

## Transmission through a Thue-Morse chain

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(Received 27 June 1991)

We study the reflection  $|r_N|$  of a plane wave (with wave number  $k > 0$ ) through a one-dimensional array of  $N$   $\delta$ -function potentials with equal strengths  $v$  located on a Thue-Morse chain with distances  $d_1$  and  $d_2$ . Our principal results are: (1) If  $k$  is an integer multiple of  $\pi/|d_1 - d_2|$ , then there is a threshold value  $v_0$  for  $v$ ; if  $v \geq v_0$ , then  $|r_N| \rightarrow 1$  as  $N \rightarrow \infty$ , whereas if  $v < v_0$ , then  $|r_N| \not\rightarrow 1$ . In other words, the system exhibits a metal-insulator transition at that energy. (2) For any  $k$ , if  $v$  is sufficiently large, the sequence of reflection coefficients  $|r_N|$  has a subsequence  $|r_{2N}|$ , which tends exponentially to unity. (3) Theoretical considerations are presented giving some evidence to the conjecture that if  $k$  is not a multiple of  $\pi/|d_1 - d_2|$ , actually  $|r_{2N}| \rightarrow 1$  for any  $v > 0$  except for a "small" set (say, of measure 0). However, this exceptional set is in general nonempty. Numerical calculations we have carried out seem to hint that the behavior of the subsequence  $|r_{2N}|$  is not special, but rather typical of that of the whole sequence  $|r_N|$ . (4) An instructive example shows that it is possible to have  $|r_N| \rightarrow 1$  for some strength  $v$  while  $|r_N| \not\rightarrow 1$  for a larger value of  $v$ . It is also possible to have a diverging sequence of transfer matrices with a bounded sequence of traces.

The experimental advance in submicrometer physics that enables the fabrication of nearly ideal one-dimensional wires<sup>1</sup> naturally leads to increasing interest in their physical features, especially their Fourier spectrum and their transport properties. The quantum-mechanical relation between electrical conductance at zero temperature and the transmission probability<sup>2</sup> indicates that some measurable physical quantities can be accurately explained on the microscopic level once a one-dimensional wire is modeled as an infinite array of potentials. Systems consist of infinite one-dimensional array of potentials are of course extensively studied in the literature in connection with Bloch theory<sup>3</sup> (if they are periodic), and Anderson localization<sup>4</sup> (if they are completely disordered). Following the discovery of quasicrystals,<sup>5</sup> interest has been focused on the mathematical and physical nature of quasiperiodic sequences<sup>6</sup> and commensurate-incommensurate systems<sup>7</sup> which are the first class of structures on the way from periodic to random matter.

In order to study transport properties of such systems one needs a theory of scattering from a semi-infinite one-dimensional array of potentials. One such a theory has been developed earlier for the study of transport in a random potential.<sup>8</sup> The basic technique is to express the transmission and reflection amplitudes through  $N+1$  scatterers in terms of the amplitudes for  $N$  scatterers (a combination of Möbius transformation and multiplication by a phase equivalent to the transfer matrix) and to let  $N \rightarrow \infty$  (the so-called thermodynamic limit). If the

system is not random and a trace map is available, this procedure is quite powerful. In two earlier publications<sup>9,10</sup> we concentrated on scattering from an infinite system of  $\delta$ -function potentials located on the Fibonacci numbers  $x_n = F_n$  and on the Fibonacci chain  $x_n = n + u [n/\tau]$ ,  $n = 1, 2, \dots, N$ , as  $N \rightarrow \infty$ , where  $u$  is a real number,  $\tau = (1 + \sqrt{5})/2$ , and  $[\dots]$  denotes integer value. To this end we have developed special mathematical tools, basically analytical and number-theoretical techniques.

In the present work we use the same mathematical framework and report the results of our study on scattering of a plane wave with wave number  $k > 0$  from a one-dimensional sequence of  $\delta$ -function potentials of strength  $v$  located on a Thue-Morse chain.<sup>11</sup> To be more specific, let  $\xi_n$  be the Thue-Morse sequence i.e.,  $\xi_n = 0$  or 1 according to the number of 1's in the binary expansion of the integer number  $n$  being odd or even, respectively. Then the Thue-Morse chain  $\{x_n\}$  is constructed such that  $y_n = x_{n+1} - x_n = d_1$  or  $d_2$  when  $\xi_n = 0$  or 1, respectively, where  $d_1, d_2 > 0$  and  $d_1 \neq d_2$ . This is a prototype of a sequence generated by substitution, in this case  $d_1 \rightarrow d_1 d_2$  and  $d_2 \rightarrow d_2 d_1$ , with highly nontrivial features. The basic difference between the Thue-Morse chain and the Fibonacci chain<sup>6,10</sup> is expressed in terms of their Fourier transforms. In the first case the Fourier transform is singular continuous and the sequence is termed as aperiodic. In the second case the Fourier transform is discrete (or atomic), and the system is said to be quasi-periodic and exhibits Bragg peaks. These aspects of

quasiperiodic and aperiodic structures have recently been investigated by Luck.<sup>12</sup> The spectrum and the nature of states pertaining to the Thue-Morse sequence have been thoroughly investigated by several authors.<sup>13</sup> We point out that in the works of Ref. 13, the aperiodic structure is introduced by a deterministic aperiodic sequence of diagonal site potentials  $\{V_n\}$  within the context of the discrete Schrödinger equation in the tight-binding approximation

$$-(\psi_{n+1} + \psi_{n-1}) + V_n \psi_n = E \psi_n .$$

Here, on the other hand, we use the ordinary Schrödinger equation and the aperiodic structure is introduced through the sequence  $\{y_n\}$  of distances between scattering centers. It affects only the phase of the wave function.

