

Trace maps of general substitutional sequences

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It is shown that for arbitrary n , there exists a trace map for any n -letter substitutional sequence. Trace maps are explicitly obtained for the well-known circle and Rudin-Shapiro sequences which can be defined by means of substitution rules on three and four letters, respectively. The properties of the two trace maps and their consequences for various spectral properties are briefly discussed.

In this paper we will deal with deterministic one-dimensional (1D) chains generated by substitution rules acting on more than two letters or building blocks. We will concentrate on the study of a broad class of physical properties that can be described in terms of unimodular 2×2 transfer matrices (by unimodular we denote here a matrix with determinant equal to one). In the case of chains generated by two-letter substitution rules, such spectral properties have been studied successfully in terms of trace maps using a dynamical-systems-theory approach.¹⁻⁴ Ali and Gumbs⁵ found the trace map for a special three-letter substitutional sequence. Some doubts have appeared recently on whether such trace maps exist for substitutional sequences with four letters.⁶ Here we will show that trace maps do indeed exist for arbitrary substitutional sequences. We will also investigate two special cases in more detail.

An n -letter substitution rule can be written as

$$a_i \rightarrow \sigma_i(a_1, \dots, a_n); \quad i = 1, \dots, n. \tag{1}$$

Here $\sigma_i(a_1, \dots, a_n)$ are arbitrarily long strings consisting of arbitrary combinations of n letters a_i ($a_1 \equiv a$, $a_2 \equiv b$, $a_3 \equiv c$, ...). The letters can represent n different building blocks of a 1D chain or layered structure. We will define n canonical chains⁴ $A_{i,\infty} = \lim_{L \rightarrow \infty} A_{i,L}$, such that $A_{i,0} \equiv a_i$, and $A_{i,L+1}$ is obtained from $A_{i,L}$ by applying the substitutions of Eq. (1). $A_{i,L}$ serves as the unit cell of the L th periodic approximant of the i th infinite canonical chain $A_{i,\infty}$.¹ Clearly,

$$A_{i,L+1} = \sigma_i(A_{1,L}, \dots, A_{n,L}), \quad i = 1, \dots, n. \tag{2}$$

Let us assume that each building block a_i is associated with a unimodular transfer matrix \mathbf{a}_i . Then the whole L th generation chain $A_{i,L}$ is represented by a unimodular transfer matrix $\mathcal{M}_{i,L}$ such that $\mathcal{M}_{i,0} \equiv \mathbf{a}_i$ and $\mathcal{M}_{i,L+1} = \sigma_i^{(r)}(\mathcal{M}_{1,L}, \dots, \mathcal{M}_{n,L})$, $\sigma_i^{(r)}$ being the reversal of string σ_i . In the periodic approximant approach, the allowed energies (frequencies) of the i th chain are those satisfying the condition $|\text{Tr} \mathcal{M}_{i,L}| \leq 2$.¹

Allouche and Peyrière⁷ showed that for $n=2$, there always exists a trace map, or recursive relation, mapping $\text{Tr} \mathcal{M}_{i,L}$ into $\text{Tr} \mathcal{M}_{i,L+1}$. For unimodular transfer matrices

this map is at most three dimensional, and its calculation has been automated recently by Kolář and Ali.⁴ Their procedure can be generalized to arbitrary n . Let \mathbf{a} , \mathbf{b} , and \mathbf{c} be unimodular matrices. Then⁴

$$\text{Tr}(\mathbf{a}^{-1}\mathbf{b}) = \text{Tra Trb} - \text{Tr}(\mathbf{ab}), \tag{3}$$

$$\text{Tr}(\mathbf{a}^2\mathbf{b}) = \text{Tra Tr}(\mathbf{ab}) - \text{Trb}.$$

Writing $\mathbf{abac} = (\mathbf{ab})^2\mathbf{b}^{-1}\mathbf{c}$, one gets from Eq. (3) the relation

$$\text{Tr}(\mathbf{abac}) = \text{Tr}(\mathbf{ab})\text{Tr}(\mathbf{ac}) + \text{Tr}(\mathbf{bc}) - \text{Trb Trc}. \tag{4}$$

