\) are quasiperiodic and those with \(n \geq 2\) are always aperiodic.

It is interesting to consider two further classes of generalized FSs:

\[
\begin{align*}
\text{FS}(1, 1) & : b \rightarrow b^{m-1}a, \quad a \rightarrow b^{m-1}ab, \quad (2.5) \\
\text{FS}(1, 2) & : b \rightarrow b^{m-2}a, \quad a \rightarrow b^{m-2}ab \quad (2.6)
\end{align*}
\]

The first class \(\text{FS}(1, 1)\) consists of the so-called Fibonacci-class sequences FC\((m, n)\), the second \(\text{FS}(1, 2)\) occurs in the renormalization-group analysis of the energy spectrum of FC\((m)\) chains. It is easy to check that the inflation schemes of these two generalized FSs are the same as those for FS\((m, 1)\), but they differ in the initial words. A natural further generalization of these sequences is given by

\[
\begin{align*}
\text{FS}(1, 1) & : b \rightarrow b^{m-k}a, \quad a \rightarrow (b^{m-k}a)b, \quad (2.7)
\end{align*}
\]

which we denote as FC\((m, k)\). Here, FC\((m, 1)\) and FC\((m, 2)\) correspond to the cases \(\text{FS}(1, 1)\) and \(\text{FS}(1, 2)\). The corresponding inflation scheme is

\[
S_0 = b, \quad S_1 = b^{m-k}a, \quad S_{l+1} = S_l^n S_{l-1}, \quad (2.8)
\]

which is the same as that of FS\((m, 1)\) apart from the different second initial word.

1. The Fibonacci sequence

Let us commence with the simplest example FS\((1, 1)\). We consider the case that the two letters \(a\) and \(b\) correspond to two basic unimodular transfer matrices \(A\) and \(B\), respectively. Denoting by \(A_l\) the total transfer matrix corresponding to a word \(S_l\), the matrix equivalent of Eq. (2.1) for FS\((1, 1)\) is

\[
A_{l+1} = A_{l-1}A_l, \quad (2.9)
\]

where \(A_1 = A\) and \(A_0 = B\) are the transfer matrices of the two building blocks \(a\) and \(b\). Note the reversed order of matrix multiplication as compared to the concatenation of letters in Eq. (2.1), which occurs in the related tight-binding model that is usually considered, whereas the order of matrix multiplications is not reversed in the optical problem, compare Eq. (1.1). The well-known trace map reads

\[
x_{l+1} = x_{l-1}x_l - x_{l-2}. \quad (2.10)
\]

Note that in part of the literature a factor \(1/2\) is introduced in the definition of \(x_l\). Here, we omitted this factor to keep symmetry between trace and antitrace. From Eq. (A.4), we obtain the antitrace map

\[
y_{l+1} = x_l y_{l-1} + y_{l-2}. \quad (2.11)
\]

The coefficients of the trace map are constants; however, those of the antitrace map include the traces. So, if we want to derive the antitrace map, the trace map must also be known. This is why we have to consider trace and antitrace maps at the same time.

2. Generalized Fibonacci sequences FS\((m, n)\)

For FS\((m, n)\), Eq. (2.1), the recursion relation for the transfer matrix is given by

\[
A_{l+1} = A_{l-1} A_l^m = \left(U_n^{l-1} A_{l-1} - U_{n-1}^{l-1} I\right) \times \left(U_m^{l-1} A_l - U_{m-1}^{l-1} I\right). \quad (2.12)
\]

Here, we used Eq. (A.4) and the definition of the functions \(U_n(x) = C_{n-1}(x/2)\) given in Appendix A in terms of the Chebyshov polynomials of the second kind \(C_n(x)\). Furthermore, we introduced the notation

\[
U_n^{l}(x) = U_n(x A_l). \quad (2.13)
\]

From Eqs. (2.12), (A.3), and (A.4), the trace and the antitrace maps are obtained as

\[
\begin{align*}
x_{l+1} &= U_n^{l-1} U_m^{l-1} v_l - U_n^{l-1} U_{m+1}^{l-1} v_l - U_{n+1}^{l-1} U_m^{l-1}, \quad (2.14) \\
v_{l+1} &= U_n^{l-1} U_m^{l+1} v_l - U_n^{l-1} U_{m+2}^{l-1} v_l - U_{n+1}^{l-1} U_m^{l+1}, \quad (2.15)
\end{align*}
\]

\[
\begin{align*}
y_{l+1} &= U_n^{l-1} \left(U_m^{l-1} w_l - U_{m-1}^{l-1} w_l - U_{m+1}^{l-1} w_l - U_{m+2}^{l-1} w_l\right) \\
&\quad - U_{n+1}^{l-1} U_m^{l+1} w_l, \quad (2.16)
\end{align*}
\]

\[
\begin{align*}
w_{l+1} &= U_n^{l-1} U_m^{l-1} w_l - U_n^{l-1} U_{m-2}^{l-1} w_l + \left(x_{l+1} - U_{n-1}^{l-1} U_{m-1}^{l-1} w_l\right) y_l, \quad (2.17)
\end{align*}
\]

where \(v_l = x_{A_l-1} A_l\) and \(w_l = y_{A_l-1} A_l\). Note that the roles of \(v_l\) and \(w_l\) are subsidiary. Eqs. (2.14) and (2.15)
constitute the trace map, Eqs. (2.16) and (2.17) give the corresponding antitrace map.

For special cases, these expressions simplify considerably. For FS(1, n), we obtain, using the properties (A.3) of the functions $U_n(x)$,

$$x_{i+1} = U_n^{(l)}(x_i) - U_{n-1}^{(l)}(x_{i-1}),$$
$$v_{i+1} = U_n^{(l)}(x_{i+1}) - U_{n-1}^{(l)}(x_{i}^2 - 1) - U_{n-1}^{(l)}(x_{i}^2 - 1),$$
$$y_{i+1} = U_n^{(l)}(x_i) - U_{n-1}^{(l)}(x_{i-1}),$$
$$w_{i+1} = x_{i+1}y_i + U_{n-1}^{(l)}y_{i-1}. $$

Similarly, for FS(m, 1), we find

$$x_{i+1} = U_m^{(l)}(x_{i+1}) - U_{m-1}^{(l)}x_{i},$$
$$v_{i+1} = U_m^{(l)}(x_{i+1}) - U_{m-1}^{(l)}x_{i-1},$$
$$y_{i+1} = U_m^{(l)}(U_{n-1}^{(l)}(x_i^2 - 1) - U_{n-1}^{(l)}(x_{i}^2 - 1)), $$
$$w_{i+1} = x_{i+1}y_i + U_{m-1}^{(l)}y_{i-1}. $$

Eqs. (2.22)–(2.25) are quite different from Eqs. (2.18)–(2.21) above. The corresponding aperiodic sequences show rather different physical properties. We also point out that the trace and antitrace maps for the sequences FC(m, k) are given by Eqs. (2.22)–(2.25) since they have the same inflation scheme.

