# Generalized measures for physical properties of nonperiodic chains

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The physical properties associated with nonperiodic deterministic sequences (such as the Fibonacci sequence) are studied by means of an information-theoretic measure, which is a generalization of one previously defined to measure the disorder of such sequences. In application to electronic or optical transmission, the measure allows the definition of an effective transmission coefficient, which is computationally more efficient to calculate, while still exhibiting the same structure (e.g., self-similarity), as the exact transmission coefficient.

# I. INTRODUCTION

Recently<sup>1</sup> we introduced a measure of disorder in nonperiodic sequences. Such sequences can be generated with substitution rules, an example of which is  $A \rightarrow A^{m}B^{n}, B \rightarrow A$ . For m = n = 1, this rule produces the well-known Fibonacci sequence ABAABABAABAAB... These sequences find their application as one-dimensional analogs of quasicrystals or of quasiperiodic superlattices. The purpose of this paper is to generalize this measure to a measure for physical properties associated with such a chain.

In particular, we will be considering the property of transmission. There has been much recent interest in optical<sup>2-4</sup> and electronic<sup>5-8</sup> transmission, and especially with how the transmission coefficient varies with energy. This variation can be analyzed to measure the resistance or conductance through the chain and to find approximate band structures. For quasicrystals, the band structures often show self-similar features and typical calculations to illustrate this require a large number of atoms or layers. In this paper, we study a measure leading to an effective transmission coefficient, using smaller numbers of atoms or layers, which produces qualitatively similar results.

In Sec. II, we discuss the general concepts underlying the measurement of properties of nonperiodic sequences, with relation to our previous work. In Sec. III, we examine the measurement of electronic transmission, in the context of three popular models (Kronig-Penney, Kronig-Penney  $\delta$  function, and tight-binding), and in Sec. IV, we proceed to the measurement of optical transmission. The work is summarized in Sec. V. Atomic units  $(\hbar = m_e = 1)$  are used throughout.

## **II. GENERAL MEASURES**

Consider a chain of letters AB..., where each letter represents an atom or a group of atoms. For each letter (or string of letters) *i* in the chain, we suppose we have  $\rho_i$ , a real positive quantity, representing a physical property of the *i*th member. The particular properties which we will be concerned with in this paper are the transmission coefficients, but in principle, the theory may be applied to any such  $\rho_i$ . Given such a chain of length N, we define the measure of the physical property as

$$h_N = -\log_2 \mu_N , \qquad (1)$$

where

$$\mu_N = \left[\prod_{i=1}^N \rho_i\right]^{1/N}.$$
(2)

Note that if  $\rho_i$  is zero for any letter of the chain, then the measure is infinite. Note also that the base of logarithms, in (1) and elsewhere, is arbitrary, although it proves to be most convenient to have it equal to the number of different letters, so we take it to be 2 here.

We will now consider the measure as  $N \rightarrow \infty$ , and obtain a probabilistic expectation value for the physical property over the infinite chain. Putting (2) into (1) leads to

$$h_N = -\frac{1}{N} \sum_{i=1}^N \log_2 \rho_i \ . \tag{3}$$

We can rewrite (3) as

$$h_N = -\sum_k \frac{n_k}{N} \log_2 \rho_k \quad , \tag{4}$$

where the sum is now over the *distinct* members of the chain, and  $n_k$  is the number of occurrences of the kth member in a chain of length N. Now, as  $N \to \infty$ , we have that  $n_k/N \to P_k$ , where  $P_k$  is the probability of that member. Thus,

$$h = \lim_{N \to \infty} h_N = -\sum_k P_k \log_2 \rho_k \quad . \tag{5}$$

By "distinct members," we may mean either the set of possible *m* strings (for example,  $\{A,B\}$ , or  $\{AA, AB, BA, BB\}$ ) or the *l*th substitution of such a set [for example,  $\{S_{I}(A), S_{I}(B)\}$  or

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 $\{S_l(AA), S_l(AB), S_l(BA), S_l(BB)\}\}$ . As a specific example for the Fibonacci sequence, if we used  $\{S_3(A), S_3(B)\}$ , then we would have two members  $S_3(A) = ABAAB$  and  $S_3(B) = ABA$ , so that we could regard the chain as being made up of ABAAB and ABA, as opposed to the usual A and B. As a second example, we can consider a completely periodic sequence ABABABAB... to be generated by the substitution rule  $A \rightarrow ABA, B \rightarrow BAB$ , and thus to be made up of the two strings ABA and BAB, both of probability 0.5. Consequently, we could work with ABA and BAB as the members, rather than the one-letter strings A and B.

