

## Structure Factor of Substitutional Sequences

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We study the structure factor for a large class of sequences of two elements  $a$  and  $b$  such that longer sequences are generated from shorter ones by a simple substitution rule  $a \rightarrow \sigma_1(a, b)$  and  $b \rightarrow \sigma_2(a, b)$ , where the  $\sigma$ 's are some sequences of  $a$ 's and  $b$ 's. Such sequences include periodic and quasiperiodic systems (e.g., the Fibonacci sequence), as well as systems such as the Thue–Morse sequence, which are neither. We show that there are values of the frequency  $\omega$  at which the structure factors of these sequences have peaks that scale with  $L$ , the size of the system like  $L^{\alpha(\omega)}$ . For a given sequence a simple one- or two-dimensional dynamical iterative map of the variable  $\omega$  can easily be abstracted from the substitution algorithm. The basin of attraction of a given fixed point or limit cycle of this map is a set of values of  $\omega$  at which there are peaks of the structure factor all of which share the same value of  $\alpha$ . Furthermore, only those values of  $\omega$  which are in the basin of attraction of the origin can have  $\alpha(\omega) = 2$ . All other peaks will grow less rapidly with  $L$ . We show how to construct many sequences which, like the Thue–Morse sequence, have no  $L^2$  peaks. Other qualitative features of the structure factors are presented. Our approach unifies the treatment of a large class of apparently very diverse systems. Implications for the band structure of these systems as well as for the analysis of sequences with more than two elements are discussed.

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Substitutional sequences are sequences of elements which are generated by a simple substitutional algorithm among the elements. In the case of two elements  $a$  and  $b$ , the algorithm takes the form

$$\begin{aligned} a &\rightarrow \sigma_1(a, b) \\ b &\rightarrow \sigma_2(a, b) \end{aligned} \tag{1}$$

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where the  $\sigma$ 's can be any string of  $a$ 's and  $b$ 's. Among the sequences so generated are the well-known Fibonacci sequence, for which  $\sigma_1 = ab$  and  $\sigma_2 = a$ , and the Thue–Morse sequence, for which  $\sigma_1 = ab$  and  $\sigma_2 = ba$ . The sequence  $F_n$  generated after  $n$  applications of the algorithm can often be more simply expressed as a sequence of appended  $F_j$ , and their complements  $\bar{F}_j$  with  $j < n$ , a famous example being the Fibonacci sequence of two elements, for which  $F_{n+1} = F_n F_{n-1}$ .

Such sequences are of very broad interest. They are of significance in fields as diverse as cryptography, time series analysis, and the study of cellular automata. In addition, there is much interest in substitutional sequences among those physicists who deal with quasiperiodic systems, and with layered materials in general (see, e.g., ref. 1). Among other things, it is possible to design and build artificial quasi-one-dimensional layered materials using, for example, molecular beam epitaxy. Many substitutional sequences have power spectra (i.e., the absolute square of the Fourier transform) that superficially resemble the power spectrum from a random sequence, even though the substitutional sequence is completely noiseless and deterministic. Using our method, it is easy to understand the most interesting features of these substitutional sequences and to see why and in what sense they resemble random sequences.

Aside from telling us about the structure factor, our work also has implications for the band structure (i.e., the energy spectrum) of a non-relativistic particle moving in a bivalued potential generated by the substitutional sequence (1). Although the band structure of such a system is not in general simply related to the structure factor of the potential, there is a relationship, and it is simple in certain limits. For example, if the perturbing potential in a tight-binding model is small, then the positions of the peaks<sup>3</sup> in the Fourier spectrum of the potential are tied to the positions of the gaps in the band structure. Very often, the gross nature of the band structure is determined largely by the symmetries of the system, and so this correspondence persists even for larger coupling constant. Thus, our approach to the structure factor will help to provide clearer qualitative insights into the band structure, particularly those aspects that are related to the symmetries of the system.