From Eq. (4), it now follows more or less directly that for every substitution rule of Eq. (1) there is a finite-dimensional trace map. Namely, repeatedly using Eq. (4), one can show that the trace of

$$\mathcal{P} = \prod_{j=1}^N \mathbf{m}_j,$$

where N is arbitrarily large, and each \mathbf{m}_j is identical with one of $\mathbf{a}_1, \dots, \mathbf{a}_n$ (mutually independent unimodular matrices) is

$$\text{Tr} \mathcal{P} = P(x_1, x_2, \dots, x_j). \tag{5}$$

Here P is a polynomial with integer coefficients, $x_j = \text{Tr} \mathbf{n}_j$, where \mathbf{n}_j are all mutually different "irreducible" products of the n matrices \mathbf{a}_i , such that each \mathbf{a}_i occurs in an \mathbf{n}_j no more than once, and $\text{Tr} \mathbf{n}_j \neq \text{Tr} \mathbf{n}_k$ for $j \neq k$. The number of such irreducible \mathbf{n}_j is equal to

$$J = \sum_{k=1}^n \binom{n}{k} \frac{k!}{k}.$$

If \mathcal{P} contains each \mathbf{a}_i no more than once, then $\text{Tr} \mathcal{P} = \text{Tr} \mathbf{n}_j$ for some j , and Eq. (5) evidently holds. Otherwise, there is an \mathbf{a}_{i_0} which occurs in \mathcal{P} at least twice. Using the invariance of the trace with respect to the cyclic permutations of a product of matrices, one can then transform $\text{Tr} \mathcal{P}$ to the form of the left-hand side of Eq. (4) with \mathbf{a}_{i_0} playing the role of \mathbf{a} . All the matrix products, the traces of which are taken on the right-hand side of Eq. (4), have the number of factors smaller by at least one less than \mathcal{P}

had. This process can be repeated until Eq. (5) is obtained. For $n=2$, we have the well-known values of $J=3$ and $n_j = a, b$, and ab .^{4,7} For $n=3$, $J=8$ and $n_j = a, b, c, ab, ac, bc, abc$, and acb . For $n=4$, $J=24$. J represents the maximum dimension of all trace maps for the given n . Substituting $a_i \rightarrow \mathcal{M}_{i,L}$ into n_j , the $x_{j,L} = \text{Tr}[n_j(\mathcal{M}_{i,L})]$ thus obtained represent suitable "trace coordinates" (cf. Refs. 1 and 4 for $n=2$). All $n_j(\mathcal{M}_{i,L+1})$ have the form of the product \mathcal{P} above, with $\mathcal{M}_{i,L}$ playing the role of a_i . Thus $x_{j,L+1}$ can be expressed in terms of $x_{j,L}$ by the relations of the type (5). These relations constitute the trace

$$\begin{aligned} a &\rightarrow cac, A_{L+1} = C_L A_L C_L, \mathcal{M}_{L+1} = \mathcal{O}_L \mathcal{M}_L \mathcal{O}_L, \\ b &\rightarrow accac, B_{L+1} = A_L C_L C_L A_L C_L, \mathcal{N}_{L+1} = \mathcal{O}_L \mathcal{M}_L \mathcal{O}_L^2 \mathcal{M}_L, \\ c &\rightarrow abcac, C_{L+1} = A_L B_L C_L A_L C_L, \mathcal{O}_{L+1} = \mathcal{O}_L \mathcal{M}_L \mathcal{O}_L \mathcal{N}_L \mathcal{M}_L. \end{aligned} \tag{6}$$

Because of the special form of these relations, we do not need all eight trace coordinates mentioned above for $n=3$. The following six coordinates will suffice:

$$\begin{aligned} x_L &= \text{Tr} \mathcal{M}_L, \quad s_L = \text{Tr}(\mathcal{O}_L \mathcal{M}_L), \\ y_L &= \text{Tr} \mathcal{N}_L, \quad u_L = \text{Tr}(\mathcal{N}_L \mathcal{M}_L), \\ z_L &= \text{Tr} \mathcal{O}_L, \quad w_L = \text{Tr}(\mathcal{M}_L \mathcal{O}_L \mathcal{N}_L). \end{aligned} \tag{7}$$