We will consider two special cases. For the first case, we take the distinct members to be strings of fixed length m and

$$\rho_k = P(x_m | x_1 x_2 \cdots x_{m-1}) , \qquad (6)$$

the conditional probability of  $x_m$  given the string  $x_1x_2 \cdots x_{m-1}$  (i.e., the probability that the string  $x_1x_2 \cdots x_{m-1}$  is followed immediately by  $x_m$ ). Here each  $x_i$  belongs to the set of letters (the "alphabet") comprising the chain. Substituting (6) into (5) gives

$$h = -\sum_{m \text{ strings}} P(x_{1} \cdots x_{m}) \log_{2} P(x_{m} | x_{1} \cdots x_{m-1})$$
  
=  $-\sum_{m \text{ strings}} P(x_{1} \cdots x_{m-1}) P(x_{m} | x_{1} \cdots x_{m-1})$   
 $\times \log_{2} P(x_{m} | x_{1} \cdots x_{m-1})$   
=  $\sum_{(m-1) \text{ strings}} P(x_{1} \cdots x_{m-1}) H(X | x_{1} \cdots x_{m-1})$ , (7)

where

$$H(X|x_{1}\cdots x_{m-1}) = -\sum_{x_{m}} P(x_{m}|x_{1}\cdots x_{m-1}) \times \log_{2} P(x_{m}|x_{1}\cdots x_{m-1}) ,$$
(8)

is the conditional entropy associated with the string  $x_1 \cdots x_{m-1}$ . The quantity h in (7) is the informationtheoretic entropy that we have used previously<sup>1</sup> as a measure of disorder in such strings. This is similar in structure to the entropy used in thermodynamics, but here we use it in a different context. We note that the minimum value of the entropy (7) is 0, which corresponds to complete order.

For the second case, we take  $\rho_k = t_k$ , the transmission coefficient through the kth member, so that, from (5),

$$h = -\sum_{k} P_k \log_2 t_k , \qquad (9)$$

where the summation is over distinct members, and of course,

$$\sum_{k} P_{k} = 1 . \tag{10}$$

Each quantity  $t_k$  is the transmission through a substring (a "member") of the chain, so that h represents a measure of transmission through the chain, which depends on the

order of the members of the chain. For the calculations of the next section, each  $P_k$  will be for a moderately long, but finite, chain C(N). In order to calculate these probabilities, the chain can be approximated by an infinite chain  $C(\infty)$ . For the latter chain, the appropriate substitution rule can be used to facilitate the calculation of the probabilities of the strings, since  $C(\infty) \rightarrow C(\infty)$ . As an example, suppose we were to use the particular choice of members (in the Fibonacci sequence) mentioned earlier. We would have two possible values of  $t_k$ , viz.  $t_1$  and  $t_2$ , one for each of the strings ABAAB and ABA, and we would need to calculate  $P_k$  for each of these. Using the substitution rule three times, when  $A \rightarrow ABAAB$  and  $B \rightarrow ABA$ , we still preserve  $C(\infty) \rightarrow C(\infty)$ . Since the chain was originally composed of strings of A's and B's, this analysis shows that it can also be regarded as a chain composed of ABAAB's and ABA's, so that, ignoring the small effects from approximating a large finite chain by an infinite chain, we have  $P_1 + P_2 = 1$ . For comparative purposes, it is useful to define an effective transmission coefficient  $t_{\rho}$  as

$$t_e = 2^{-h}$$
 (11)