In this paper we will present a formalism for studying the structure factor of iterative strings composed of two elements  $a$  and  $b$ . We will show that for sequences of this type the structure of the Fourier spectrum can be related to properties of a simple one- or two-dimensional nonlinear

<sup>3</sup> In this paper the word “peak” in reference to a power spectrum or Fourier transform of a chain of length  $L$  will mean a contribution to the intensity at frequency  $\omega$  which has an asymptotic (large- $L$ ) form  $C(\omega) L^{z(\omega)}$ , where  $C$  is an  $L$ -independent factor.

iterative map of the frequency. In particular, we will show that the peaks in the power spectrum can be grouped into classes such that the heights of all peaks in a given class scale with the size of the system  $L$  as  $L^{\alpha(\omega)}$  with the same value of  $\alpha$  for all members of a given class. All frequencies that are in the basin of attraction of a given fixed point have the same value of  $\alpha$ . Furthermore, all the frequencies that are in the basin of attraction of a given limit cycle are in the same class and share a common value of  $\alpha$ . We will also argue that the only peaks for which  $\alpha = 2$  (which is the usual case seen in periodic and quasiperiodic systems) are those that are associated with the fixed point at  $\omega = 0$ : Only those frequencies which lie in the basin of attraction of this (trivial) fixed point can have peaks that scale like  $L^2$ . For all other frequencies the scaling exponent must be less than 2, or else it is not well defined.

These observations concerning peaks that scale like  $L^2$  are consistent with the result obtained by Bombieri and Taylor<sup>(2)</sup> for a physically somewhat different set of quasiperiodic systems. They showed that the existence of peaks that scale like  $L^2$  implies the existence of a single root of absolute value greater than one to a characteristic equation. However, not all sequences with a single characteristic root of absolute value greater than one have structure factor peaks with  $\alpha = 2$ , as we discuss in some detail below.

Our method lets us treat a very wide variety of sequences on an equal footing. Periodic and quasiperiodic sequences, as well as sequences such as the Thue–Morse sequence,<sup>(3,4)</sup> which is neither periodic nor quasiperiodic, can all be analyzed using the same techniques. Moreover, using our picture, the reasons behind the qualitatively different structure factors of these different kinds of systems become clear. In addition, we are able to relate various aspects of the structure factor of apparently very different systems to each other. For instance, we find that the structure factors of the Thue–Morse sequence and of a simple periodic sequence have the same support, i.e., peaks appear in the respective power spectra at the same frequencies, albeit with different values of  $\alpha$ . As a by-product of our investigations, we are able to develop some simple rules using which we can determine certain general qualitative features of the structure factor of a sequence by inspection. In the remainder of this paper we will describe the relationship between the power spectrum of a sequence and the associated iterative map. Fuller details profusely illustrated with interesting examples will be presented elsewhere.<sup>(5)</sup>

Consider a sequence generated by the substitution rules (1). Suppose the initial sequence consists of a single element, either  $a$  or  $b$ . Let  $F_0 = a$  and  $G_0 = b$ . Then, after  $n$  applications of the rules (1) to the initial sequence  $F_0$  a sequence  $F_n$  will be generated. Similarly,  $n$  applications of the

substitution rules to  $G_0$  will yield a sequence  $G_n$ . From (1), it is clear that  $G_{n+1}$  and  $F_{n+1}$  can be written in terms of  $G_n$  and  $F_n$  as

$$\begin{aligned} F_{n+1} &= \sigma_1(F_n, G_n) \\ G_{n+1} &= \sigma_2(F_n, G_n) \end{aligned} \tag{2}$$

For example, the Fibonacci sequence that begins with the element  $a$  has the form  $F_{n+1} = F_n G_n$ , but  $G_{n+1} = F_n$ , so that we recover the familiar form  $F_{n+1} = F_n F_{n-1}$ . Similarly, the Thue–Morse sequence can be written as  $F_{n+1} = F_n G_n$  with  $G_n = G_{n-1} F_{n-1}$ . But in this case, a further simplification is possible: The symmetry of the substitution rules clearly indicates that  $G_n = \bar{F}_n$ , where the bar indicates the complement, which means interchanging  $a \leftrightarrow b$ . Thus, for the Thue–Morse case,  $F_{n+1} = F_n \bar{F}_n$ .