Eliminating the subsidiary variables $v_i$ and $w_i$ in Eqs. (2.14)–(2.17) for the general case FS(m, n), we obtain

$$x_{i+1} = \frac{U_m^{(l)}U_{n}^{(l-1)}}{U_{n}^{(l-1)}} \left( U_{n+1}^{(l)}x_i - U_{n+2}^{(l)}x_{i-1} + U_{n-1}^{(l)}y_{i-1} \right),$$
$$y_{i+1} = \frac{U_m^{(l)}U_{n}^{(l-1)}}{U_{n}^{(l-1)}} \left( U_{n+1}^{(l)}y_i - U_{n+2}^{(l)}y_{i-1} + U_{n-1}^{(l)}y_{i-1} \right).$$

Here, we used Eq. (A.3) to simplify the result. The above two equations are alternative forms of the trace and the antitrace map.

Again, for the special cases $m = 1$ or $n = 1$, these equations simplify. For FS(1, n), we find

$$x_{i+1} = U_n^{(l)}(x_i^2 - 1) + U_{n+1}^{(l)}x_i,$$
$$y_{i+1} = U_n^{(l)}(x_i^2 - 1) - U_{n+1}^{(l)}x_i,$$

The result for FS(m, 1) reads

$$x_{i+1} = \frac{U_m^{(l)}}{U_{m+1}^{(l)}} \left( U_{m+1}^{(l)}x_i - x_{i-2} \right) - U_{m-1}^{(l)}x_{i-1}.$$

For FS(1, 1), Eqs. (2.26)–(2.31) reduce to Eqs. (2.10) and (2.11), as expected. For some other special values of $m$ and $n$, the trace and antitrace maps of FS(m, n) are given in Appendix B.

\section*{B. Generalized Thue-Morse sequences}

Another type of aperiodic sequence is the celebrated TMS and its generalizations. Here, we consider generalized sequences TMS(m, n) with inflation scheme

$$b \rightarrow b^m a^n, \quad a \rightarrow a^n b^m. $$

Equivalently, TMS(m, n) can be constructed as

$$S_0 = b, \quad S_0 = a,$$

$$S_{i+1} = S_i^m S_i^n, \quad S_{i+1} = S_i^m S_i^n. $$

For $m = n = 1$, this reduces to the standard TMS. The recursion relation for transfer matrices of TMS(m, n) reads

$$A_{i+1} = B_i^m A_i^n, \quad B_{i+1} = A_i^m B_i^n$$

where $A_0$ is the matrix corresponding to the building block $b$, and $B_0$ corresponds to $a$, respectively. Using the same method as above, we get

$$x_{i+1} = U_n^{(l)}(U_{m+1}^{(l)}v_i - U_{m+2}^{(l)}v_{i-1} - U_{m+1}^{(l)}v_{i-1} - U_{m+2}^{(l)}v_{i-2}),$$
$$y_{i+1} = U_n^{(l)}(U_{m+1}^{(l)}y_i - U_{m+2}^{(l)}y_{i-1} - U_{m+1}^{(l)}y_{i-1} - U_{m+2}^{(l)}y_{i-2}).$$

where $v_i = x_{B_i A_i}$. These two equations determine the trace map.

It is somewhat more complicated to derive the antitrace map because $y_{A_i} \neq y_{B_i}$. We define $y_i = y_{A_i}$ and $\tilde{y}_i = y_{B_i}$. Then, from Eqs. (2.26), (A.4), (A.12), and (A.13), we have

$$y_{i+1} = U_n^{(l)}(U_{m+1}^{(l)}w_i - U_{m+2}^{(l)}w_{i-1} - U_{m+1}^{(l)}w_{i-1} - U_{m+2}^{(l)}w_{i-2}),$$
$$\tilde{y}_{i+1} = U_n^{(l)}(U_{m+1}^{(l)}\tilde{w}_i - U_{m+2}^{(l)}\tilde{w}_{i-1} - U_{m+1}^{(l)}\tilde{w}_{i-1} - U_{m+2}^{(l)}\tilde{w}_{i-2}),$$

$$w_{i+1} = \left( U_{m+1}^{(l)}v_i - U_{m+2}^{(l)}v_{i-1} - U_{m+1}^{(l)}v_{i-1} - U_{m+2}^{(l)}v_{i-2}) - U_{m+1}^{(l)}v_{i-1} - U_{m+2}^{(l)}v_{i-2} \right),$$

$$\tilde{w}_{i+1} = \left( U_{m+1}^{(l)}\tilde{v}_i - U_{m+2}^{(l)}\tilde{v}_{i-1} - U_{m+1}^{(l)}\tilde{v}_{i-1} - U_{m+2}^{(l)}\tilde{v}_{i-2}) - U_{m+1}^{(l)}\tilde{v}_{i-1} - U_{m+2}^{(l)}\tilde{v}_{i-2} \right).$$
Here, \( w_l = y_{B_lA_l} \) and \( \tilde{w}_l = y_{A_lB_l} \). The antitrace map is completely determined by Eqs. (2.35)-(2.40).

For \( n = 1 \) and \( m = 1 \), Eqs. (2.35)-(2.40) reduce to

\[
\begin{align*}
    x_{l+1} &= v_l, \\
v_{l+1} &= x_l^2(v_l - 2) + 2, \\
y_{l+1} &= w_l, \\
\tilde{y}_{l+1} &= \tilde{w}_l, \\
w_{l+1} &= x_l[(x_{l+1} - 1)y_l + \tilde{y}_l], \\
\tilde{w}_{l+1} &= x_l[(x_{l+1} - 1)\tilde{y}_l + y_l].
\end{align*}
\]

This yields the well-known trace map of the TMS

\[
x_{l+1} = x_{l-1}^2(x_l - 2) + 2,
\]

and the antitrace map

\[
\begin{align*}
v_{l+1} &= x_{l-1}[(x_l - 1)y_{l-1} + \tilde{y}_{l-1}], \\
\tilde{y}_{l+1} &= x_{l-1}[(x_l - 1)\tilde{y}_{l-1} + y_{l-1}].
\end{align*}
\]

The above two equations give

\[
y_{l+1} = x_{l-1}[(x_l + x_{l-2} - 2)y_{l-1} + x_{l-3}x_{l-2}(2 - x_{l-2})y_{l-3}]
\]

which is an alternative form of the antitrace map.