In the following sections we will consider (9) and (11)in reference to electronic and optical transmission through one-dimensional chains. To illustrate this idea, we take the Fibonacci golden-mean sequence, which is generated by the substitution  $A \rightarrow AB$ ,  $B \rightarrow A$ . To model the chain, we use as distinct members the set  $\{S_7(AB), S_7(BA), S_7(AA)\}$ , omitting  $S_7(BB)$ , since BB does not occur. The reason for the choice of this set is that, in order to get reasonable convergence from a set of  $S_1$  (*m* strings), it is necessary to have fairly long chains. These can be obtained using large m and small l, which produces a large number of members, or small m and moderate l, which produces a small number of members. We find the latter case preferable, and for the particular choice made above, we have three members whose chain lengths are 55, 55, and 68, respectively. We note that

$$P(xy) = P(S_l(xy)) , \qquad (12)$$

where  $x, y \in \{A, B\}$ , and these probabilities have been calculated in Ref. 1 as P(AB) = P(BA) = 0.381966 and P(AA) = 0.236068. As a check on the convergence of these calculations, the values of  $t_e$  were compared with the exact transmission coefficients for very long chains, and were found to be in good agreement, but the approximation  $t_e$  proved to be much quicker computationally.

It is important to emphasize that the  $t_k$ 's of Eq. (9), which are combined to form  $t_e$  in (11), are obtained from full quantum-mechanical calculations for model chains. In the next section, we discuss the models used to calculate the transmission coefficients for the three representative chains considered. In practice the size of the chains in any application will be large and the exact size will almost certainly be unknown so that, in principle, the calculations involving our smaller representative chains form just as valid a model as the large chains involving several hundred atoms. Since the calculations are in agreement with those for longer chains we believe that we have found a more effective measure for the transmission through the system. Of course if we increase the size of the representative chains, then for sufficiently long chains, the transmission coefficients will be virtually the same. However, for the size of chains used here, this is not the case but, nevertheless, the measure leads to the same qualitative band structures as that obtained with more precise numerical calculations. In particular, the self-similarity features, which are typically found for these band structures, are found (approximately) in most of the models used here. On the other hand, if very short subchains (of length 2, say) were to be used, then one would not expect the resulting band structure to reflect the actual band structure realistically. However, the efficiency can only be assessed by numerical comparisons. For the nonperiodic sequences considered in this paper, the results indicate that good qualitative band structures can be obtained from intermediate-length subchains.

## **III. ELECTRONIC TRANSMISSION**

We here consider electronic transmission through a one-dimensional chain of length N, using three different models:<sup>9</sup> Kronig-Penney (KP), Kronig-Penney  $\delta$  function (KP $\delta$ ), and tight-binding (TB).

#### A. Kronig-Penney model

The KP model is a one-dimensional array of rectangular barriers of height  $V_{j+1}$  and width  $d_{j+1}$ , bounded by zero-potential regions of width  $a_j$  and  $a_{j+2}$ . (The index jis taken to be odd). The regions of nonzero potential start at  $X_j$  and end at  $X_{j+1}$  (see Fig. 1). The Schrödinger equation is solved in each region and the wave functions and their derivatives are matched at each point  $X_j$ . In regions j and j+1, we take  $X_j$ , to be the origin, and the forms of the wave functions are

$$\psi_j = A_j \cos kx + B_j \sin kx \quad , \tag{13}$$

where

$$k = (2E)^{1/2}, E > 0,$$
 (14)



FIG. 1. Kronig-Penney model of a rectangular potential barrier.

and

$$\psi_{j+1} = A_{j+1} \cosh k_{j+1} x + B_{j+1} \sinh k_{j+1} x$$
, (15)

with

$$k_{j+1} = [2(V_{j+1} - E)]^{1/2}, E < V_{j+1}.$$
 (16)