Then from Eq. (6) one gets

$$\begin{aligned} x_{L+1} &= \text{Tr} \mathcal{M}_{L+1} = \text{Tr}(\mathcal{O}_L^2 \mathcal{M}_L), \\ y_{L+1} &= \text{Tr} \mathcal{N}_{L+1} = \text{Tr}[(\mathcal{M}_L \mathcal{O}_L)^2 \mathcal{O}_L], \\ z_{L+1} &= \text{Tr} \mathcal{O}_{L+1} = \text{Tr}[(\mathcal{M}_L \mathcal{O}_L)^2 \mathcal{N}_L], \\ s_{L+1} &= \text{Tr}(\mathcal{O}_{L+1} \mathcal{M}_{L+1}) = \text{Tr}[(\mathcal{O}_L^2 \mathcal{M}_L)^2 \mathcal{O}_L \mathcal{N}_L \mathcal{M}_L \mathcal{O}_L^{-1}], \\ u_{L+1} &= \text{Tr}(\mathcal{N}_{L+1} \mathcal{M}_{L+1}) = \text{Tr}[(\mathcal{O}_L^2 \mathcal{M}_L)^2 \mathcal{O}_L \mathcal{M}_L], \\ w_{L+1} &= \text{Tr}(\mathcal{M}_{L+1} \mathcal{O}_{L+1} \mathcal{N}_{L+1}) \\ &= \text{Tr}\{[(\mathcal{M}_L \mathcal{O}_L)^2 \mathcal{O}_L]^2 \mathcal{M}_L \mathcal{O}_L \mathcal{N}_L\}. \end{aligned}$$

One can apply directly the second formula of Eq. (3) to all these expressions and obtain the 6D trace map,

$$\begin{aligned} x_{L+1} &= z_L s_L - x_L, \quad s_{L+1} = x_{L+1} z_{L+1} - u_L, \\ y_{L+1} &= s_L x_{L+1} - z_L, \quad u_{L+1} = x_{L+1} y_{L+1} - s_L, \\ z_{L+1} &= s_L w_L - y_L, \quad w_{L+1} = y_{L+1} s_{L+1} - w_L. \end{aligned} \tag{8}$$

It now would be easy to expand the right-hand sides of all these relations in terms of old trace coordinates x_L, y_L, z_L, s_L, u_L , and w_L , if so desired. This map is volume preserving (its Jacobian is identically equal to 1) and invertible. Thus every point (x, y, z, s, u, w) in the 6D trace space has exactly one predecessor. In these two properties the map of Eq. (8) resembles the trace map of the Fibonacci golden-mean sequence.¹ The quantity

$$I_c = y_L z_L + s_L u_L - x_L w_L \tag{9}$$

is an invariant of the map (8). There is no other polynomial invariant of degree less than or equal to 3. The 3D subspace ($z=y, u=s, w=ys-x$) is an invariant sub-

space of the circle map, and I_c in this subspace has the Fibonacci-like form $I_c = x^2 + y^2 + s^2 - xys$. The circle map in this subspace reduces to a 3D map (in coordinates x, y , and s) identical to the trace map of the two-letter substitution rule ($a \rightarrow bab, b \rightarrow ab^2ab$) (note that this corresponds, e.g., to $\mathcal{O}_0 \equiv \mathcal{N}_0$). This rule can be composed of three Fibonacci golden-mean rules, and it belongs to the class of quasi-PM (precious mean) rules whose trace maps have the same invariant as the Fibonacci map.⁴ As in the Fibonacci case, we can show that the interior of the central part of the $x^2 + y^2 + s^2 - xys = 4$ surface (in the above-mentioned 3D subspace) is an invariant continuous manifold of nonescaping initial points. A similar 3D nonescaping manifold exists in the subspace ($z=-y, s=-u, w=ys+x$) (e.g., $\mathcal{O}_0 \equiv -\mathcal{N}_0$). These seem to be just subsets of a 6D continuous manifold of nonescaping initial points near the origin: we have observed that if the initial point of map (8) is in the 6D cube of the unit edge centered at the origin, it seems to never escape to infinity (see Fig. 1). From the 6D cube with edge of length 2 centered at the origin, less than 2% of all points (out of 64000000 regularly spaced initial points) escape to infinity during the first 100 iterations. For example, along the diagonal, all points $x=y=z=s=u=w \in (\approx -0.66, 2]$ do not escape. From this 6D manifold of nonescaping initial points many lower-dimensional continua of periodic points protrude up to infinity, such as four 1D continua of fixed points: ($x=s=u=w=0, z=-y$), ($x=y=z=w=0, u=-s$), ($x=y=z=w, s=2, u=x^2-2$), and ($x=-y=-z=w, s=-2, u=2-x^2$); seven 2D continua of period-2 points:

$$\begin{aligned} [x = -y(s-1), z = -y, u = y(x-s/x), w = y], \\ [x = -y(s+1), z = -y, u = y(x+s/x), w = -y], \\ [x = y(s-1), z = y, u = y(x-s/x), w = y], \\ [x = y(s+1), z = y, u = y(x+s/x), w = -y], \end{aligned}$$

and the xw -, yz -, and su -planes; or at least six continua of period-12 periodic points one of which is ($x=y=z=s=0, u=1$).