From Eqs. (2.35)-(2.40), we can solve for the subsidiary quantities \( v_l, w_l, \) and \( \tilde{w}_l \), for instance,

\[
v_{l+1} = \frac{U_{m}^{(l)}U_{m+2}^{(l)}}{U_{m+1}^{(l)}} x_l + U_{m-1}^{(l)} \left( U_{m}^{(l-1)} x_l - U_{m-1}^{(l-1)} \right) + U_{m-2}^{(l)} \left( U_{m-1}^{(l)} x_l - U_{m-2}^{(l)} \right) - U_{m-3}^{(l)} \left( U_{m-2}^{(l)} x_l - U_{m-3}^{(l)} \right).
\]

The combination of Eqs. (2.35) and (2.51) gives an alternative form of the trace map of TMS(\( m, n \)).

### III. Arbitrary Substitution Sequences

As there exist trace maps for arbitrary substitution sequences, \[
A_1, A_2, \ldots, A_n
\]
one natural question is whether antitrace maps also exist for arbitrary sequences. The answer is affirmative. We commence our argument in analogy with the discussion in Ref. [22] and restrict ourselves to the case of unimodular matrices.

Let \( A_1, A_2, \ldots, A_n \) be \( 2 \times 2 \) matrices and define the following \( 2^n \) matrices

\[
B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r} = A_1^{\epsilon_1} A_2^{\epsilon_2} \ldots A_r^{\epsilon_r}
\]

where each coefficient is a polynomial in the traces \( x_{A_j} \), \( 1 \leq j \leq r \). Then, from Eq. (3.3), any monomial \( A_{j_1} A_{j_2} \ldots A_{j_s} \), with \( 1 \leq j_i \leq r \) and \( 1 \leq i \leq s \), can be written as a linear combination of the matrices \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r} \), namely,

\[
A_{j_1} A_{j_2} \ldots A_{j_s} = \sum_{\epsilon_1=0}^{1} \sum_{\epsilon_2=0}^{1} \cdots \sum_{\epsilon_r=0}^{1} c_{\epsilon_1 \epsilon_2 \ldots \epsilon_r} B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r}
\]

where each coefficient is a polynomial in the traces \( x_{A_j} \), \( 1 \leq j \leq r \), and the traces \( x_{A_i A_k} \), \( 1 \leq j < k \leq r \).

This result not only yields the trace map, but also gives the antitrace map for any substitution sequence. We define

\[
B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l} = A_1^{\epsilon_1} A_2^{\epsilon_2} \ldots A_r^{\epsilon_r}
\]

with \( \epsilon_j \in \{0, 1\} \), \( 1 \leq j \leq r \), and \( l \geq 0 \), where \( A_{jl} \) is the unimodular \( 2 \times 2 \) matrix associated to the \( l \)-th iterate of the \( j \)-th letter. Since each matrix in \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l+1} \) is, by definition, a monomial in the matrices \( A_{jl} \), they can be expanded in terms of the matrices \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l} \) according to (3.2). Then the trace of \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l+1} \) is a polynomial in the \( 2^r - 1 \) traces of \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l} \), and the antitrace of \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l+1} \) is a polynomial in the \( 2^r - 1 \) antitraces of \( B_{\epsilon_1 \epsilon_2 \ldots \epsilon_r, l} \). Therefore, we conclude that both the trace and antitrace maps exist for arbitrary substitution sequences, and the dimension of the antitrace map is \( 2^n - 1 \).

Next, we present a concrete example to illustrate this conclusion.

The Rudin-Shapiro sequence can be defined by means of a substitution rule on four letters. The substitution rule is

\[
\begin{align*}
    a &\rightarrow ac, \\
b &\rightarrow dc, \\
c &\rightarrow ab, \\
d &\rightarrow db,
\end{align*}
\]

and the corresponding matrix recursion relations are

\[
\begin{align*}
    A_{t+1} &= C_t A_t, \\
    B_{t+1} &= C_t D_t, \\
    C_{t+1} &= B_t A_t, \\
    D_{t+1} &= B_t D_t.
\end{align*}
\]

We have the useful relation

\[
D_t = C_t A_t^{-1} B_t
\]

which effectively reduces the sequence to three basic letters. Now, we choose the seven matrices \( A_t, B_t, C_t, D_t, A_t C_t, A_t B_t, \) and \( B_t C_t \) as our basic set of matrices.
In what follows, we denote the traces and antitraces by
\[ a_t = x_{A_t}, \quad b_t = x_{B_t}, \quad c_t = x_{C_t}, \quad d_t = x_{D_t}, \]
\[ e_t = x_{A_tC_t}, \quad f_t = x_{A_tB_t}, \quad g_t = x_{B_tC_t}, \]
\[ \tilde{a}_t = y_{A_t}, \quad \tilde{b}_t = y_{B_t}, \quad \tilde{c}_t = y_{C_t}, \quad \tilde{d}_t = y_{D_t}, \]
\[ \tilde{e}_t = y_{A_tC_t}, \quad \tilde{f}_t = y_{A_tC_t}, \quad \tilde{g}_t = y_{B_tC_t}. \] (3.7)

By using Eqs. (A.3) and (A.12), we obtain
\[ A_{t+1} = C_tA_t, \]
\[ B_{t+1} = c_tD_t - a_TB_t + A_tB_t, \]
\[ C_{t+1} = B_tA_t, \]
\[ D_{t+1} = (a_tg_t - c_df_t)B_t - c_tD_t + b_tD_t \]
\[ + (f_t - a_tB_t)C_tA_t, \]
\[ A_{t+1}C_{t+1} = f_tC_tA_t - b_tC_t + C_tC_t, \]
\[ A_{t+1}B_{t+1} = a_t[(1 - a_t^2)B_t + c_tD_t + a_TB_tC_t] \]
\[ - C_tC_tB_t, \]
\[ B_{t+1}C_{t+1} = b_tC_t[(f_ta_t - a_t^2b_t + b_t)C_t] \]
\[ + a_tD_t - C_tC_tB_t - (f_t - a_tB_t)C_tC_tA_t \]
\[ - b_tC_t[(f_t - a_tB_t)(a_tI - A_t) \]
\[ + b_tI + (a_t^2 - 1)B_t - a_TB_tC_t \]
\[ - c_tC_t + I. \] (3.8)

Note that the order of multiplication of two matrices on the right-hand sides of these equations may differ from the order of our basic matrix products \( A_tC_t, A_tC_t, \) or \( B_tC_t. \) We can use Eq. (A.3) to reverse the order to obtain a systems of equations that closes with our seven basic matrices.