Now define a function  $F_n(x)$  for integer  $x$  between 1 and  $L$ , which takes on two possible numerical values (e.g.,  $\pm 1$ ), depending on whether the  $x$ th element in the string  $F_n$  is  $a$  or  $b$ . Consider the Fourier transforms  $f_n(\omega)$  and  $g_n(\omega)$  of the sequences  $F_n$  and  $G_n$ , respectively defined by

$$f_n(\omega) = \sum_{x=1}^L e^{2\pi i \omega x} F_n(x)$$

and similarly for  $g_n(\omega)$ . Here  $L$  is the length of the  $n$ th-order string (e.g., for the Thue–Morse case,  $L = 2^n$ ). Since the  $\sigma_i$  are strings of their arguments, it is not difficult to see that the Fourier transforms  $f_{n+1}(\omega)$  and  $g_{n+1}(\omega)$  can be expressed in terms of  $f_n(\omega)$  and  $g_n(\omega)$  in the following form:

$$[t_{n+1}(\omega)]_i = [M_n(\omega)]_{ij} [t_n(\omega)]_j \tag{3}$$

where the vector  $t_n(\omega) = (f_n(\omega), g_n(\omega))$ , and  $M$  is a two-by-two matrix. The elements of  $M$  have a very specific form. Each element is just a sum of phases of the form  $\exp[2\pi i(kp_n + lq_n)\omega]$ , where  $p_n$  is length of the string  $F_n$ ,  $q_n$  is the length of the string  $G_n$ , and  $k$  and  $l$  are integers. For example, for the Fibonacci sequence,

$$M_n(\omega) = \begin{bmatrix} 1 & \exp(2\pi i p_n \omega) \\ 1 & 0 \end{bmatrix} \tag{4}$$

while for the sequence defined by  $a \rightarrow aba$  and  $b \rightarrow ba$ ,

$$M_n(\omega) = \begin{bmatrix} 1 + \exp[2\pi i(p_n + q_n)\omega] & \exp(2\pi i p_n \omega) \\ \exp(2\pi i q_n \omega) & 1 \end{bmatrix} \tag{5}$$

To understand how the sizes of the peaks in the power spectrum depend on the length of the chain, we note first that since there are, in general, two coupled sequences of length  $p_n$  and  $q_n$ , the matrices  $M_n(\omega)$  can be written in the following form, in which all the  $n$  dependence is carried by the arguments of the matrices:

$$M_n(\omega) = M(\Theta_n) \tag{6}$$

with

$$\Theta_n = (p_n \omega, q_n \omega) \tag{7}$$

Furthermore,  $M_j(\omega) = M(\Theta_j) = M(\Theta_j \bmod 1)$ , so that if we define  $\Omega_j = \Theta_j \bmod 1$  (by which we mean that  $\bmod 1$  applies to each component of the vector), then, using Eqs. (3) and (6), we can write the Fourier transform of the  $n$ th iterate in the matrix product form

$$[t_n(\omega)]_i = \left[ \prod_{j=1}^n M(\Omega_j) \right]_{ik} [t_0(\omega)]_k \tag{8}$$

Many of the properties of the power spectra (or structure factors) can be understood by studying the  $j$  dependence of  $\Omega_j$ . It is easy to show that

$$\Omega_{n+1} = A[\Omega_n] = M(\mathbf{0}) \cdot \Omega_n \bmod 1, \quad 0 \leq \Omega_n < 1 \tag{9}$$

$A$  is a nonlinear operator which is independent of  $n$  and depends on the substitution rules. Its action consists of multiplication by  $M(\mathbf{0})$  followed by taking  $\Omega_{n+1} \bmod 1$  in each of its components.<sup>4</sup>

Equation (9) defines a two-dimensional nonlinear iterative map from which many of the features of the power spectra can be gleaned. If  $\sigma_1$  and  $\sigma_2$  both contain the same number of elements, then the two-dimensional map is degenerate and reduces to a one-dimensional map. For pedagogical purposes, it is simplest to consider such an equal-length case and study the resulting one-dimensional map, and in the ensuing discussion we shall often do that. Most of the statements made in that context apply (with obvious modification) to the two-dimensional maps as well.<sup>(5)</sup>

For the cases in which  $\sigma_1$  and  $\sigma_2$  are of equal length, (9) reduces to

$$\omega_{n+1} = R\omega_n \bmod 1 \tag{10}$$

where  $R$  is the length of  $\sigma_1$  and of  $\sigma_2$ . In the Thue–Morse case, for example,  $R = 2$ .