The central question which will be addressed in this study does not concern the spectral properties but, rather, the question of transmission and reflection. We want to find out whether a one-dimensional Thue-Morse chain is a conductor ( $|r_N| \rightarrow 1$ ) or an insulator ( $|r_N| \rightarrow 0$ ). To be more specific, is there a curve in the  $(v, k)$  plane separating the conductor and insulator "phases"? The finer details pertaining to the behavior of  $|r_N|$  as a function of  $N$  are also discussed albeit briefly. We point out that this problem is related to the study of the spectrum in the following heuristic manner: If an energy  $E = k^2$  does not belong to the spectrum we expect that  $|r_N| \rightarrow 1$  exponentially. On the other hand, if the energy is in the spectrum, then the behavior of  $|r_N|$  for large  $N$  determines the nature of the pertinent eigenstate (localized, extended, or critical). In the present work we simply study the transmission for all energies, both in the spectrum and outside it. Any result which applies to "almost every energy" will then apply to the spectrum as well.

Although every sequence has its own characteristics we believe that the mathematical framework developed here is capable of solving the scattering problems encountered in other one-dimensional arrays, especially if a trace map exists. This is the case for two-letters substitution sequences.<sup>14</sup> Recently, trace maps have also been constructed for general substitution sequences, with applications to the circle sequence and the Rudin-Shapiro sequence.<sup>15</sup>

It has been recognized that in these kinds of problems, mathematical rigor is essential. That is the reason why the presentation below is mathematically oriented. Yet, the reader should be aware of the physical basis for the present study. For the sake of smooth reading we present the proofs of most of our statements in the Appendix. With that notion of apology we start our study proper.

Consider a one-dimensional array of  $N$   $\delta$ -function potentials

$$V_N(x) = v \sum_{n=1}^N \delta(x - x_n) , \quad (1)$$

where  $v > 0$  and  $\{x_n\}$  is an infinite deterministic real sequence whose difference sequence  $x_{n+1} - x_n$  assumes two possible (positive) values  $d_1$  and  $d_2$ . In fact, due to translation invariance what really counts is the sequence

of differences  $y_n = x_{n+1} - x_n$ . Some of our results will apply to any sequence  $y_n$  assuming only two values, but the more detailed study is concentrated on the Thue-Morse chain, for which some deeper results are obtained. In the special case of a Thue-Morse chain the sequence  $\{y_n\}$  is defined by

$$y_n = x_{n+1} - x_n = \begin{cases} d_1 & \text{if } \xi_n = 0 \\ d_2 & \text{if } \xi_n = 1 . \end{cases} \quad (2)$$

where  $\xi_n = [1 + (-1)^{s(n)}]/2$  and  $s(n)$  the number of 1's in the binary expansion of  $n$ .

A plane wave at momentum  $k, e^{-ikx}$ , coming from the right will have reflection and transmission amplitudes  $r_N$  and  $t_N$ , respectively. For  $N=1$ , these amplitudes are given by

$$r = \frac{v}{2ik - v}, \quad t = \frac{2ik}{2ik - v}, \quad (3)$$

which satisfy unitarity

$$|r|^2 + |t|^2 = 1, \quad tr^* + t^*r = 0, \quad (4a)$$

and continuity at the point  $x = x_0$ ,

$$t = 1 + r . \quad (4b)$$

The unitarity relation (4a) is valid of course for any  $N$ . For  $N > 1$  scattering centers, the reflection and transmission amplitudes can be determined from a recursion relation as follows: We introduce the dimensionless parameter  $q = v/2k$  and define

$$\begin{aligned} a_n &= t_n^{-1}, \quad b_n = r_n t_n^{-1}, \\ C &= \begin{bmatrix} t^{-1} & -rt^{-1} \\ rt^{-1} & (t^2 - r^2)t^{-1} \end{bmatrix} = \begin{bmatrix} 1+iq & iq \\ -iq & 1-iq \end{bmatrix}, \\ \Lambda_n &= \begin{bmatrix} e^{-iky_n} & 0 \\ 0 & e^{iky_n} \end{bmatrix}, \quad D_n = C \Lambda_n, \end{aligned} \quad (5)$$

with

$$\det(C) = \det(\Lambda_n) = \det(D_n) = 1 . \quad (6)$$

The matrix  $D_n$  is recognized as the transfer matrix at site  $n$ . We then have

$$\begin{bmatrix} a_{n+1} \\ b_{n+1} \end{bmatrix} = C \Lambda_n \begin{bmatrix} a_n \\ b_n \end{bmatrix} . \quad (7)$$

Anticipating the use of product of  $n$  transfer matrices we also define

$$M_n = \Lambda_n C \Lambda_{n-1} \cdots C \Lambda_1 C . \quad (8)$$

The conductance (at zero temperature and in units of  $e^2/h$ ) of this system is given by the Landauer formula  $g = |t_N/r_N|^2$ . Therefore, we need to study the limit of  $|t_N|^2 = 1/|a_N|^2$  as  $N \rightarrow \infty$ . Equivalently, we may inspect the limit of  $|r_N|^2 = |b_N/a_N|^2$  and use unitarity. If  $|t_N| \rightarrow 0$  (equivalently  $|r_N| \rightarrow 1$ ) we say that the system is an insulator. If  $|t_N|$  does not tend to 0 the system may conduct. Our aim is to find out for which values of the momentum  $k$  and the strength  $v$  the system is an insula-

tor and for which it may conduct. It is also of interest to know when the sequence  $|r_N|$  has a subsequence converging to 1 (or a subsequence converging to 0).

Now, we point out that in general (independently of the sequence  $x_n$ ), all the matrices  $C$ ,  $\Lambda_n$ , and  $M_n$ , belong to the following multiplicative group of  $2 \times 2$  matrices:

$$SU(1,1) = \left\{ \begin{bmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{bmatrix} \mid \alpha, \beta \in \mathbb{C}, |\alpha|^2 - |\beta|^2 = 1 \right\}. \quad (9)$$

Denote

$$\left| \left| \begin{bmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{bmatrix} \right| \right| = |\alpha| + |\beta|. \quad (10)$$

Following our previous work<sup>10</sup> the following proposition is implied.

*Proposition 1.* For any sequence  $n_j$  we have  $|r_{n_j}|_{j \rightarrow \infty} \rightarrow 1$  if and only if  $\|M_{n_j}\|_{j \rightarrow \infty} \rightarrow \infty$ .

Actually, using basically the same ideas, one can prove the following proposition.