Now, from Eq. (3.3) and (A.4), the trace and antitrace maps are obtained as
\[ a_{t+1} = e_t, \]
\[ b_{t+1} = c_tD_t - a_TB_t + f_t, \]
\[ c_{t+1} = f_t, \]
\[ d_{t+1} = b_tD_t - a_TC_t + e_t, \]
\[ e_{t+1} = c_tD_t - b_tC_t + g_t, \]
\[ f_{t+1} = c_tD_t - a_t^2b_t + a_TB_t + b_t - g_t, \]
\[ g_{t+1} = b_tC_t(a_tC_tf_t - c_tD_t - a_t^2b_tC_t + a_TB_tC_t + b_tC_t) \]
\[ + a_tD_t + g_t - b_t^2 - c_t^2 + 2, \]
\[ \tilde{a}_{t+1} = c_tD_t + a_tC_t - \tilde{e}_t, \]
\[ \tilde{b}_{t+1} = c_tD_t - a_tC_t + \tilde{f}_t, \]
\[ \tilde{c}_{t+1} = b_tD_t - a_tC_t + \tilde{g}_t, \]
\[ \tilde{d}_{t+1} = (a_tg_t - a_TB_tC_t)\tilde{b}_t + \tilde{b_tD_t} - (g_t - b_tC_t)\tilde{f}_t \]
\[ + (f_t - a_TB_t)(\tilde{b_tC_t} - \tilde{g}_t) + a_tC_t - \tilde{e}_t, \]
\[ \tilde{e}_{t+1} = f_t(c_tD_t + a_tC_t - \tilde{e}_t) + c_tD_t - \tilde{g}_t, \]
\[ \tilde{f}_{t+1} = \tilde{c}_t(-a_t^2\tilde{b}_t + c_tD_t + \tilde{f}_t) - \tilde{b_tC_t} + \tilde{g}_t, \]
\[ \tilde{g}_{t+1} = b_t(1 - a_t^2)(\tilde{f}_t - aTB_t)\tilde{a}_t + b_t(1 - a_t^2 - c_t^2)\tilde{b}_t \]
\[ - c_tC_t + a_TB_tC_t\tilde{d}_t + b_tC_t(f_t - a_TB_t)\tilde{e}_t + a_TB_tC_t \tilde{f}_t \]
\[ + b_tC_t\tilde{g}_t. \] (3.9)

Thus, we derived the trace and antitrace maps of the Rudin-Shapiro sequence.

Now, we discuss the dimension of the antitrace map. Let \( A, B, \) and \( C \) be \( 2 \times 2 \) matrices. Then
\[ ABC = [(x_{ABC} - x_{AIBC} - x_{AIBC} + x_{AIBC})I \]
\[ + (x_{BC} - x_{BIBC})A - x_{ACB} \]
\[ + (x_{AB} - x_{ABIC})B \]
\[ + x_{CAB} + x_{BIBC} + x_{ABC}] / 2. \] (3.10)

Taking the trace on both sides of Eq. (3.10), we are led to a trivial identity. However, if we take the antitrace, we obtain
\[ y_{ABC} = [(x_{BC} - x_{BIBC})y_A - x_{ACB} \]
\[ + (x_{AB} - x_{ABIC})y_B \]
\[ + x_{CAB} + x_{BIBC} + x_{ABC}] / 2. \] (3.11)

The antitrace of any monomial can be written as a linear combination of the antitraces \( y_{A_{j,k}}, 1 \leq j \leq r, \) and the antitraces \( y_{A_{j,k}}, 1 \leq j < k \leq r. \) Each coefficient is a polynomial in the traces \( x_{A_{j,k}}, 1 \leq j \leq r \) and the traces \( x_{A_{j,k}}, 1 \leq j < k \leq r. \) From this observation we conclude that the dimension of our antitrace map is \( r(r + 1)/2, \) i.e., the dimension is reduced from \( 2^r - 1. \) Here, for the dimension of the antitrace map, do not take into account the dimension of the trace map, which enters the coefficients of the antitrace map. Thus, the full dimension of the trace and antitrace map is given by the sum of their respective dimensions.

Let us consider two ternary sequences as examples.

Our first example of a three-letter substitution rule and a corresponding recursion relation for the transfer matrices is
\[ a \rightarrow b, \quad b \rightarrow c, \quad c \rightarrow ca, \]
\[ A_{t+1} = B_t, \quad B_{t+1} = C_t, \quad C_{t+1} = A_tC_t. \] (3.12)

Using Eqs. (A.10) and (A.12), we obtain
\[ A_{t+1} = B_t, \]
\[ B_{t+1} = C_t, \]
\[ C_{t+1} = A_tC_t, \]
\[ B_{t+1}A_{t+1} = C_tC_t, \]
\[ C_{t+1}B_{t+1} = x_tC_tA_tC_t - A_t, \]
\[ A_{t+1}C_{t+1} = B_tC_tC_t, \]
\[ B_{t+1}A_{t+1}C_{t+1} = B_tC_tC_t + x_{BC}A_tC_tC_t - x_{ABC}I. \] (3.13)

Taking the trace of the above equation, we obtain the trace map. The dimension of the trace map is \( 2^3 - 1 = 7. \)

Taking the antitrace of the sixth line of the above equation, we can expand it according to Eq. (5.11). Therefore, the last equality in Eq. (3.13) is not necessary, and the dimension of the antitrace map is \( 3(3 + 1)/2 = 6. \)
Our second example is the three-component FS generated by

\[ a \to b, \quad b \to c, \quad c \to abc, \]

\[ A_{l+1} = B_l, \quad B_{l+1} = C_l, \quad C_{l+1} = C_l B_l A_l. \quad (3.14) \]

The corresponding maps for the matrices are

\[ A_{l+1} = B_l, \]
\[ B_{l+1} = C_l, \]
\[ C_{l+1} = C_l B_l A_l, \]
\[ B_{l+1} A_{l+1} = C_l B_l, \]
\[ C_{l+1} B_{l+1} = B_l A_l - x_{B_l A_l} I + x_{C_l B_l A_l} C_l, \]
\[ C_{l+1} B_{l+1} A_{l+1} = A_l - x_{A_l} I + x_{C_l B_l A_l} C_l B_l. \quad (3.15) \]

We see that, for this particular sequence, both the trace and antitrace maps are six-dimensional.