<sup>4</sup> This procedure for defining  $A$  is possible only because the elements of the matrix  $M(\mathbf{0})$  are all integers. See ref. 5 for further details.

Consider now  $t_n(\omega)$  for large  $n$ . It is useful to distinguish among three qualitatively different behaviors for the iterates  $\Omega_n$ : asymptotic fixed point behavior, limit cycle behavior, and "chaotic" behavior. These different behaviors will be associated with different behaviors for the peaks in the power spectra of the associated sequence. Recall that by a peak in the power spectrum at a frequency  $\omega$  we mean a contribution to the intensity which has an asymptotic form  $C(\omega)L^{\alpha(\omega)}$ , where  $C$  is an  $L$ -independent amplitude. We will see that values of  $\omega$  for which there is a well-defined exponent  $\alpha$  are those associated with the fixed point and limit-cycle behavior of the map (9). Values of  $\omega$  which lie in the basin of attraction of an aperiodic or chaotic attractor do not have simple scaling peaks in the structure factor.

First, consider a fixed point  $\Omega_n^*$  of the map (9). From (8), it is clear that for all values of  $\omega$  such that an associated  $\Omega_n$  lies in the basin of attraction of the fixed point, the power spectra  $|[t_n(\omega)]_i|^2$  will generically contain a peak which scales asymptotically with the size of the system  $L$  as  $L^{\alpha(\omega)}$  with the same value of the  $\alpha$  for all such  $\omega$ .<sup>5</sup> This is because the  $\Omega_n$  will eventually be arbitrarily close to  $\Omega_n^*$ , so that for large  $n$  most of the factors of  $M$  in (8) will be evaluated at or very near the fixed point. (In fact, in the examples we have studied, the fixed point basins of attraction are discrete sets of points, and the most important power spectrum peaks are associated with values of  $\omega$  that reach their fixed points in a finite number of iterations. See below for more details.) Generically, the asymptotic behavior of the power spectrum will be dominated by the largest eigenvalue of the matrix  $M$  in Eq. (8), evaluated at  $\Omega_n^*$ . If  $\lambda$  is the largest eigenvalue, and if the length of the sequence grows by a factor of  $R$  with each iteration, then it is easy to see that

$$\alpha(\omega) = 2 \ln |\lambda(\Omega_n^*)| / \ln R \quad (11)$$

If  $\sigma_1$  and  $\sigma_2$  are of equal length (such as in the Thue–Morse problem), then Eq. (8) can be simplified to a nonmatrix form. In such a case,  $\alpha$  is given simply by  $\alpha(\omega) = \ln |M(\Omega^*)|^2 / \ln R$ .

The second type of behavior which the  $\Omega_n$  can express is limit cycle behavior. The frequencies which lie in the basin of attraction of a  $k$ -cycle (including of course the  $k$  stopover points) will have peaks in the power

<sup>5</sup> Of course, for a given sequence generated from a given zeroth-order chain, the values of  $\omega$  at which there are scaling peaks in the structure factor may depend on the zeroth-order chain. In the context of the two-dimensional map, this just reflects the fact that the starting value  $\Omega_0$  lies on some line in the two-dimensional plane determined by the form of the zeroth-order chain. In general, only a subset of the entire basin of attraction (in the  $\Omega$  plane) of some fixed point or limit cycle may be associated with a sequence generated from a given zeroth-order chain.

spectrum all of which asymptotically grow with the same exponent. It is easy to see that this is so by considering the  $k$ th iterate  $M^{[k]}$  of the matrix  $M$ . Any point  $\Omega_n$  which is a stopover point of a  $k$ -cycle will be a fixed point with respect to  $M^{[k]}$ . Thus, after substituting  $M^{[k]}$  for  $M$  in Eq. (8), we can apply the fixed point discussion presented above almost without change to this case also. It is clear that the form of  $M^{[k]}$  is the same for any  $\Omega_n$  in the limit cycle, and so all stopovers of a given limit cycle share the same  $\alpha(\omega)$ . Similarly, the  $\omega$ 's associated with the basin of attraction of the limit cycle will have the same asymptotic  $\alpha(\omega)$  as the elements of the limit cycle. If, for simplicity, we again consider those cases in which the matrix equation can be reduced to a simple scalar form, then it is easy to show that  $\alpha(\omega) = \ln |M^{[k]}|^2 / (k \ln R)$ .