The proper circle sequence^{6,8} is binary. It can be obtained from A_∞ of Eq. (6) if we assume that the a and b

building blocks are identical, or $\mathcal{N}_0 = \mathcal{M}_0$. Then the initial conditions satisfy the constraints $y_0 = x_0$, $u_0 = x_0^2 - 2$, $w_0 = x_0 s_0 - z_0$, and we are left with only three independent input parameters $x_0 = \text{Tr} \mathcal{M}_0$, $z_0 = \text{Tr} \mathcal{O}_0$, and $s_0 = \text{Tr}(\mathcal{O}_0 \mathcal{M}_0)$, as it should be for a binary sequence. For the often discussed diagonal model (with energy origin such that the two different diagonal elements of the potential are $+V$ at the a and b sites and $-V$ at the c sites), $x_0 = E - V$, $z_0 = E + V$, and $s_0 = x_0 z_0 - 2$. As the energy E changes, the initial point $(x_0, y_0, z_0, s_0, u_0, w_0)$ moves along a 1D curve that seems to avoid for $V \neq 0$ the central continuous nonescaping region as it has been observed in other quasicrystals. For $V = 0$ (periodic chain), this curve lies in the invariant 3D subspace mentioned above, and its portion corresponding to the continuous allowed band $E \in [-2, 2]$, can be found on the central nonescaping part of the $I_c = 4$ surface, where $|x_L| \leq 2$ everywhere. Energy $E = 0$ corresponds to the period-2 periodic point $(0, 0, 0, -2, -2, 0)$ at the intersection of the second and seventh continua of the period-2 points listed above. Energies $E = \pm 2$ correspond to the fixed points $(\pm 2, \pm 2, \pm 2, -2, -2, \pm 2)$, both lying in the third continuum of fixed points which in turn is a subset of the third continuum of the period-2 points above.

Rudin-Shapiro sequence can also be defined by means of a substitution rule, this time on four letters.⁶ We will need one more letter, d , the corresponding L th generation chain will be D_L , and the corresponding transfer matrix \mathcal{P}_L . Equations (1) and (2), and the corresponding recursion relations for the transfer matrices in this case read

$$\begin{aligned} a &\rightarrow ac, & A_{L+1} &= A_L C_L, & \mathcal{M}_{L+1} &= \mathcal{O}_L \mathcal{M}_L, \\ b &\rightarrow dc, & B_{L+1} &= D_L C_L, & \mathcal{N}_{L+1} &= \mathcal{O}_L \mathcal{P}_L, \\ c &\rightarrow ab, & C_{L+1} &= A_L B_L, & \mathcal{O}_{L+1} &= \mathcal{N}_L \mathcal{M}_L, \\ d &\rightarrow db, & D_{L+1} &= D_L B_L, & \mathcal{P}_{L+1} &= \mathcal{N}_L \mathcal{P}_L. \end{aligned} \quad (10)$$

Because of the regular form of these relations, only 12 trace coordinates need to be introduced out of the maximum of 24 for $n = 4$. A suitable choice is

$$\begin{aligned} x_L &= \text{Tr} \mathcal{M}_L, & s_L &= \text{Tr}(\mathcal{O}_L \mathcal{M}_L) - \text{Tr} \mathcal{O}_L \text{Tr} \mathcal{M}_L, \\ y_L &= \text{Tr} \mathcal{N}_L, & t_L &= \text{Tr}(\mathcal{O}_L \mathcal{P}_L) - \text{Tr} \mathcal{O}_L \text{Tr} \mathcal{P}_L, \\ z_L &= \text{Tr} \mathcal{O}_L, & q_L &= \text{Tr}(\mathcal{M}_L \mathcal{P}_L), \\ w_L &= \text{Tr} \mathcal{P}_L, & r_L &= \text{Tr}(\mathcal{N}_L \mathcal{O}_L), \\ o_L &= \text{Tr}(\mathcal{O}_L \mathcal{M}_L \mathcal{N}_L \mathcal{P}_L), & \bar{s}_L &= \text{Tr}(\mathcal{N}_L \mathcal{P}_L) - \text{Tr} \mathcal{N}_L \text{Tr} \mathcal{P}_L, \\ p_L &= \text{Tr}(\mathcal{O}_L \mathcal{P}_L \mathcal{N}_L \mathcal{M}_L), & \bar{t}_L &= \text{Tr}(\mathcal{N}_L \mathcal{M}_L) - \text{Tr} \mathcal{N}_L \text{Tr} \mathcal{M}_L. \end{aligned} \quad (11)$$