IV. MAPS FOR MATRIX ELEMENTS

As discussed in Sec. [1], we need to know all elements of the global transfer matrix in order to compute certain physical quantities. Thus, the trace and antitrace maps may not be sufficient, and one would like to determine analogous maps for each of the matrix elements.

Actually, from Eq. (3.3), we know that such matrix element maps exist for any substitution rule, and Eqs. (3.8), (3.12), and (3.13) already contain examples of matrix element maps. Now, we investigate the maps for the matrix elements of the FS(\(m, n\)) and TMS(\(m, n\)).

Using Eqs. (3.4), (3.12), and (3.13), we obtain the matrix maps of FS(\(m, n\)) as

\[ M_{l+1} = U^{(l-1)}_{m-1} M_l + U^{(l)}_{m-1} A_l + (x_{l} - U^{(l-1)}_{m-1}) A_l - U^{(l)}_{m-2} A_{l-1} + U^{(l-1)}_{m-1} A_{l-1}. \]

(4.1)

where \(M_l = A_{l-1} A_l\). The traces \(v_{l+1}\) and \(v_{l+1}\) appearing on the right-hand side of Eq. (4.1) are given in terms of \(v_{l}\) via Eqs. (2.14) and (2.15), respectively.

Similarly, the matrix map of TMS(\(m, n\)) is obtained as

\[ A_{l+1} = U^{(l)}_{m} \left( U^{(l)}_{m} N_l - U^{(l)}_{m-1} B_l \right) - U^{(l-1)}_{m} \left( U^{(l)}_{m} A_l - U^{(l)}_{m-1} I \right), \]

\[ B_{l+1} = U^{(l)}_{m} \left( U^{(l)}_{m} \tilde{N}_l - U^{(l)}_{m-1} B_l \right) - U^{(l-1)}_{m} \left( U^{(l)}_{m} A_l - U^{(l)}_{m-1} I \right), \]

\[ N_{l+1} = \left( U^{(l)}_{m} U^{(l)}_{m} v_l - U^{(l)}_{m-1} U^{(l)}_{m+1} \right) - U^{(l)}_{m+1} \left( U^{(l)}_{m} A_l - U^{(l)}_{m-1} I \right). \]

(4.2)

(4.3)

(4.4)

\[ \tilde{N}_{l+1} = \left( U^{(l)}_{m} U^{(l)}_{m} v_l - U^{(l)}_{m-1} U^{(l)}_{m+1} \right) - U^{(l)}_{m+1} \left( U^{(l)}_{m} B_l - U^{(l)}_{m-1} I \right) \]

\[ + U^{(l)}_{m} A_l - U^{(l)}_{m-1} I, \]

where \(N_l = B_l A_l\) and \(\tilde{N}_l = A_l B_l\). We can eliminate the subsidiary matrices \(M_l, N_l,\) and \(\tilde{N}_l\) from Eqs. (4.12) and (4.13) and (4.14). For example, Eq. (4.11) becomes

\[ M_l = \frac{1}{U^{(l)}_{m}} \left( U^{(l-1)}_{m-1} A_l + U^{(l-2)}_{l-2} A_{l-2} - U^{(l-2)}_{m-1} I \right) + v_l A_{l-1} I + x_l A_{l-1}. \]

(4.6)

Thus, we obtain another form of the matrix map of FS(\(m, n\)) given by Eqs. (2.12) and (4.6).

For \(m = n = 1\), Eqs. (2.12) and (4.6) reduce to

\[ A_{l+1} = (x_{l+1} - x_l) A_{l-1} + B_{l-1} + x_l x_{l-1}. \]

(4.7)

This is the matrix map of the FS. For the TMS, we find from Eqs. (4.12) and (4.5) for \(m = n = 1\)

\[ A_{l+1} = x_{l-1} [x_{l-1} A_{l-1} + B_{l-1} - x_l x_{l-1} I] + x_l A_{l-1} + x_{l-1} I, \]

(4.8)

\[ B_{l+1} = x_{l-1} [x_{l-1} B_{l-1} + A_{l-1} - x_l x_{l-1} I] + x_l A_{l-1} + x_{l-1} I. \]

(4.9)

The maps for the matrix elements are easily obtained from the matrix map, thus we do not give them explicitly.

Specifically, we consider the FS. From Eq. (4.7), it is interesting to find that the maps for the non-diagonal elements, and for the difference of the diagonal elements, coincide with the antitrace map, Eq. (2.12). From Eqs. (4.3) and (4.9), this fact also holds for the TMS. Actually, as again follows from Eq. (3.2), we arrive at the important conclusion that the maps for the antitrace, the non-diagonal elements, and the difference of the diagonal elements are all the same for arbitrary substitution rules. This means that the knowledge of the trace and antitrace maps suffices to compute any physical quantities related to the global transfer matrix.

V. APPLICATIONS

We now turn our attention to applications of the dynamical map method developed in this paper. In what follows, we are going to consider three examples.

A. Optical Multilayers

As our first example, we show how to use the antitrace map to calculate light transmission coefficients.

The transmission of light through aperiodic multilayers arranged according to the FS [28] the “non-Fibonacci”
quasiperiodic multilayers as optical switches and memo-

by Huang et al. and Yang et al. found an interesting switch-like property in the light transmission through a FC(m) multilayer.

Using the antitrace map, we re-investigate the light transmission through FC(m) which is sandwiched by two media of type b. In analogy with the discussion of Ref. 19, we write the corresponding transfer matrices as

\[ A_1 = P_b, \]
\[ A_2 = P_b^{m-1} P_a P_a P_{ab}, \]
\[ A_{i+1} = A_i^m A_{i-1}. \] (5.1)

The recursion relation for the transfer matrix (5.1) is a sequence, and the corresponding transfer matrices as in Table I, also show this periodicity. The initial conditions, given in Table II, also show this periodicity. The initial conditions for FC(2q), q = 1, 2, 3, . . . , or for FC(2q + 1), only differ by the sign of the parameter R. Thus, it is natural to divide the FC(m) into two classes, FC(2q) and FC(2q + 1).

From the initial conditions and recursion equations, we can directly obtain the trace, the antitrace and the transmission coefficients of FC(2q), which are given in Table III. It can be seen that the trace and the antitrace vanish alternately. The trace shows periodicity with period four for odd values of q, and period two for even q, but the antitrace shows no periodicity. Thus, the transmission coefficient also is not periodic in l. For even l, the transmission coefficient does not depend on m. However, for odd l, the transmission coefficient depends on m and l, see Table III.