The other generic type of behavior the  $\Omega_n$  can display is chaotic or aperiodic behavior, by which we mean that the sequence of  $\Omega$ 's does not repeat in a finite number of iterates. In general there will not be a well-defined  $\alpha(\omega)$  associated with this kind of behavior. For these values of  $\omega$  the asymptotic behavior of the power spectrum will generally not be that of a simple power law.<sup>6</sup>

To illustrate our procedure, let us turn to some simple examples. First, consider the well-studied Fibonacci sequence. In this case there is only one fixed point of the two-dimensional map (9), which is at the origin,  $\Omega = 0$ . It is easy to see that all the frequencies associated with points in the basin of attraction of this fixed point at the origin have power spectrum peaks which scale with the size of the system as  $L^2$ ; i.e., for these  $\omega$ 's,  $\alpha(\omega) = 2$ . Furthermore, it can be shown (with some tomentose algebra)<sup>(2,5)</sup> that there are no other  $\omega$ 's for which the power spectrum has peaks which scale like  $L^2$ . Thus, the usual power spectrum peaks of the Fibonacci lattice are those associated with the basin of attraction of the fixed point at the origin.

In fact, this is a general property of these substitutional sequences: It can be shown<sup>(2,5)</sup> that for any sequences generated by expressions of the form (1), all the peaks that scale with  $\alpha = 2$  are located at values of  $\omega$  which are associated with  $\Omega$ 's which lie in the basin of attraction of the fixed point at the origin. (For a closely related class of systems, Bombieri and Taylor<sup>(2)</sup> also showed that a necessary, but not sufficient condition for this scenario is the existence of a single characteristic root of absolute value greater than one.) We emphasize that this result applies not only to the

<sup>6</sup> However, for finite-length sequences these aperiodic points may, within the resolution of the structure factor, be degenerate with a nearby (in  $\omega$ ) scaling peak. Furthermore, although for any finite number of iterations  $\alpha(\omega)$  is not defined, insofar as there is no systematic  $L$  dependence of the power at a chaotic value of  $\omega$ , it may be said that  $\alpha(\omega)$  is zero on average. See ref. 4 for more details.

standard quasiperiodic sequences which can be produced by (1), but also to other more general types of sequences that do not naturally fall into this category, but which are generated by (1).

In addition to these  $L^2$  peaks, there are other peaks, associated with limit cycles of the map (9), but they grow less rapidly with  $L$ , and thus diminish relative to the primary  $L^2$  peaks in the infinite-volume limit. Thus, for such substitutional sequences, and for the much studied quasiperiodic sequences in particular, there is an enormous amount of subsidiary structure associated with the limit cycles of the maps (9) which is of significance for finite-size systems.

Among the other, nonquasiperiodic sequences which can be generated by the rules (1) is the very interesting Thue–Morse lattice.<sup>(3,4)</sup> To understand further the potential of our analysis, it is useful to quickly review some of the properties of that system. In particular, it will be illuminating to compare the Thue–Morse sequence with an ordinary periodic sequence with period 2. As stated earlier, the Thue–Morse sequence is determined by (1) with  $\sigma_1 = ab$  and  $\sigma_2 = ba$ , while the ordinary period-2 sequence is defined by  $\sigma_1 = ab$  and  $\sigma_2 = ab$ . The map (10) associated with both these systems is the same and is shown in Fig. 1. It is clear that the fixed point at  $\Omega = 0$  has a nonnull basin of attraction in these cases. The structure factor of the periodic system contains the usual  $L^2$  peak associated with period 2. On the other hand, the structure factor of the Thue–Morse system