*Proposition 2.* There exist positive constants  $c_1 < c_2$  (depending on  $k, v$ , and the sequence  $y_n$ ) such that

$$c_1 / \|M_n\|^2 \leq 1 - |r_n| \leq c_2 / \|M_n\|^2, \quad n \geq 1. \quad (11)$$

For a fixed  $k$  it seems plausible that the larger  $v$  is, the better are the ‘‘chances’’ that  $|r_N|_{N \rightarrow \infty} \rightarrow 1$ . Surprisingly, however, it is possible that the reflection coefficient tends to unity for some value of  $v$  but not for a larger value of  $v$  (see also Example 1). Nevertheless, our next result shows that the set of  $v$ 's for which  $|r_N|_{N \rightarrow \infty} \rightarrow 1$  is quite nice. Recall that a set in a metric space is called an  $F_\sigma$  set if it is a countable union of closed sets, and an  $F_{\sigma\delta}$  set if it is a countable intersection of  $F_\sigma$  sets.

*Proposition 3.* For any sequence  $\{y_n\}_{n=1}^\infty$  and  $k > 0$ , the set  $\{v : |r_N|_{N \rightarrow \infty} \rightarrow 1\}$  is an  $F_{\sigma\delta}$  set. The proof is given in the Appendix. One actually has the more general re-

$$v = v_0 \implies c_1/n^2 \leq 1 - |r_n| \leq c_2/n^2, c_2 > c_1 > 0 \text{ const,}$$

$$v > v_0 \implies c_1 e^{-\alpha n} \leq 1 - |r_n| \leq c_2 e^{-\alpha n}, \quad c_2 > c_1 > 0, \text{ and } \alpha > 0 \text{ const depending on } v.$$

(2) In the second part of Proposition 4, the sequence  $r_n$  is ‘‘usually’’ dense in the circle it lies on, but sometimes is periodic and so concentrated on a finite subset of the circle (see Ref. 10 for more details).

(3) If  $k$  is also an integer multiple of  $\pi$  (which is possible if  $d_1 - d_2$  is rational), then  $|r_n|$  converges to 1 for every  $v > 0$  ( $\|M_n\|$  grows linearly with  $n$ , so that  $1 - |r_n|$  behaves as  $c/n^2$  for some constant  $c$ ).

We now turn to study in detail the Thue-Morse chain for which the sequence  $y_n$  is defined through Eq. (2). Recall that the Thue-Morse sequence  $\xi_n$  is defined as follows:

$$\xi_1 = 0, \quad \xi_{2^m+i} = 1 - \xi_i, \quad m \geq 0, \quad 1 \leq i \leq 2^m. \quad (15)$$

The sequence  $\{y_n\}$ , Eq. (2) can be defined also as

$$y_n = d_1 + (d_2 - d_1)\xi_n, \quad n \geq 1, \quad (16)$$

sult specified below.

*Proposition 3'.* In the setup of Proposition 3, for any sequence  $\{N_j\}_{j=1}^\infty$  of positive integers the set  $\{v : |r_{N_j}|_{N_j \rightarrow \infty} \rightarrow 1\}$  is an  $F_{\sigma\delta}$  set. The proof is identical with that of Proposition 3.

Our main problem is to decide, given the sequence  $\{y_n\}_{n=1}^\infty$ , for which values of  $k$  and  $v$  do we have  $|r_N|_{N \rightarrow \infty} \rightarrow 1$ . Before studying the Thue-Morse chain we present a statement concerning any sequence  $y_n$  which assumes only two values  $d_1$  and  $d_2$ .

*Proposition 4.* Suppose  $y_n$  assumes only two values  $d_1$  and  $d_2$ . Then for every  $k$  which is an integer multiple of  $\pi/(d_1 - d_2)$ , there is a threshold value  $v_0$  for  $v$  such that

(1)

$$\begin{aligned} |r_N| \rightarrow 1 &\iff v \geq v_0 (> 0), \\ v_0 &= \begin{cases} 2k \operatorname{tg} \frac{k}{2} \operatorname{sink} > 0 \\ -2k \operatorname{ctg} \frac{k}{2} \operatorname{sink} < 0. \end{cases} \end{aligned} \quad (12)$$

(2) If  $|r_N| \not\rightarrow 1$  then the sequence  $r_n$  itself lies on a circle in the complex plane whose diameter is  $q/|\operatorname{sink} - q \operatorname{cosk}| (< 1)$  passing through the origin, and in particular

$$\overline{\lim} |r_N| < 1; \underline{\lim} |r_N| = 0. \quad (13)$$

The proof of Proposition 4 is identical to the one we gave in Ref. 10 where we have studied the Fibonacci chain. It is to be noted that the proof does not rely on the nature of the sequence but merely on the fact that the sequence of differences assumes only two values.

*Remarks.* (1) Using Proposition 2 one can improve somewhat the first part to obtain

$$\text{[Equation content from previous block]} \quad (14)$$

where, as we have already indicated,  $d_1$  and  $d_2$  are positive numbers. The case  $d_1 = d_2$  amounts to an ordered system for which  $y_n$  is constant (a trivial case in the present context) and hence it is assumed that  $d_1 \neq d_2$ . Proposition 4 covers values of  $k$  which are integer multiples of  $\pi/(d_1 - d_2)$  and we henceforth assume  $k \notin \pi/(d_1 - d_2)\mathbb{Z}$  unless stated otherwise. We set

$$\phi = kd_1, \quad \psi = kd_2, \quad (17)$$

and define two sequences of matrices  $\{P_n\}_{n=1}^\infty$  and  $\{Q_n\}_{n=1}^\infty$  in  $SU(1,1)$  by

$$P_0 = \begin{bmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{bmatrix} C, \quad Q_0 = \begin{bmatrix} e^{-i\psi} & 0 \\ 0 & e^{i\psi} \end{bmatrix} C, \quad (18a)$$

$$P_n = Q_{n-1} P_{n-1}, \quad Q_n = P_{n-1} Q_{n-1}, \quad (18b)$$

where  $C$ , the transfer matrix through the  $\delta$ -function po-

tential, is defined in Eq. (5). Then direct calculation yields the following.