In region j+2, we take the origin at  $X_{j+2}$  and

$$\psi_{j+2} = A_{j+2} \cos kx + B_{j+2} \sin kx \quad . \tag{17}$$

The continuity conditions at the boundaries lead to the recursive relationship

$$\begin{vmatrix} A_{j+2} \\ B_{j+2} \end{vmatrix} = M(j) \begin{vmatrix} A_j \\ B_j \end{vmatrix},$$
(18)

where

$$M(j) = \begin{pmatrix} k \cos\theta_j & \sin\theta_j \\ -k \sin\theta_j & \cos\theta_j \end{pmatrix} \begin{pmatrix} \cosh y_j & \sinh y_j \\ k_{j+1} \sinh y_j & k_{j+1} \cosh y_j \end{pmatrix} \\ \times \begin{pmatrix} 1/k & 0 \\ 0 & 1/k_{j+1} \end{pmatrix},$$
(19)

$$\theta_j = ka_{j+2} \text{ and } k_{j+1}d_{j+1} = y_j. \text{ Note that}$$

$$\det M(j) = 1.$$
(20)

Thus, we can build up an expression of the form

$$\begin{bmatrix} \boldsymbol{A}_{2N+1} \\ \boldsymbol{B}_{2N+1} \end{bmatrix} = \boldsymbol{M} \begin{bmatrix} \boldsymbol{A}_1 \\ \boldsymbol{B}_1 \end{bmatrix}, \qquad (21)$$

where

$$M = \prod_{r=1}^{N} M(2r-1) .$$
 (22)

Since we are considering a plane wave in incident region 1 and moving towards the right, it is more convenient to consider the wave functions in regions 1 and 2N + 1 in the forms

$$\psi_1 = e^{ikx} + Ce^{-ikx} \tag{23}$$

and

$$\psi_{2N+1} = De^{ikx} , \qquad (24)$$

where  $|C|^2$  denotes the reflection coefficient and  $|D|^2$  the transmission coefficient. Comparing (23) and (24) with (13), it is clear that we have

$$A_1 = 1 + C$$
,  $B_1 = (1 - C)i$ ,  $A_{2N+1} = D$ ,  $B_{2N+1} = iD$ .  
(25)

From (21) and (25) we obtain

$$\begin{pmatrix} D \\ iD \end{pmatrix} = M \begin{pmatrix} 1+C \\ (1-C)i \end{pmatrix} ,$$
 (26)

and we can calculate the transmission coefficient for the kth member to be

$$t_k = |D|^2 = 4/(M_{11}^2 + M_{12}^2 + M_{21}^2 + M_{22}^2 + 2) , \qquad (27)$$



FIG. 2. Effective coefficient of electronic transmission  $t_e$  versus energy E for the KP model, with  $d_A = 0.8$ ,  $d_B = 0.5$ ,  $a_A = a_B = 1.0$ , and  $V_A = V_B = 1.0$ .

where  $M_{ii}$  are the elements of M.

In Figs. 2 and 3, we present calculations of the effective transmission coefficient  $t_e$  versus energy E, for the case of the barriers arranged in a Fibonacci sequence. To show the qualitative structure, model parameters have been used, varying (i)  $d_A$  and  $d_B$  (Fig. 2), and (ii)  $a_A$  and  $a_B$  (Fig. 3). Both graphs exhibit a band structure, and include isolated peaks of high transmission. There are clearly several main bands, with a division of each one into subbands, and we can see indications of the self-similarity typically observed in such calculations. For example, in Fig. 2, the band in the energy region (0.65, 1.0)



FIG. 3. Effective coefficient of electronic transmission  $t_e$  versus energy E for the KP model, with  $d_A = d_B = 0.8$ ,  $a_A = 2.0$ ,  $a_B = 1.0$ , and  $V_A = V_B = 1.0$ .

shows a main central structure and two side structures, each of which is further split into substructures. Calculations made varying  $V_A$  and  $V_B$  give very much the same results as those obtained by varying  $d_A$  and  $d_B$ . This is an expected result, since the transmission tends to vary with the area Vd under the barriers.