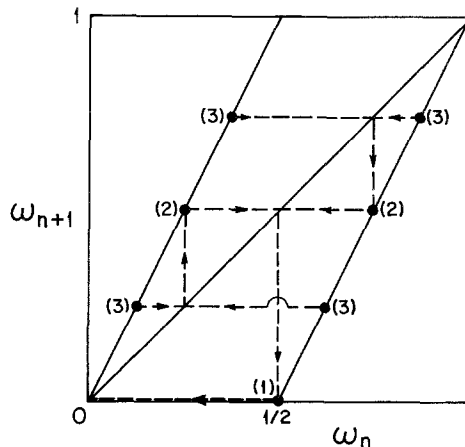


Fig. 1. The iterative map, Eqs. (9) and (10), for the Thue–Morse and period-2 simple periodic sequences. The line  $\omega_{n+1} = \omega_n$  is also shown. Some of the points in the basin of attraction of the fixed point at  $\omega = 0$  are indicated. Their route to the fixed point under the iteration (10) is shown by the arrows. The numbers in parentheses next to the points indicate how many iterations are necessary to reach the fixed point.



has no spectral peaks that grow like  $L^2$ . In the light of our previous statements, how can we understand this difference?

According to our earlier discussion, since the map of Fig. 1 is the same for both cases, then the values of  $\omega$  for which there may be peaks that scale like  $L^2$  is the same. Furthermore, the matrix  $M$  is very similar in the two cases, being

$$M_n(\omega) = \begin{cases} \begin{bmatrix} 1 & \exp(2\pi i p_n \omega) \\ \exp(2\pi i p_n \omega) & 1 \end{bmatrix} & \text{Thue-Morse} \\ \begin{bmatrix} 1 & \exp(2\pi i p_n \omega) \\ 1 & \exp(2\pi i p_n \omega) \end{bmatrix} & \text{periodic} \end{cases} \quad (12)$$

It is clear that for  $\omega = 0$  the matrices are identical, and so are their eigenvalues. In this case, the largest eigenvalue at  $\omega = 0$  is 2, corresponding, according to Eq. (11), to an  $L^2$  peak at the origin. For general  $a$  and  $b$  there will be an  $L^2$  peak at  $\omega = 0$  in both these cases. This peak just counts the average value of the elements in the sequence which is the same in both cases. (Of course, if  $b = -a$ , then the coefficient of this peak will be zero, since zero will be the average value of the elements.) Now consider other values of  $\omega$  that lie in the basin of attraction of  $\omega = 0$ . Look first at  $\omega = 1/2$ , which is one iteration away from  $\omega = 0$ . Multiplying  $M(0) \cdot M(1/2)$  for the periodic case gives a result proportional to the identity matrix, while for the Thue-Morse case it gives a null matrix. Thus, in the Thue-Morse system the final two iterates to the fixed point are orthogonal. Since every  $\omega$  in the basin of attraction of zero must pass through  $\omega = 1/2$  on the way to  $\omega = 0$ , this orthogonality effectively sets the coefficient of every would-be  $L^2$  peak to zero. For the periodic case, on the other hand, there is a peak at  $\omega = 1/2$ . However, the matrices at  $\omega = 1/4$  and  $3/4$  are orthogonal to  $M(1/2)$ , so that the coefficients of the  $L^2$  peaks at the other values of  $\omega$  in the basin of attraction of  $\omega = 0$  are all zero. This is the most striking difference between the Thue-Morse sequence with its bizarre structure and the ordinary periodic sequence: The support over  $\omega$  for spectral peaks that scale like  $L^2$  is the same in both cases, but because of an altered minus sign, the coefficient of all the  $L^2$  peaks is zero in the Thue-Morse case.<sup>7</sup>

We can easily deduce some other interesting properties of the Thue-Morse and periodic lattices from our approach. First, since the map in Fig. 1 is the same for both cases, the support for spectral peaks in the structure factor is the same in both cases. What is different between the two

<sup>7</sup> Notice that both the Thue-Morse and periodic systems have a single characteristic root of absolute value greater than one, yet there are no  $L^2$  peaks in the Thue-Morse system. Although Bombieri and Taylor,<sup>(2)</sup> correctly conclude that  $L^2$  peaks require a single characteristic root of absolute value greater than one, such a condition is not sufficient to ensure the existence of  $L^2$  peaks. This has also been noted independently by Aubry *et al.*<sup>(6)</sup>