*Lemma 1.* For the sequence of matrices  $\{M_N\}_{N=1}^\infty$  defined in Eq. (8) one has

$$M_{2^n} = P_n, \quad n \geq 0. \tag{19}$$

At present we do not have the tools to study the whole sequence  $\{M_N\}_{N=1}^\infty$  and our strategy will be to study its subsequence  $\{M_{2^n}\}_{n=1}^\infty$ . Numerical simulations indicate that any statement concerning the behavior of the subsequence is valid for the whole sequence. We shall investigate the sequence  $\{P_n\}_{n=1}^\infty$  using the trace map. Denote

$$\chi_n = \text{tr}(P_n), \quad n \geq 0. \tag{20}$$

Note that  $\text{tr}(Q_n) = \chi_n$  for  $n \geq 1$ . Our task is to find out for which values of  $k$  and  $v$  the sequence of norms  $\{\|P_n\|\}_{n=1}^\infty$  tends to infinity and for which it does not. To this end we shall consider the sequence of traces  $\{\chi_n\}_{n=1}^\infty$ . If  $|\chi_n|_{n \rightarrow \infty} \rightarrow \infty$  then  $\|P_n\|_{n \rightarrow \infty} \rightarrow \infty$ , whereas if  $|\chi_n|_{n \rightarrow \infty} \not\rightarrow \infty$  then we have a clue hinting that perhaps  $\|P_n\|_{n \rightarrow \infty} \not\rightarrow \infty$  (however, it is possible to have  $|\chi_n|_{n \rightarrow \infty} \not\rightarrow \infty$  but  $\|P_n\|_{n \rightarrow \infty} \rightarrow \infty$ , as is demonstrated in Example 1 below). The following Lemma is well known.

*Lemma 2.* If  $\{P_n\}_{n=0}^\infty$  and  $\{Q_n\}_{n=0}^\infty$  are any two sequences of matrices in  $SU(1,1)$  satisfying the recursion relations (18.b) and  $\chi_n = \text{tr}(P_n)$ , then

$$\chi_{n+2} = \chi_n^2(\chi_{n+1} - 2) + 2, \quad n \geq 1. \tag{21}$$

For completeness we present the proof of Lemma 2 in the Appendix.

To study the behavior of the sequence  $\{\chi_n\}_{n=1}^\infty$  it is thus natural to consider the mapping  $H: \mathbb{R}^2 \rightarrow \mathbb{R}^2$  defined by

$$H(x,y) = (y, x^2y - 2x^2 + 2), \quad (x,y) \in \mathbb{R}^2. \tag{22}$$

In fact, in view of Lemma 2 we have

$$(X_n, \chi_{n+1}) = H(X_{n-1}, \chi_n) = H^{n-1}(X_1, \chi_2), \quad n \geq 1, \tag{23}$$

so that the  $H$  orbit of  $(X_1, \chi_2)$  contains all information regarding the traces of the matrices  $P_n$ .

The dynamical system defined by  $H$  has been studied by various authors.<sup>13</sup> The questions we are interested in, as well as our approach, are somewhat different, though. We shall now replace  $H$  by a somewhat simpler transformation which is adapted to our future discussion. Let  $\mathbb{R}_+ = \{x \in \mathbb{R}: x \geq 0\}$ . Define maps  $\gamma: \mathbb{R}^2 \rightarrow \mathbb{R}_+ \times \mathbb{R}$  and  $K: \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}_+ \times \mathbb{R}$  by

$$\gamma(x,y) = (x^2, y), \quad (x,y) \in \mathbb{R}^2, \tag{24}$$

$$(1) \quad K^n(x,y) \xrightarrow{n \rightarrow \infty} (\infty, \infty), \quad (x,y) \in \mathcal{U}_0 = \{(x,y): x > 0, y > 2\}, \tag{28}$$

$$(2) \quad K^2(x,y) \xrightarrow{n \rightarrow \infty} (\infty, -\infty), \quad x \geq 1, y \leq -1, (x,y) \neq (1, -1). \tag{29}$$

The second part of Lemma 5 is proved in the Appendix.

It is now possible to study the behavior of the set of potential strengths  $\{v\}$  for which the reflection coefficient tends to 1 in the special case of a Thue-Morse chain. Re-

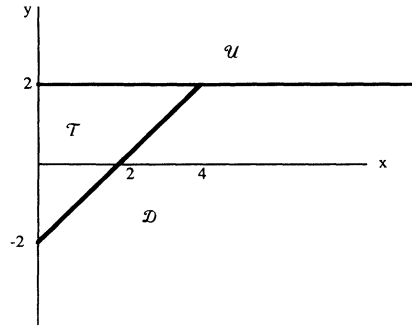


FIG. 1. Decomposition of the right half plane into the three sets  $\mathcal{U}$ ,  $\mathcal{D}$ , and  $\mathcal{T}$  following Lemma 4.

$$K(x,y) = (y^2, xy - 2x + 2), \quad (x,y) \in \mathbb{R}_+ \times \mathbb{R}. \tag{25}$$

We then have the following lemma.

*Lemma 3.* The following equality holds:

$$\gamma \circ H = K \circ \gamma, \tag{26}$$

which is proved in the Appendix.

In the terminology of dynamical systems we say that the transformations  $H$  and  $K$  are semiconjugate via  $\gamma$ . Clearly, the Lemma implies that we may as well study  $K$  instead of  $H$ . In fact, we may replace Eq. (23) by the following relation:

$$(\chi_n^2, \chi_{n+1}) = K^{n-1}(\chi_1^2, \chi_2), \quad n \geq 1. \tag{27}$$

Thus, our main objective now is to find out which points in  $\mathbb{R}_+ \times \mathbb{R}$  have  $K$  orbits going to infinity and which do not.

*Lemma 4.* The following three subsets of  $\mathbb{R}_+ \times \mathbb{R}$  are invariant under  $K$ :

- (1)  $\mathcal{U} = \{(x,y): x \geq 0, y \geq 2\}$ .
- (2)  $\mathcal{D} = \{(x,y): x \geq 0, y \leq 2, y \leq x - 2\}$ .
- (3)  $\mathcal{T} = \{(x,y): x \geq 0, x - 2 \leq y \leq 2\}$ .

The proof of Lemma 4 (for  $\mathcal{T}$  only) is given in the Appendix.