However, even this number can be reduced to eight. Starting from the second iteration, one can drop \bar{s}_L , \bar{t}_L , o_L , and p_L as they can be expressed in terms of other coordinates. Using Eqs. (4) and (10), one can write for $L > 0$,

$$\begin{aligned} s_{L+1} &= \text{Tr}(\mathcal{N}_L \mathcal{M}_L \mathcal{O}_L \mathcal{M}_L) - \text{Tr}(\mathcal{N}_L \mathcal{M}_L) \text{Tr}(\mathcal{O}_L \mathcal{M}_L) \\ &= \text{Tr}(\mathcal{N}_L \mathcal{O}_L) - \text{Tr} \mathcal{N}_L \text{Tr} \mathcal{O}_L = r_L - y_L z_L. \end{aligned}$$

In the same way, the same result is obtained for \bar{s}_{L+1} . Similarly, $t_{L+1} = \bar{t}_{L+1} = q_L - x_L w_L$. Also, we have q_{L+1}

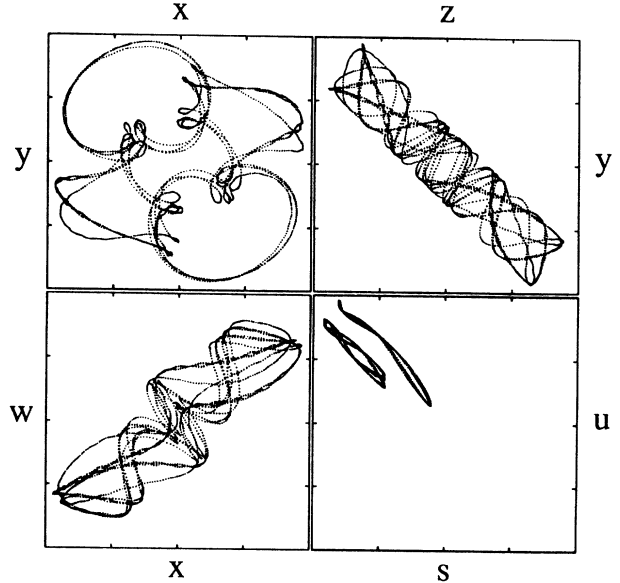


FIG. 1. Circle map: Projections on four different coordinate planes of a nonescaping orbit (first 5000 iterations) starting with $x_0 = -0.5$, $y_0 = 0.34$, $z_0 = -0.2$, $s_0 = -0.1$, $u_0 = 0.12$, and $w_0 = -0.4$. All axes range from -0.6 to 0.6 .

$= o_L$ and

$$\begin{aligned} o_{L+1} &= \text{Tr}[(\mathcal{O}_L \mathcal{M}_L)^2 \mathcal{M}_L^{-1} \mathcal{P}_L (\mathcal{N}_L \mathcal{P}_L)^2 \mathcal{P}_L^{-1} \mathcal{M}_L] \\ &= x_{L+1} w_{L+1} r_{L+1} - x_L^2 z_{L+1} - w_L^2 z_{L+1} + 2. \end{aligned}$$

Therefore, we can write $q_{L+1} = x_L w_L r_L - x_L^2 z_L - w_L^2 z_L + 2$ for $L > 0$. Similar results can be obtained for r_{L+1} and p_{L+1} , eliminating in this way p_L . The remaining recursion relations are easy to obtain, and for $L > 0$ we get the 8D trace map;

$$\begin{aligned} x_{L+1} &= x_L z_L + s_L, & s_{L+1} &= r_L - y_L z_L, \\ y_{L+1} &= z_L w_L + t_L, & t_{L+1} &= q_L - x_L w_L, \\ z_{L+1} &= x_L y_L + t_L, & q_{L+1} &= x_L w_L r_L - x_L^2 z_L - w_L^2 z_L + 2, \\ w_{L+1} &= y_L w_L + s_L, & r_{L+1} &= y_L z_L q_L - y_L^2 - z_L^2 + 2. \end{aligned} \quad (12)$$