is the set of matrix eigenvalues associated with the various limit cycles of the map. In the Thue–Morse case, these eigenvalues give rise to nontrivial values of the exponents  $\alpha(\omega)$ . Moreover, because of the absence of  $L^2$  peaks, a set of peaks associated with a period-two limit cycle of Fig. 1 and for which  $\alpha(\omega) = \ln 3 / \ln 2$  are the most significant peaks in the large- $L$  limit. (These include the dominant peak at  $\omega = 1/3$ .) On the other hand, in the periodic case, these peaks as well as those associated with other limit cycles of the map in Fig. 1 are merely the finite-size corrections to the infinite- $L$  structure factor for the simple periodic system. On the basis of a simple physical argument,<sup>(5)</sup> we expect all these peaks (for all limit cycles) to have  $\alpha(\omega) = 0$ . Due to a remarkable trigonometric identity, this is indeed the case. Thus, the persistent finite-size corrections of the structure factor in the periodic case occur at those values of  $\omega$  (and only those values of  $\omega$ ) for which there are peaks in the Thue–Morse structure factor.

A number of other intriguing general properties of the structure factors of substitutional sequences should be mentioned here. They will be explicitly demonstrated in a subsequent publication.<sup>(5)</sup> First, it is possible to construct many sequences which, like the Thue–Morse sequence, have no peaks that scale like  $L^2$  (except possibly for a trivial peak at  $\omega = 0$ ). Consider a sequence of the form

$$F_{n+1} = \Sigma(F_j; \bar{F}_j), \quad j = 1, \dots, n \quad (13)$$

where  $\Sigma$  is some string of the  $F$ 's and  $\bar{F}$ 's. If for every  $j$  for which there is at least one  $F_j$  ( $\bar{F}_j$ ) in the string there is also at least one  $\bar{F}_j$  ( $F_j$ ), then the sequence will have no nontrivial  $L^2$  peaks. An example is the sequence  $F_{n+1} = F_n \bar{F}_n \bar{F}_n$ , which is generated by the rules  $\sigma_1 = abb$  and  $\sigma_2 = baa$ . The mechanism by which this occurs is very similar to that of the Thue–Morse case. Second, the formalism presented here for sequences with two elements can easily be generalized to substitutional sequences containing any number of distinct elements. In particular, the structure factor of substitutional sequences with  $k$  elements is related to the behavior of a  $k$ -dimensional iterative map in a way similar to that which we have described here for the  $k=2$  case. Finally, for those sequences for which  $\sigma_1$  and  $\sigma_2$  are each a  $k$ -string (e.g., the Thue–Morse or periodic case in which both  $\sigma$ 's are two-strings, but not the Fibonacci case), each action of the map, Eq. (9), can be directly related to an operator which shifts the decimal point one place to the right in a base- $k$  representation of the original frequency  $\omega$ .

In this paper we have considered the structure factors for a large class of substitutional sequences which encompass a very diverse set of objects, including periodic and quasiperiodic systems, as well as other sequences with a more complex structure. The structure factors for all these systems, although apparently very different, can all be very simply treated in the

same unified picture. We have shown that the peaks in the structure factor of such a sequence can be grouped into classes such that all members of a given class scale with  $L$ , the size of the system, with the same exponent  $\alpha$ . The values of  $\omega$  at which there are peaks belonging to a given class can be determined by a simple iterative map that can easily be abstracted from the algorithm of the substitutional sequence. All those  $\omega$ 's that lie in the basin of attraction of the same fixed point or limit cycle of the map will have peaks in the structure factor that scale with the same value of  $\alpha$ . We further indicated how to calculate  $\alpha$  explicitly. Moreover, the only peaks that scale with  $\alpha = 2$  (the usual situation of peaks that survive in the infinite-volume limit) are associated with  $\omega$ 's that lie in the basin of attraction of the fixed point at zero. All other peaks will grow less rapidly with  $L$  for large  $L$ . In addition, using our approach, we were able to abstract a number of other useful characteristics of the structure factors, including simple sufficient conditions on the substitutional algorithm such that the structure factor is guaranteed to have no peaks that grow proportional to  $L^2$ .

In addition to its intrinsic theoretical interest, our picture should help to unify and clarify a number of important aspects of these unusual sequences, and in particular should be a very useful tool in helping to design artificial quasi-one-dimensional materials with specific structural and electronic properties.

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