In particular, the borderline between  $\mathcal{U}$  and  $\mathcal{D} \cup \mathcal{T}$ , namely, the half line  $\{(x,2): x \geq 0\}$ , is  $K$  invariant; in fact it is carried to the single point  $(4,2)$ . The decomposition of the right half plane  $\mathbb{R}_+ \times \mathbb{R}$  into the sets  $\mathcal{U}$ ,  $\mathcal{D}$ , and  $\mathcal{T}$  is illustrated in Fig. 1.

*Lemma 5.* We have

call that, according to Proposition 3', for any  $k > 0$  the set  $\{v: |r_{2^n}| \rightarrow_{n \rightarrow \infty} 1\}$  is an  $F_{\sigma\delta}$  set. The following proposition, which we prove in the Appendix, may hint that in our case this set might be even more well behaved.

*Proposition 5.* For any  $k > 0$ , the set  $\{v:|\chi_n|_{n \rightarrow \infty} \rightarrow \infty\}$  is open. Note that the set considered in Proposition 5 is just a subset of the set  $\{v:|r_{2^n}|_{n \rightarrow \infty} \rightarrow 1\}$ ; not the whole of this set (see Example 1).

In Lemma 5 we found two unbounded sets in  $\mathbb{R}_+ \times \mathbb{R}$  consisting of points whose orbits under  $K$  go to infinity. As  $\mathcal{T}$  is a compact  $K$ -invariant set, its points have bounded  $K$  orbits. The two shaded regions in Fig. 2 depict the set of points the behavior of whose  $K$  orbits is not covered by Lemmas 4 and 5.

*Remarks.* (1) It is inconsequential for the problem at hand, but it would be of interest to better understand the behavior of  $K$  on the triangle  $\mathcal{T}$ . On the boundary of  $\mathcal{T}$ , this is relatively simple. The top side  $\{(x, 2): x \leq 4\}$  is carried to the  $K$ -fixed point  $(4, 2)$ , whereas the left side  $\{(0, y): -2 \leq y \leq 2\}$  is carried to the top side. To describe the action of  $K$  on the bottom right side of  $\mathcal{T}$ , namely, the line interval  $\mathcal{J} = \mathcal{T} \cap \mathcal{D}$ , we first note that

$$\mathcal{J} = \{(4 \cos^2 \alpha, 2 \cos 2\alpha) : \alpha \in [0, 2\pi)\} . \tag{30}$$

A straightforward calculation gives

$$K(4 \cos^2 \alpha, 2 \cos 2\alpha) = (4 \cos^2 2\alpha, 2 \cos 4\alpha), \quad \alpha \in [0, 2\pi) . \tag{31}$$

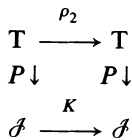
Thus, letting  $\rho_2$  denote multiplication by 2 on the circle group  $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$ ,

$$\rho_2(t) = 2t, \quad t \in \mathbb{T}, \tag{32}$$

and  $P: \mathbb{T} \rightarrow \mathcal{J}$  be defined by

$$P(t) = (4 \cos^2 t, 2 \cos 2t), \quad t \in \mathbb{T}, \tag{33}$$

we find that the following diagram



is commutative. Now  $\rho_2$  is a mixing algebraic endomorphism of  $\mathbb{T}$ , and its action has been extensively studied. Furthermore, the action of  $K$  on  $\mathcal{J}$  is semiconjugate to

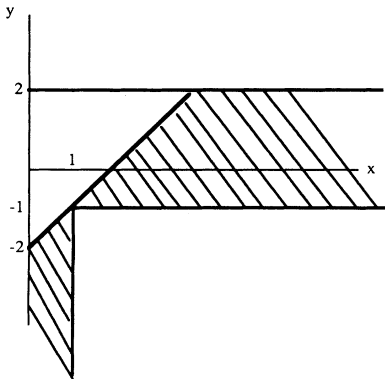


FIG. 2. The set of points the behavior of whose  $K$  orbits is not described by Lemmas 4 and 5.

that of  $\rho_2$  on  $\mathcal{J}$ , where it is also well understood. It would then be worthwhile to explore the behavior of  $K$  on the whole of  $\mathcal{J}$ .

(2) The family of solutions of the trace recursion relation (21) is two-parametric. A one-parameter subfamily can be written down explicitly. Start with any matrix  $R \in \text{SU}(1, 1)$ , put  $P_0 = Q_0 = R$  and define  $\{P_n\}_{n=1}^\infty$  and  $\{Q_n\}_{n=1}^\infty$  by Eq. (18b). (Taking just commuting  $P_0$  and  $Q_0$  does not provide more generality.) Then Eq. (21) still holds. The sequence of traces is easily found out to be of the form

$$\chi_n = \lambda^{2^n} + \lambda^{-2^n}, \quad n \geq 0 . \tag{34}$$

This sequence is real if and only if  $\lambda$  is either real or lies on the unit circle in the complex plane. In the first case the sequence  $(\chi_n^2, \chi_{n+1})$  lies on the ray  $\{(x, x-2): x \geq 4\}$ , while in the second case it lies on the interval  $\mathcal{J}$  (note that both sets are portions of the same line). This shows with more clarity why  $K$  acts on  $\mathcal{J}$  (almost) as multiplication by 2 on  $\mathbb{T}$ , and on  $\{(x, x-2): x \geq 4\}$  as squaring on  $\mathbb{R}_+$ .

There exist points with bounded  $K$  orbits in addition to those of  $\mathcal{J}$ . In fact, any point entering  $\mathcal{J}$  after finitely many iterates of  $K$  is such. To describe this set  $\cup_{i=1}^\infty K^{-i}(\mathcal{J})$  we first note that

$$K^{-1}(\mathcal{J}) = \mathcal{J} \cup \{(x, 2): x \geq 0\} , \tag{35}$$

and therefore

$$K^{-2}(\mathcal{J}) = K^{-1}(\mathcal{J}) \cup \{(0, y): y \in \mathbb{R}\} . \tag{36}$$

Letting  $P: \mathbb{R}^2 \rightarrow \mathbb{R}$  be the projection on the first coordinate we obtain

$$K^{-(i+1)}(\mathcal{J}) = K^{-i}(\mathcal{J}) \cup \{(x, y): P \circ K^{i-1}(x, y) = 0\}, \quad i \geq 1 . \tag{37}$$

Some of the one-dimensional sets we encounter in the process have simple representations. Thus, to get from  $K^{-2}(\mathcal{J})$  to  $K^{-5}(\mathcal{J})$  we add successively the sets  $\{(x, 0): x \geq 0\}$ ,  $\{(x, 2-2/x): x > 0\}$  and  $\{(2/y^2(2-y), y): 0 \neq y < 2\}$ . However, as  $P \circ K^j$  is a polynomial of degree  $2^j$ , these curves become more and more cumbersome.