## B. Kronig-Penney $\delta$ -function model

The KP $\delta$  model is a modification of the KP model, discussed in the previous subsection, such that  $V_{j+1} \rightarrow \infty$ ,  $d_{j+1} \rightarrow 0$ , where  $V_{j+1}d_{j+1} \rightarrow C_j$  a finite nonzero quantity. Essentially, this scheme changes the barriers to  $\delta$ -function potentials. From these assumed limits, we can deduce that  $y_j \rightarrow 0$  and  $k_{j+1}y_j = k_{j+1}^2 d_{j+1} \rightarrow C_j$ . We can now write the last two factors of (19) in the form

$$\begin{pmatrix} (\cosh y_j)/k & (\sinh y_j)/k_{j+1} \\ (k_{j+1}\sinh y_j)/k & \cosh y_j \end{pmatrix} \rightarrow \begin{pmatrix} 1/k & 0 \\ C_j/k & 1 \end{pmatrix} .$$
(28)

Consequently, (19) reduces to

$$M(j) = \begin{bmatrix} k \cos\theta_j & \sin\theta_j \\ -k \sin\theta_j & \cos\theta_j \end{bmatrix} \begin{bmatrix} 1/k & 0 \\ C_j/k & 1 \end{bmatrix}, \quad (29)$$

and the calculation of the transmission coefficient  $t_k$  is identical to that of the previous section, apart from the change in the definition of M(j).

Calculations for the KP $\delta$  model are presented, which were obtained by varying simultaneously both sets of parameters  $C_A$ ,  $C_B$  and  $a_A$ ,  $a_B$ . The results are given in Fig. 4, and similar results were obtained by varying only one of the sets of parameters. There are actually several bands, but the energy range of Fig. 4 has been chosen to show only one of them. Qualitatively, the structure is the same as that observed in Figs. 2 and 3 for the KP model. The band edges are clearly defined as the transition



FIG. 4. Effective coefficient of electronic transmission  $t_e$  versus energy E for the KP $\delta$  model, with  $a_A = 3.0$ ,  $a_B = 5.0$ ,  $V_A = 0.6$ , and  $V_B = 1.0$ .

points between regions of zero and nonzero transmission. Again there is subdivision of the band, with a self-similar structure. Note that the structure is not precisely symmetric about the band center, due to the fact that we have calculated an effective transmission coefficient by an averaging process, whereas a graph of the exact transmission coefficient would exhibit such symmetry.

## C. Tight-binding model

Here we consider a linear chain of N atoms, at points  $X_1, \ldots, X_N$ , bounded by conducting regions with  $X_0$  and  $X_{N+1}$  as reference points in these regions. Within the chain of N atoms, we use the TB model, where the wave function is assumed to have the form

$$\psi = \sum_{n=1}^{N} c_n \phi_n , \qquad (30)$$

with  $\phi_n$  being the atomic orbital centered at  $X_n$ . This leads to the usual system of difference equations<sup>9</sup>

$$(\alpha_n - E)c_n - \beta_n c_{n+1} - \beta_{n-1} c_{n-1} = 0$$
,  $n = 1, 2, ..., N$ ,  
(31)

where  $\alpha_n$  is the Coulomb integral at site  $X_n$ , and  $\beta_n$  is the resonance integral between sites  $X_n$  and  $X_{n+1}$ . We can write (31) in the matrix form

$$\begin{pmatrix} c_{n+1} \\ c_n \end{pmatrix} = \boldsymbol{M}(n) \begin{pmatrix} c_n \\ c_{n-1} \end{pmatrix}, \qquad (32)$$

where

$$\boldsymbol{M}(n) = \begin{bmatrix} (\alpha_n - E)/\beta_n & -\beta_{n-1}/\beta_n \\ 1 & 0 \end{bmatrix}, \qquad (33)$$

so that

$$\begin{pmatrix} c_{N+1} \\ c_N \end{pmatrix} = M \begin{pmatrix} c_1 \\ c_0 \end{pmatrix}, \qquad (34)$$

where

$$M = \prod_{n=1}^{N} M(n) .$$
(35)

We assume identical conducting regions on each side of the chain of atoms, so that we may take  $\beta_0 = \beta_N$ . In the conducting region to the left of the chain, we have (analogously to the KP model)

$$\psi = e^{ikx} + Ce^{-ikx} . \tag{36}$$

Choosing  $X_0$  as origin in this region, with  $|X_0X_1| = 1$ , the fact that  $c_0 = \psi(0)$  and  $c_1 = \psi(1)$  leads to

where

$$S = \begin{bmatrix} \cos k & \sin k \\ 1 & 0 \end{bmatrix}.$$
 (38)