Table III shows the results for FC(2q + 1). In this case, the trace, the antitrace and the transmission coefficient are periodic in l with period six. The transmission coefficients are the same for l = 2, l = 3, and l = 6 and do not depend on m. We find that the multilayer is transparent for \( l = 6i + 1, i = 0, 1, 2, . . . \).

Here, we not only recover the recent results of Ref. 19, but also give a natural classification of FC(m) and derive the periodicities of the trace and antitrace maps.

### B. Harmonic Chains

As our second example, we show how to apply the map for the matrix elements to calculate some physical quantities for a harmonically coupled Fibonacci chain. The transmission coefficient and the Lyapunov exponent were already given in Eqs. (1.4) and (1.8). We know the trace (2.10) and antitrace maps (2.11) for this system. In order to determine the transmission coefficient, we additionally need to know the map for the difference \( z_l \) of the diagonal elements in Eq. (1.7). As discussed in Sec. IV, the map for \( z_l \) is the same as the map for the antitrace \( y_l \).

Now, this leaves us with the problem to determine the initial conditions. By a so-called transfer matrix “renormalization” the transfer matrix product can be re-written in terms of “renormalized” transfer matrices such that these are arranged according to the FS. Following the discussion in Ref. [21], we choose a special value of parameters

\[ \Omega = \frac{\alpha - 2\beta + 1}{\alpha(1 - \beta)} = \frac{m_a \omega^2}{K_{ab}} \] (5.8)

where \( \alpha = m_b / m_a \) and \( \beta = K_a / K_{ab} \). The first two renormalized transfer matrices are

\[ A_1 = \begin{pmatrix} 1 & 0 \\ \eta_1 & 1 \end{pmatrix}, \]
the trace map is periodic in \( \eta \) where

\[
A_2 = \begin{pmatrix} -1 & 0 \\ \eta_2 & -1 \end{pmatrix},
\]

(5.9)

where \( \eta_1 = 2(\alpha - 2) \) and \( \eta_2 = 2(1 - \alpha) \). Note that these two matrices commute with each other for arbitrary values of \( \eta_1 \) and \( \eta_2 \). From this equation, we obtain

\[
A_3 = A_1 A_2 = \begin{pmatrix} -1 & 0 \\ \eta_2 - \eta_1 & -1 \end{pmatrix}.
\]

(5.10)

Thus, the initial conditions are given by

\[
x_1 = 2, \quad x_2 = -2, \quad x_3 = -2,
\]

\[
y_1 = \eta_1, \quad y_2 = \eta_2, \quad y_3 = \eta_2 - \eta_1,
\]

\[
z_1 = z_2 = z_3 = 0.
\]

(5.11)

From the antitrace map (2.11), we find that \( z_1 = 0 \) for all \( l \). Using the trace map (2.11), we easily obtain \( x_{3l+1} = 2, \ x_{3l+2} = -2, \) and \( x_{3l} = -2 \). That is, the trace map is periodic in \( l \) with period three. Then, from Eqs. (1.7) and (1.8), the transmission coefficient and the Lyapunov exponent have the simple forms

\[
t_l^{-1} = 1 + \frac{y_l^2}{4 \sin^2 k},
\]

(5.12)

\[
\Gamma_l = N^{-1} \ln(y_l^2 + 2).
\]

(5.13)

From the initial conditions for \( y_l \) and the antitrace map (2.11), we easily find that the modulus of \( y_l \) is

\[
|y_l| = |F_l \eta_2 - F_{l-1} \eta_1|, \quad l \geq 3,
\]

(5.14)

where \( F_l \) denotes the Fibonacci number defined by the recursion \( F_l = F_{l-1} + F_{l-2} \) with \( F_0 = 1 \).

Finally, the transmission coefficient and the Lyapunov exponent are obtained as

\[
t_l^{-1} = 1 + \frac{\left( F_l \eta_2 - F_{l-1} \eta_1 \right)^2}{4 \sin^2 k},
\]

(5.15)

\[
\Gamma_l = N^{-1} \ln[(F_l \eta_2 - F_{l-1} \eta_1)^2 + 2].
\]

(5.16)

Thus, using our matrix element maps, we have re-derived the result of Ref. [1].

### C. Electronic systems

We now apply the trace and antitrace method to the transmission problem in electronic systems for the examples of the FS and the TMS. In what follows, we choose the parameters as \( \epsilon_a = -\epsilon_b = \epsilon, \ t_{ab} = 1, \) and \( t_{aa} = t_{bb} = t \).

\[ \text{1. Fibonacci sequence} \]

For the FS, there are actually four different local transfer matrices \( M_n \) [4], because the hopping matrix elements depend on three subsequent letters in the FS. Nevertheless, the transfer matrix product can be re-written in terms of two matrices

\[
M_b = \begin{pmatrix} E - \epsilon & -1 \\ 1 & 0 \end{pmatrix}, \quad M_a = \begin{pmatrix} E - \epsilon & -t \\ 1 & 0 \end{pmatrix} \times \begin{pmatrix} E + \epsilon & -1 \\ 1 & 0 \end{pmatrix},
\]

(5.17)

such that the resulting transfer matrix product is again arranged according to the Fibonacci sequence.

For the trace and antitrace maps, we only need to know the first three matrices \( A_1 = M_a, \ A_2 = M_b M_a, \) and \( A_3 = M_a M_b M_a \). From Eq. (5.17), these matrices and thus the initial conditions are easily obtained. In order to obtain an analytical result, we restrict ourselves to the case \( E = \epsilon = 0 \). For this particular choice of parameters, Eq. (1.10) simplifies to

\[
t_l = \frac{4}{x_l^2 + y_l^2},
\]

(5.18)

which is formally the same as Eq. (1.4). The initial conditions become

\[
x_1 = 0, \quad x_2 = 0, \quad x_3 = 2,
\]

\[
y_1 = -t - 1/t, \quad y_2 = t + 1/t, \quad y_3 = 0.
\]

(5.19)

From the trace and antitrace map equations (2.10)–(2.11) for the FS, we can easily find that both the trace \( t_l \) and the antitrace \( y_l \) are periodic in \( l \) with period six. In one period the traces are \( 0, 0, 0, 0, -2, \) and the antitraces are \( -t-1/t, t+1/t, 0, t+1/t, t+1/t, 0 \). From Eq. (5.18), we deduce that the transmission coefficient \( t_l \) is periodic in \( l \) with period three. For one period, the transmission coefficients are given by \( 4/(t+1/t)^2, 4/(t+1/t)^2, \) and \( 1 \). If the hopping parameter \( t = 1 \), the transmission coefficient \( t_l = 1 \) for all values of \( l \), which is the trivial (periodic) case. Next we consider the electronic transmission for the TMS.