Similarly, all points entering  $(1, \infty) \times (-\infty, -1)$  under some power of  $K$  have orbits going to infinity. It is therefore easy to reduce the shaded regions in Fig. 2 by taking out of them the inverse images of this set under higher and higher powers of  $K$ . However, we could not answer the following questions.

(1) Are there any points outside  $\cup_{i=1}^\infty K^{-i}(\mathcal{J})$  having bounded orbits?

(2) Let  $(x, y) \in \mathbb{R}_+ \times \mathbb{R}$  be a point with an unbounded  $K$  orbit and let  $(x_n, y_n) = K^n(x, y)$ . Is it necessarily the case that  $x_n \rightarrow \infty$  (and  $|y_n| \rightarrow \infty$ )?

*Lemma 6.* Let  $\{s_n\}_{n=1}^\infty$  be a sequence of positive numbers satisfying

$$s_{n+2} = \rho s_n^2 s_{n+1}, \quad n \geq 1 . \tag{38}$$

for some  $\rho > 0$ . Then

$$s_n = \rho^{-1/2} [\rho^{-1/6} s_1^{-1/3} s_2^{1/3}]^{(-1)^n} [(\rho s_1 s_2)^{1/6}]^{2^n}, \quad n \geq 1 . \tag{39}$$

The Lemma is easily proved by passing to logarithms and solving the resulting inhomogeneous linear recurrence with constant coefficients.

*Lemma 7.* Let  $(x, y) \in \mathbb{R}_+ \times \mathbb{R}$  and  $(x_n, y_n) = K^n(x, y)$  for  $n \geq 0$ . If  $x_n \rightarrow \infty$ , then

$$x_n \geq a\xi^{2^n}, \quad n \geq 0, \tag{40}$$

for some  $a > 0$  and  $\xi > 1$ .

Lemma 7 is proved in the Appendix.

*Lemma 8.* For every  $q > 0$  (recall that  $q = v/2k$ ), we have  $\chi_2 < \chi_1^2 - 2$ . The proof of Lemma 8 is given in the Appendix.

Thus, all possible pairs  $(\chi_1^2, \chi_2)$  lie, in our case, to the

$$\begin{aligned} q_{1,2} &= \{ -\sin(\phi + \psi) \pm [\sin^2(\phi + \psi) - \sin\phi \sin\psi \cos(\phi + \psi)]^{1/2} \} / 2 \sin\phi \sin\psi \\ &= [ -\sin(\phi + \psi) \pm (\sin^2\phi + \sin^2\psi)^{1/2} ] / 2 \sin\phi \sin\psi . \end{aligned} \tag{41}$$

Depending on  $\phi$  and  $\psi$ , none, exactly one, or both  $q_1$  and  $q_2$  may be positive. Thus, the case of bounded traces is possible. The question whether solutions  $q > 0$  exist for the equation  $\chi_j(q) = 0$  for  $j \geq 2$  involves the solution of equations of higher degrees than (41). One would expect, though, that infinitely many of the solutions would turn out to be positive and thus relevant in the present context.

If  $\chi_j = 0$  for some  $j \geq 0$  then the answer to our basic question is known for any  $N$ , not only for  $N = 2^n$ . Indeed, since  $P_{j+2} = Q_{j+2} = I$ , we have [see Eq. (8)]  $M_N = I$  for every  $N \equiv 0 \pmod{2^{j+2}}$ , where  $r_N = 0$  for each such  $N$ . Note that the sequence  $\{r_N\}_{N=1}^\infty$  is nonperiodic. Rather, it moves from 0 to 0 on two different paths, the order corresponding to the rule of the Thue-Morse sequence. Obviously, in this case,  $\max_N |r_N| < 1$ .

*Lemma 10.* (1) For every sufficiently large  $q$  we have  $|\chi_n|_{n \rightarrow \infty} \rightarrow \infty$ . (2) If  $|\chi_n|_{n \rightarrow \infty} \rightarrow \infty$  for some  $q$ , then  $|\chi_n| \geq a\xi^{2^n}$  for some  $a > 0$  and  $\xi > 1$ . Lemma 10 is proved in the Appendix.

We are now in a position to state our central result. Propositions 1, 2, 4, and Lemma 10 now yield the following theorem.

*Theorem 1.* For every  $k$ , if  $v$  is sufficiently large, then  $|r_{2^n}|_{n \rightarrow \infty} \rightarrow 1$ . Moreover, the convergence is exponential, namely,

$$1 - |r_{2^n}| \leq a\xi^{2^n}, \quad n \geq 0, \quad a > 0, \quad 0 < \xi < 1. \tag{42}$$

Recall that we assumed  $k(d_1 - d_2)$  not to be an integer multiple of  $\pi$ . The theorem actually holds in that case as well, but in the particular case of  $k$  itself being also a multiple of  $\pi$  (which is possible if  $d_1 - d_2$  is rational), the convergence is not exponential, and the right-hand side of (42) is replaced by  $a/4^n$ .

*Example 1.* We shall see here that it is possible to have  $|r_N|_{N \rightarrow \infty} \rightarrow 1$  for a certain value of  $v$  and yet  $\lim_{N \rightarrow \infty} |r_N| < 1$  for some larger value of  $v$ . In some sense, this result is counterintuitive since for a positive potential, increasing  $v$  means stronger repulsion. In the context of one-dimensional barrier penetration it can be viewed as a resonance tunneling but we are unaware of its

right of the line  $\{(x, x - 2) : x \geq 0\}$ , on which they lie if we start with commuting  $P_0, Q_0 \in \text{SU}(1, 1)$  (see the second remark following Lemma 5). However, since points outside  $\mathcal{S}$  can be carried to  $\mathcal{S}$  by  $K$ , we may still get bounded traces. The following Lemma shows that in this case bounded traces actually mean bounded matrices.