Similarly, in the conducting region to the right, we have

$$\psi = De^{ikx} , \qquad (39)$$

and taking the origin to be at  $X_N$ , with  $|X_N X_{N+1}| = 1$ , gives

$$\begin{pmatrix} c_{N+1} \\ c_N \end{pmatrix} = S \begin{pmatrix} D \\ iD \end{pmatrix}.$$
 (40)

Inserting (37) and (40) into (34) gives

$$\begin{bmatrix} D \\ iD \end{bmatrix} = S^{-1}MS \begin{bmatrix} 1+C \\ i(1-C) \end{bmatrix}, \qquad (41)$$

which is the same form as (26) for the KP model, except that the transfer matrix is now  $T=S^{-1}MS$ . We note that the choice  $\beta_0=\beta_N$  ensures that detT=1, and we can calculate the transmission coefficient in the same way as for the KP model.

Calculations are presented varying (i)  $\alpha_A$  and  $\alpha_B$  (Fig. 5) and (ii)  $\beta_{AA}$  and  $\beta_{AB}$  (Fig. 6) for the two possible sites. In each case, we take  $\beta_0=1$  for the conducting regions. Once again, band structure and subdivision within the bands is observable, as is a self-similarity in the structure [see especially Fig. 6(b)]. It is reassuring that all three models of this section produce the same qualitative features, illustrating that they are "physical," and not an artifact of some particular model.

## **IV. OPTICAL TRANSMISSION**

In this section, we consider optical transmission through a one-dimensional system, made up of two types of layers, A and B, with  $X_i$  denoting the interface points. Here we take the layers to be arranged in a Fibonacci sequence, although the theory can be applied to any arrangement of the layers.



FIG. 5. Effective coefficient of electronic transmission  $t_e$  versus energy E for the TB model, with  $\alpha_A = 0.6$ ,  $\alpha_B = -0.6$ , and  $\beta_{AA} = \beta_{AB} = 1.0$ .

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The electric field for each layer has the form

$$\mathbf{E}_{p} = E_{p}^{1} \exp[i(\mathbf{k}_{p}^{1} \cdot \mathbf{x} - \omega t)] + E_{p}^{2} \exp[i(\mathbf{k}_{p}^{2} \cdot \mathbf{x} - \omega t)], \quad p = A, B, \quad (42)$$

where the first term represents the transmitted wave and the second represents the reflected wave. Writing

$$E_p^+ = E_p^1 + E_p^2$$
,  $E_p^- = (E_p^1 - E_p^2)/i$ , (43)

then for any medium between points  $X_i$  and  $X_{i+1}$ , we have

$$T_p S_p \begin{pmatrix} E_p^+ \\ E_p^- \end{pmatrix}_{X_i} = S_p \begin{pmatrix} E_p^+ \\ E_p^- \end{pmatrix}_{X_{i+1}}, \qquad (44)$$



FIG. 6. (a) Effective coefficient of electronic transmission  $t_e$  versus energy E for the TB model, with  $\alpha_A = \alpha_B = -0.6$ ,  $\beta_{AA} = 0.5$ , and  $\beta_{AB} = 1.0$ . (b) As in (a), but magnifying the region  $0.0 \le E \le 0.7$ .

where

$$S_p = \begin{bmatrix} 1 & 0\\ 0 & n_p \cos\theta_p \end{bmatrix} . \tag{45}$$

The introduction of the matrix  $S_p$  is required to ensure that the laws of refraction hold at the interface of the media, since between two different media we have

$$\begin{bmatrix} E_A^+ \\ E_A^- \end{bmatrix}_{X_i} = S_A^{-1} S_B \begin{bmatrix} E_B^+ \\ E_B^- \end{bmatrix}_{X_i},$$
(46)

where

$$S_{A}^{-1}S_{B} = \begin{bmatrix} 1 & 0 \\ 0 & n_{B}\cos\theta_{B}/n_{A}\cos\theta_{A} \end{bmatrix} .$$
 (47)