The initial conditions are $x_1 = \text{Tr}(\mathcal{O}_0 \mathcal{M}_0)$, $y_1 = \text{Tr}(\mathcal{O}_0 \mathcal{P}_0)$, $z_1 = \text{Tr}(\mathcal{N}_0 \mathcal{M}_0)$, $w_1 = \text{Tr}(\mathcal{N}_0 \mathcal{P}_0)$, $s_1 = r_0 - y_0 z_0$, $t_1 = q_0 - x_0 w_0$, $q_1 = \text{Tr}(\mathcal{O}_0 \mathcal{M}_0 \mathcal{N}_0 \mathcal{P}_0)$, and $r_1 = \text{Tr}(\mathcal{O}_0 \mathcal{P}_0 \mathcal{N}_0 \mathcal{M}_0)$. The map of Eq. (12) is volume nonpreserving and noninvertible. A general point $(x_{L+1}, y_{L+1}, z_{L+1}, \dots)$ need not have any predecessor (x_L, y_L, z_L, \dots) at all. An example of such a point is the origin. Most of the points have a finite number of predecessors. There are two 3D subspaces, $(z = y, w = x, t = -2, q = r = 2)$ and $(z = y, w = x, s = -2, q = r = 2)$ [both contained in the 6D invariant subspace $(z = y, w = x)$], whose every point has infinitely many predecessors. Among these points with infinitely many predecessors is also the fixed point $(2, 2, 2, 2, -2, -2, 2, 2)$. Thus this point is the attractor of the Rudin-Shapiro map, probably with a fractal basin of attraction similar to that of the in detail investigated 2D copper-mean² or Thue-Morse³ (TM) maps. The existence of points with infinitely many predecessors also implies un-

der certain conditions the nonexistence of a polynomial invariant. We believe that also in this aspect the Rudin-Shapiro map resembles the copper mean and TM maps.

The proper Rudin-Shapiro sequence is binary.⁶ In its usual notation it can be obtained from A_∞ of Eq. (10) by substituting a and c with 1, and b and d with -1 . In other words, the building blocks a and c , and b and d , must have identical properties, or $\mathcal{O}_0 = \mathcal{M}_0$ and $\mathcal{P}_0 = \mathcal{N}_0$. For this case the trace map of Eq. (12) can be used from $L = 0$ if the initial conditions are chosen as $x_0 = z_0 = \text{Tr} \mathcal{M}_0$, $y_0 = w_0 = \text{Tr} \mathcal{N}_0$, $s_0 = -2$, $q_0 = r_0 = \text{Tr}(\mathcal{M}_0 \mathcal{N}_0)$, and $t_0 = q_0 - x_0 y_0$. Again, there are only three independent input parameters x_0 , y_0 , and q_0 . For the diagonal model, $x_0 = E - V$, $y_0 = E + V$, and $q_0 = x_0 y_0 - 2$. For $E = 0$ (center of the central gap of Fig. 8 of Ref. 6) and $L \geq 2$, x_L is a polynomial in V^2 of degree 2^{L-1} . Its two lowest terms are $x_{2l} = 2 - \alpha_l V^4 + \dots$ or $x_{2l+1} = 2 - \beta_l V^2 + \dots$, where α_l and β_l are positive integers. For $V = 0$, the initial point (x_0, y_0, \dots) ends up in the fixed point $(2, 2, 2, 2, -2, -2, 2, 2)$ in just two iterations. For all $L \geq 2$, the equation $x_L(E = 0, V) = 0$ has a finite number (increasing with L) of solutions V_{Li} . In the immediate vicinity of these roots, $|x_L| \leq 2$, and thus $E = 0$ is allowed for such values of V and the central gap closes. As $L \rightarrow \infty$, the roots V_{Li} remain clustered in the same regions, which explains the dependence of the central gap width on V in Fig. 8 of Ref.

6. This dependence should be the same down to $V = 0$. However, none of the roots V_{Li} seem to be fixed as $L \rightarrow \infty$, and we believe that eventually $|x_L| \rightarrow \infty$ for any $V \neq 0$ and $E = 0$. Though arbitrarily small for some values of V , the central gap would thus always be of nonzero width, and the curve in Fig. 8 of Ref. 6 would never actually touch the horizontal axis except at $V = 0$. For comparison, in the case of circle sequence, the polynomial equation $x_L(E = 0, V) = 0$ has the only real solution $V = 0$ for all L , which leads to a monotonous dependence of the central gap width on V .⁶

We have shown that for an arbitrary n -letter substitutional sequence, there always exists a trace map that determines the spectral properties of the system. We have found these trace maps for two special cases and studied their most important properties including the invariants, periodic points, and the manifolds of nonescaping points.

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