*Lemma 9.* If  $\chi_j = 0$  for some  $j \geq 1$ , then  $P_n = I$  for  $n \geq j + 2$ , and therefore the sequence  $\{M_n\}_{n=1}^\infty$  defined in Eq. (8) takes only finitely many values. For the proof of Lemma 9, see the Appendix.

It is possible to have  $\chi_j = 0$  already for  $j = 1$ . In fact, from (A8) it follows that  $\chi_1$  vanishes for the following two values of  $q = v/2k$  [recall the definitions of  $\phi$  and  $\psi$  Eq. (17)]:

presence for aperiodic systems.

We shall also encounter in this example a nontrivial case where the sequence of traces  $\{\chi_n\}_{n=1}^\infty$  is bounded but  $\|P_n\|_{n \rightarrow \infty} \rightarrow \infty$ . Thus, the consequences drawn from the use of the trace map should be taken with some care.

Consider the specific case in which we take  $k, d_1, d_2$ , so that  $\phi = kd_1 = 5\pi/6$  and  $\psi = kd_2 = 3\pi/4$ . By (41),  $\chi_1(q)$  vanishes for  $q_1 = (\sqrt{3} + 1 + \sqrt{6})/2$  and  $q_2 = (\sqrt{3} + 1 - \sqrt{6})/2$ . In view of Lemma 9,  $P_3 = I$  and  $|r_N| < 1$  for these values of  $q$ . We mention that, taking  $q_3 = 1$ , we may verify that  $\chi_3(q_3) = 0$ , so that  $P_5 = I$  and hence  $\max_N |r_N| < 1$  for  $q_3$  as well. Now consider  $q_4 = (\sqrt{3} + 1)/2$ . Denoting  $R = \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$  and  $\mu = i(\sqrt{3} - 1)/4$ , we find after lengthy calculations that

$$P_2 = I + 2\mu R, \quad Q_2 = I + \mu R, \quad P_3 = Q_3 = I + 3\mu R. \tag{43}$$

It follows that  $\chi_n = 2$  for  $n \geq 3$  and

$$M_N = P_3^N = I + 3N\mu R, \quad N \geq 0. \tag{44}$$

Thus,  $\|M_N\|_{N \rightarrow \infty} \rightarrow \infty$ , so that  $|r_N|_{N \rightarrow \infty} \rightarrow 1$  for  $q = q_4$ . Notice incidentally that in view of Proposition 2 the convergence in this special case is not exponential.

ACKNOWLEDGMENTS

We are grateful to H. Furstenberg, T. Spencer, J. M. Luck, and R. M. Redheffer for valuable discussions on this subject and to D. Glaubman for verifying the calculations in Example 1 using the MATHEMATICA® software. This work was sponsored in part by a Grant from the United States-Israel Binational Science Foundation and in part by an NSF Grant No. 8505550. This work was partially supported by the Laboratoire de la Direction des Sciences de la Matière du Commissariat à l’Energie Atomique and by the Israel Ministry of Science.

APPENDIX

*Proof of Proposition 3.* Denote

$$L_{jN} = \{v : \|M_N\| \geq j\}, \quad j, N = 1, 2, \dots \tag{A1}$$

Since  $M_N$  depends continuously on  $v$ , each  $L_{jN}$  is a closed set. Obviously

$$\begin{aligned} \{v: |r_N|_{N \rightarrow \infty} \rightarrow 1\} &= \{v: \|M_N\|_{N \rightarrow \infty} \rightarrow \infty\} \\ &= \bigcap_{j=1}^{\infty} \bigcap_{i=1}^{\infty} \bigcap_{N=i}^{\infty} L_{jN}, \end{aligned} \quad (\text{A2})$$

$$\begin{aligned} \chi_{n+2} &= \text{tr}(P_{n+2}) = \text{tr}(P_n Q_n Q_n P_n) = \text{tr}(P_n^2 Q_n^2) = \text{tr}[(\chi_n P_n - I)(\chi_n Q_n - I)] \\ &= \chi_n^2 \text{tr}(P_n Q_n) - \chi_n \text{tr}(P_n) - \chi_n \text{tr}(Q_n) + \text{tr}(I) = \chi_n^2 \chi_{n+1} - 2\chi_n^2 + 2 = \chi_n^2 (\chi_{n+1} - 2) + 2. \end{aligned} \quad (\text{A3})$$

*Proof of Lemma 3.* For any  $(x, y) \in \mathbb{R}$

$$\begin{aligned} (\gamma \circ H)(x, y) &= \gamma(y, x^2 y - 2x^2 + 2) \\ &= (y^2, x^2 y - 2x^2 + 2) \end{aligned} \quad (\text{A4})$$

and

$$(K \circ \gamma)(x, y) = K(x^2, y) = (y^2, x^2 y - 2x^2 + 2). \quad (\text{A5})$$

*Proof of Lemma 4.* We shall only show that, say,  $\mathcal{T}$  is  $K$  invariant. In fact, if  $(x, y) \in \mathcal{T}$  then

$$xy - 2x + 2 \leq 2x - 2x + 2 = 2 \quad (\text{A6})$$

and

$$\begin{aligned} y^2 - 2 &= xy - 2x + 2 - [y - (x - 2)](2 - y) \\ &\leq xy - 2x + 2, \end{aligned} \quad (\text{A7})$$

so that  $K(x, y) \in \mathcal{T}$ .

*Proof of Lemma 5.* We prove the second part Eq. (27). Let us first show that the set  $\mathcal{D}_1 = [1, \infty) \times (\infty, 1]$  is  $K$  invariant. In fact, if  $(x, y) \in \mathcal{D}_1$ , then  $y^2 \geq 1$  and

$$xy - 2x + 2 \leq y + 2(1 - x) \leq y \leq -1, \quad (\text{A8})$$

which shows that our set is indeed an  $F_{\sigma\delta}$  set. This proves the proposition.

*Proof of Lemma 2.* Employing the Cayley-Hamilton theorem we readily obtain

where  $K(x, y) \in \mathcal{D}_1$ .