\[ \text{2. Thue-Morse sequence} \]

We consider the on-site model for the TMS, i.e., the hopping parameter \( t = 1 \). So there are only two kinds of transfer matrices

\[
B_0 = \begin{pmatrix} E + \epsilon & -1 \\ 1 & 0 \end{pmatrix}, \quad A_0 = \begin{pmatrix} E - \epsilon & -1 \\ 1 & 0 \end{pmatrix}.
\]

(5.20)

From these, we can calculate the matrices \( A_1, B_1, A_2, \) and \( B_2, \) and thus the initial conditions for the trace and antitrace map. Again, in order to obtain an analytical result, we limit ourselves to the case where the parameter \( \epsilon \) and the energy \( E \) fulfill a particular relation, \( E = \sqrt{2 + \epsilon^2} \). In this case, the initial conditions become

\[
x_0 = \sqrt{2 + \epsilon^2} - \epsilon, \quad x_1 = 0, \quad x_2 = -2 - 4\epsilon^2,
\]

9
\[ y_0 = \tilde{y}_0 = 2, \quad y_1 = \tilde{y}_1 = 2\sqrt{2 + 2\epsilon^2}, \quad y_2 = -\tilde{y}_2 = 4\epsilon, \]
\[ z_0 = \sqrt{2 + 2\epsilon^2} - \epsilon, \quad \tilde{z}_0 = \sqrt{2 + 2\epsilon^2} + \epsilon, \]
\[ z_1 = \tilde{z}_1 = 2, \quad z_2 = -\tilde{z}_2 = 4\epsilon\sqrt{2 + 2\epsilon^2}, \quad (5.21) \]

where \( z_l = (A_l)_{11} - (A_l)_{22} \) and \( \tilde{z}_l = (B_l)_{11} - (B_l)_{22} \). From Eq. (2.47), we deduce that the traces \( x_l = 2 \) for all \( l \geq 3 \). From the antitrace map equations (2.48)–(2.49) and the above initial conditions, we easily find that \( y_l = \tilde{z}_l = 0 \) for \( l \geq 3 \). Thus, we obtain the result that the transmission coefficient \( t_l = 1 \) for \( l \geq 3 \). For \( l = 1 \) and \( l = 2 \), the transmission coefficients are given by \( t_1 = (2 - \epsilon^2)/(2 + \epsilon^2) \) and \( t_2 = (2 - \epsilon^2)/(2 + 7\epsilon^2 + 4\epsilon^4) \), respectively.

The examples considered here show that trace and antitrace maps provide a convenient tool for the computation of physical quantities related to the global transfer matrices of aperiodic substitution systems. In the applications presented above, we mainly concentrated on obtaining analytical results, and therefore had to restrict the discussion to specific values of the parameters. The trace and antitrace map equations, of course, are not restricted to these cases, but there will be no simple closed-form solutions to the recursion relations in general. The particular parameter values considered above correspond to periodic orbits of the associated dynamical systems. These cases, and probably all examples where simple solutions exist, share the property that, at a certain stage, different transfer matrices commute with each other, and thus are simultaneously diagonalizable. This also explains why these systems turn out to be transparent, because it does not matter in which order one multiplies matrices that commute with each other. In spite of these comments, the method presented here is expedient and useful for the investigation of physical systems built on aperiodic substitution sequences, because the trace and antitrace map equations can very efficiently be used in numerical investigations of large, but finite, systems.

VI. CONCLUSIONS

In conclusion, we have extended the well-studied trace-map method for the investigation of aperiodic substitution systems by considering corresponding maps for the antitrace and the matrix elements of the transfer matrices. Our main results are the following.

Firstly, we obtained the trace and antitrace maps for various aperiodic sequences, such as generalized FSs and TMSs, the periodic-doubling sequence, examples of ternary sequences, and the four-letter Rudin-Shapiro sequence. The dimension of the dynamical systems defined by the trace map and our antitrace maps is \( r(r+1)/2 \) plus the dimension of the trace map itself, where \( r \) denotes the number of basic letters in the aperiodic sequence. Secondly, we showed that trace and antitrace maps can be constructed for arbitrary substitution rules. Thirdly, we introduced analogous maps for specific matrix elements of the transfer matrix, but it turns out that the maps for the off-diagonal elements and those for the difference of the diagonal elements coincide with the antitrace map. Thus, from the trace and antitrace map, we can determine any physical quantity related to the global transfer matrix of the system. Finally, as examples of applications of the trace and antitrace map method, we investigated the transmission problem for optical multilayers, harmonic chains, and electronic systems arranged according to the FS or the TMS.

The trace and antitrace map method developed here can be expected to have many applications in the study of one-dimensional aperiodic systems.

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APPENDIX A: RELATIONS FOR UNIMODULAR MATRICES

For convenience, we present a collection of relevant identities, which are used in the construction of the trace and antitrace maps in Secs. II, III, and IV.

The \( n \)th power of a unimodular 2x2 matrix \( A \) can be written as
\[ A^n = U_n(x_A)A - U_{n-1}(x_A)I, \quad (A.1) \]
where \( I \) is the unit matrix and
\[ U_n(x_A) = \frac{\lambda_+^n - \lambda_-^n}{\lambda_+ - \lambda_-}, \]
\[ \lambda_{\pm} = \frac{x_A \pm \sqrt{x_A^2 - 4}}{2}. \quad (A.2) \]

Here \( x_A \) and \( \lambda_{\pm} \) denote the trace and the two eigenvalues of \( A \), respectively, and \( \lambda_+ \lambda_- = \det A = 1 \). The functions \( U_n(x) \) are related to the Chebyshev polynomials of the second kind \( C_n(x) \) by \( U_n(x) = C_{n-1}(x/2) \). From the definition of the functions \( U_n(x) \), it follows
\[ U_{-1}(x) = -1, \quad U_0(x) = 0, \]
\[ U_1(x) = 1, \quad U_2(x) = x, \]
\[ U_3(x) = x^2 - 1, \quad U_4(x) = x^3 - 2x, \]
\[ U_{n+1}(x) = xU_n(x) - U_{n-1}(x), \]
\[ U_n^2(x) = U_{n+1}(x)U_{n-1}(x) + 1. \quad (A.3) \]