Here  $n_p$  is the refractive index for medium p, and  $\theta_p$  is the angle between the normal to the interface and the direction of polarization. The matrix  $T_p$  is the transfer matrix for medium p, and is given by

$$T_p = \begin{bmatrix} \cos \delta_p & -\sin \delta_p \\ \sin \delta_p & \cos \delta_p \end{bmatrix}, \qquad (48)$$

where  $\delta_p = n_p k d_p \cos \theta_p$ , k is the wave number in vacuum, and  $d_p$  is the thickness of the layer.<sup>10</sup> Thus, from (44) we have

where

$$\det M_p = 1 . (50)$$



FIG. 7. Effective coefficient of optical transmission  $t_e$  versus energy E, with  $n_A = 2.0$ ,  $n_B = 3.0$ ,  $d_A = 3.0$ , and  $d_B = 2.0$ .

For a chain of N such media, bounded by  $X_0$  and  $X_N$ , we have

$$\begin{bmatrix} E_{p_N}^+ \\ E_{p_N}^- \end{bmatrix}_{X_N} = M \begin{bmatrix} E_{p_1}^+ \\ E_{p_1}^- \end{bmatrix}_{X_0},$$
 (51)

where

$$\boldsymbol{M} = \prod_{i=1}^{N} \boldsymbol{M}_{p_i} \ . \tag{52}$$

From these results, we can calculate the transmission coefficient as  $^{10}$ 

$$t_k = |D|^2 = 4/(M_{11}^2 + M_{12}^2 + M_{21}^2 + M_{22}^2 + 2) , \qquad (53)$$

where  $M_{ij}$  are the matrix elements of M. We note that (53) is identical in form to (27), obtained for the transmission coefficient for electronic transmission.

We have calculated  $t_e$  as a function of energy, by arranging both the refractive indices  $(n_A, n_B)$  and layer thicknesses  $(d_A, d_B)$  according to the Fibonacci sequence, and taking the light to travel normal to the interfaces so that  $\theta_A = \theta_B = 0$ . The results are given in Fig. 7, showing a "close-up" of one particular region of nonzero transmission. Qualitatively, the figure is much like those

of the previous section for electronic transmission, and specifically, a degree of self-similarity is again in evidence, as may be expected for such chains.

## **V. CONCLUSIONS**

In this paper, we have defined a measure of transmission (or, more generally, any physical property) through nonperiodic sequences, such as a Fibonacci chain. We have looked specifically at electronic and optical transmission, and in the former case, we have utilized three commonly studied models and have seen that they all give qualitatively similar behavior. In all of the calculations performed, we have obtained subdivided band structures, which show self-similarity. These are qualitatively the same as calculations done with a large number of atoms or layers, but the computational effort is smaller. We note that it is trivial to calculate an effective resistivity  $(1-t_e)/t_e$  in the same way.

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- <sup>1</sup>B. L. Burrows and K. W. Sulston, J. Phys. A 24, 3979 (1991).
- <sup>2</sup>M. Kohmoto, B. Sutherland, and K. Iguchi, Phys. Rev. Lett. **58**, 2436 (1987).
- <sup>3</sup>G. Gumbs and M. K. Ali, J. Phys. A 22, 951 (1989).
- <sup>4</sup>M. Kolar, M. K. Ali, and F. Nori, Phys. Rev. B **43**, 1034 (1991).
- <sup>5</sup>Y.Avishai and D. Berend, Phys. Rev. B 41, 5492 (1990).

- <sup>6</sup>D. Kiang, T. Ochiai, and S. Date, Am. J. Phys. 58, 1200 (1990).
- <sup>7</sup>R. K. Pattnaik and E. A. Whittaker, J. Phys. A 25, 577 (1992).
- <sup>8</sup>P. K. Thakur, C. Basu, A. Mookerjee, and A. K. Sen, J. Phys. Condens. Matter 4, 6095 (1992).
- <sup>9</sup>S. G. Davison and M. Steslicka, *Basic Theory of Surface States* (Clarendon, Oxford, 1992).
- <sup>10</sup>M. Born and E. Wolf, *Principles of Optics*, 3rd ed. (Pergamon, Oxford, 1965).