Thus, starting with  $(x, y) \in \mathcal{D}_1$ , and denoting  $(x_n, y_n) = K^n(x, y)$  for  $n \geq 0$ , we have  $(x_n, y_n) \in \mathcal{D}_1$  for each  $n$ . As in Eq. (A8), we have  $y_1 \leq y = y_0$ , and by the same token the sequence  $\{y_n\}_{n=0}^{\infty}$  is nonincreasing. It then follows that the sequence  $\{x_n\}_{n=0}^{\infty}$  is nondecreasing. Set  $L = \lim_{n \rightarrow \infty} y_n$ . Then  $x_n = y_{n-1}^2 \rightarrow L^2$ . The foregoing discussion implies that, if  $L > -\infty$ , then the point  $(L^2, L)$  must be a fixed point of  $K$ . It is, however, easily verified that the only fixed points of  $K$  are  $(1, 1)$ ,  $(1, -1)$ , and  $(4, 2)$ . Consequently,  $L = -\infty$  unless  $(x, y) = (1, -1)$ . This proves part (2) of the Lemma.

*Proof of Proposition 5.* In view of Lemma 5 we have

$$\{v: |\chi_n| \xrightarrow[n \rightarrow \infty]{} \infty\} = \bigcup_{i=1}^{\infty} \{v: |\chi_i|, |\chi_{i+1}| > 2\}. \quad (\text{A9})$$

Now, each trace  $\chi_i$  considered as a function of  $v$ , is clearly continuous. Hence, each of the sets in the union on the right-hand side of (A9) is open, where so is their union. This proves the proposition.

*Proof of Lemma 7.* Since  $x_n \rightarrow \infty$  we have  $y_n \rightarrow \infty$  as well. Hence, for all sufficiently large  $n$

$$|y_{n+2}| = |x_{n+1} y_{n+1} - 2x_{n+1} + 2| = |y_n^2 y_{n+1} - 2y_n^2 + 2| \geq y_n^2 |y_{n+1} - 2| - 2 \geq y_n^2 |y_{n+1}| / 2. \quad (\text{A10})$$

By Lemma 6 we then get  $|y_n| \geq b \xi^{2^n}$  for some  $b > 0$  and  $\xi > 1$ , and hence  $x_n = y_{n-1}^2 \geq b^2 \xi^{2^{n-1}}$ , which proves the Lemma.

*Proof of Lemma 8.* Recall the definitions of  $\phi$  and  $\psi$  [Eq. (17)] and of the matrices  $\{P_n\}_{n=1}^{\infty}$  and  $\{Q_n\}_{n=1}^{\infty}$  [Eqs. (18)]. We routinely get

$$\text{tr}(P_0) = 2(\cos\phi + q \sin\phi), \quad (\text{A11})$$

$$\text{tr}(Q_0) = 2(\cos\psi + q \sin\psi), \quad (\text{A12})$$

$$\begin{aligned} \chi_1 &= \text{tr}(P_1) = 4q^2 \sin\phi \sin\psi + 4q \sin(\phi + \psi) + 2 \cos(\phi + \psi), \\ & \quad (\text{A13}) \end{aligned}$$

$$\begin{aligned} \chi_2 &= \text{tr}(P_0 Q_0 Q_0 P_0) \\ &= \text{tr}(P_0^2 Q_0^2) \\ &= \text{tr}[\text{tr}(P_0) P_0 - I][\text{tr}(Q_0) Q_0 - I] \\ &= 4(\cos\phi + q \sin\phi)(\cos\psi + q \sin\psi) \chi_1 \\ &\quad - 4(\cos\phi + q \sin\phi)^2 - 4(\cos\psi + q \sin\psi)^2 + 2, \end{aligned} \quad (\text{A14})$$

$$\chi_2 - \chi_1^2 + 2 = -4q^2 \sin^2(\phi - \psi). \quad (\text{A15})$$

The right-hand side of Eq. (A15) is strictly positive since the case  $\phi - \psi = k(d_1 - d_2)$  being an integer multiple of  $\pi$  has been excluded. Hence the Lemma is proved.

*Proof of Lemma 9.* First, note that if  $\text{tr}(A) = 0$  for some  $A \in \text{SU}(1, 1)$ , then  $A^2 = \text{tr}(A)A - I = -I$ . Consequently, if  $\text{tr}(A) = \text{tr}(B) = 0$ , then  $ABBA = A(-I)A = I$ . In our case, since  $\chi_i = 0$ , namely,  $\text{tr}(P_i) = \text{tr}(Q_i) = 0$ , we get  $P_{i+2} = P_i Q_i Q_i P_i = I$ , and similarly  $Q_{i+2} = I$ . By induction this implies  $P_n = Q_n = I$  for  $n \geq i + 2$ , which proves Lemma 9.

*Proof of Lemma 10.* (1) From (A13) and (A14) we see that, in general,  $\chi_1(q)$  is a quadratic polynomial in  $q$  and  $\chi_2(q)$  is a quartic. Their leading coefficients are  $4 \sin\phi \sin\psi$  and  $(4 \sin\phi \sin\psi)^2$ , respectively. Hence, if both  $\sin\phi \neq 0$  and  $\sin\psi \neq 0$ , the Lemma follows from (25) and Lemma 5. Now suppose that exactly one of the sines is nonzero, say  $\sin\phi \neq 0$  but  $\sin\psi = 0$ . Then  $\sin(\phi + \psi) = \pm \sin\phi \neq 0$ , so that, by (A13),  $\chi_1(q)$  as a function of  $q$  is nonconstant. Furthermore, according to (A14),  $\chi_2(q)$  is a quadratic polynomial with leading

coefficient

$$16 \sin \phi \cos \psi \sin(\phi + \psi) - 4 \sin^2 \phi \\ = 16 \sin^2 \phi \cos^2 \psi - 4 \sin^2 \phi = 12 \sin^2 \phi \neq 0,$$

and we conclude as in the former case. Finally, the

remaining case  $\sin \phi = \sin \psi = 0$  is excluded since we have assumed that  $k(d_1 - d_2) = \phi - \psi$  is not an integer multiple of  $\pi$ .

(2) The proof of this part follows straightforwardly from Lemma 7.

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