In order to study the antitrace maps, we need the following identity
\[ y_{AB} = x_B y_A + x_A y_B - y_{BA}. \quad (A.4) \]
for the antitraces of two unimodular $2 \times 2$ matrices $A$ and $B$. Now, we briefly prove this identity by introducing an auxiliary matrix

$$
\gamma = \begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix}, \quad \gamma^2 = -I, \quad \det(\gamma) = 1.
$$

(A.5)

For the matrix $A$, we have

$$
y_A = x_A \gamma.
$$

(A.6)

Then the antitrace of $AB$ is given by

$$
y_{AB} = x_{AB} \gamma = -x_\gamma A \gamma B.
$$

(A.7)

Let $A$, $B$, and $C$ be unimodular matrices. Then

$$
x_{ABAC} = x_{AB} x_{AC} + x_{BC} - x_B x_C.
$$

(A.8)

Applying the above identity to Eq. (A.7) and using Eq. (A.6) again, we obtain Eq. (A.4).

It should be pointed out that Eq. (A.4) is valid for any pair of $2 \times 2$ matrices, and it follows directly from the identity

$$
AB = (x_{AB} - x_A x_B) I + x_A B + x_B A - BA
$$

(A.9)

which holds for any pair of $2 \times 2$ matrices. The detailed proof of this identity can be found in Ref. [2]. Here, we only need to consider unimodular matrices.

For $n = 2$, Eq. (A.3) becomes

$$
A^2 = x_A A - I.
$$

(A.10)

This is the well-known Cayley-Hamilton theorem. From the theorem, we have

\begin{align*}
A + A^{-1} &= x_A I, \\
x_{A^{-1}} &= x_A, \\
x_{BA} + x_{BA^{-1}} &= x_A x_B, \\
y_{BA} + y_{BA^{-1}} &= x_A y_B.
\end{align*}

(A.11)

From Eqs. (A.9) and (A.11), we can prove the following useful relations

$$
BA = A - A x_A I + x_{AB} B = x_A B - A^{-1} B, \\
BA^{-1} B = (x_A x_B - x_{AB}) B - A.
$$

(A.12)

Finally, from Eqs. (A.1), (A.3), and (A.10), we obtain the following relations

\begin{align*}
x_{A^2} &= x_A^2 - 2, \\
x_{A^n} &= U_{n+1}(x_A) - U_{n-1}(x_A), \\
y_{A^2} &= x_{A^2} A, \\
y_{A^n} &= U_n(x_A) y_A.
\end{align*}

(A.13)

This completes our collection of identities.

**APPENDIX B: ANTITRACE MAPS FOR SOME METALLIC MEAN SEQUENCES**

The trace and antitrace maps for the golden mean and the copper mean sequences were discussed explicitly in the main part of this paper. Here, we give the trace and antitrace maps for some other prominent examples of metallic mean sequences.

From Eqs. (2.26), (2.27), and (A.3), the trace and antitrace maps for the silver mean case ($m = 2, n = 1$) are obtained as

$$
x_{l+1} = \frac{x_l}{x_{l-1}} [x_l (x_{l-1}^2 - 1) - x_{l-2}] - x_{l-1},
$$

(B.1)

$$
y_{l+1} = \frac{x_l}{x_{l-1}} [(y_{l-2} + y_l) + (x_l^2 - 1) y_{l-1}].
$$

(B.2)

For the bronze mean sequence ($m = 3, n = 1$), we find

$$
x_{l+1} = \frac{x_l^2 - 1}{x_{l-1}^2 - 1} [x_l (x_{l-1}^3 - 2x_{l-1} - x_{l-2})]
$$

(B.3)

$$
y_{l+1} = \frac{x_l^2 - 1}{x_{l-1}^2 - 1} (y_{l-2} + x_{l-1} y_l) + (x_l^3 - 2x_l) y_{l-1}.
$$

(B.4)

Finally, for the nickel mean case ($m = 1, n = 3$), the result reads

$$
x_{l+1} = \frac{x_l^2 - 1}{x_{l-1}^2 - 1} (x_l x_{l-1}^3 - x_{l-2}^3 + 3x_{l-2})
$$

(B.5)

$$
y_{l+1} = \frac{x_l^2 - 1}{x_{l-1}^2 - 1} (x_l^2 - 2) y_{l-2} + x_l (x_{l-1}^2 - 1) y_{l-1} - x_{l-1} y_l.
$$

(B.6)

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TABLE I. The initial conditions for the trace and antitrace map.

|   | $m = 1$ | $m = 2$ | $m = 3$ | $m = 4$ |
|---|---------|---------|---------|---------|
| $x_1$ | 0       | 0       | 0       | 0       |
| $x_2$ | 0       | $-g_1$  | 0       | $g_1$  |
| $v_2$ | $-g_1$  | 0       | $g_1$  | 0       |
| $y_1$ | 2       | 2       | 2       | 2       |
| $y_2$ | $g_1$  | 0       | $-g_1$ | 0       |
| $w_2$ | 0       | $-g_1$  | 0       | $g_1$  |

TABLE II. The trace, antitrace, and transmission coefficients for FC($m$) with $m = 2q$. The upper (lower) signs refer to even (odd) values of $q$.

| $l$ | $x_l$ | $y_l$ | $t_l$ |
|-----|-------|-------|-------|
| 1   | 0     | 2     | 1     |
| 2   | $\pm g_1$ | 0     | $4/g_1^2$ |
| 3   | 0     | $1/g_m$ | $4/g_m^2$ |
| 4   | $g_1$ | 0     | $4/g_1^2$ |
| 5   | 0     | $1/g_m$ | $4/g_m^2$ |
| 6   | $\pm g_1$ | 0     | $4/g_1^2$ |
| 7   | 0     | $1/g_m$ | $4/g_m^2$ |

TABLE III. The trace, antitrace, and transmission coefficients for FC($m$) with $m = 2q + 1$. The upper (lower) signs refer to even (odd) values of $q$.

| $l$ | $x_l$ | $y_l$ | $t_l$ |
|-----|-------|-------|-------|
| 1   | 0     | 2     | 1     |
| 2   | 0     | $1/g_1$ | $4/g_1^2$ |
| 3   | $-g_1$ | 0     | $4/g_1^2$ |
| 4   | 0     | $\mp 1/g_{m+1}$ | $4/g_{m+1}^2$ |
| 5   | 0     | $1/g_m$ | $4/g_m^2$ |
| 6   | $g_1$ | 0     | $4/g_1^2$ |