Green's functions, density of states, and dynamic structure factor
for a general one-dimensional quasicrystal

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Using an analytic method involving continued fractions, we calculate the site-site, two-time Green's functions for a general one-dimensional crystal. These Green's functions give the electron correlations for a tight-binding model in the noninteracting-electron approximation, or the displacement correlations of a vibrating system with harmonic interatomic forces. The Green's functions can be summed in closed form to give the density of states for either model. The resulting expression depends only on the trace of a "transfer matrix," and on its derivative with respect to energy. We use this formula to determine the densities of states of a large class of quasiperiodic models, and we check our results against perturbation-theory calculations of the band structure of our models. From the Green's functions, we also derive an expression for the dynamic structure factor of our vibrating-lattice model, and we derive a class of iteration relations which allow us to evaluate it very rapidly for quasiperiodic chains. We give results for two different quasicrystals, and compare them against known general restrictions on the form of the dynamic structure factor.

I. INTRODUCTION

In recent years considerable effort has been expended in the theoretical investigation of the physical properties of quasiperiodic systems, particularly since the discovery of real physical examples—the so-called quasicrystals.[1] Naturally occurring quasicrystals[2] are all built upon quasiperiodic lattices in two or three dimensions. Unfortunately however, analytical work on these lattices has proved extremely difficult, and most of the important results have come from numerical studies.[3-8] One-dimensional quasilattices, on the other hand, have proved amenable to analytical methods and have yielded many interesting results. There are known to be some qualitative differences between one-dimensional quasicrystals and higher-dimensional ones (see, for example, Ashraff, Luck, and Stinchcombe[9]), but there are also many similarities and it is hoped that the study of these systems will give us some feeling for the properties we should expect in more than one dimension. And lest we convey the impression that one-dimensional quasicrystals are unphysical, we should also point out that at least one such structure has been created in the laboratory—the Fibonacci-chain superlattice of Merlin *et al.*[10]

The greater part of the work so far performed on one-dimensional quasicrystals has been on systems built around the Fibonacci chain.[11] This is a one-dimensional equivalent of the Penrose tiling[12] given by the repetition, *ad infinitum*, of the (concurrent) "inflation rules"

$$A \rightarrow AB \quad \text{and} \quad B \rightarrow A,$$

starting from a single letter A. For a tight-binding model built on this lattice, with hopping coefficients varying with the pattern of A's and B's along the chain, a transfer-matrix method was devised by Kohmoto, Kadanoff, and Tang,[13] and independently also by Ostlund and Pandit,[14] which yields the allowed electron energies. The results of these and other calculations[15] show that the spectrum of the model is a Cantor set of measure zero, and by making use of the inflation symmetry of the lattice, scaling laws for the spectra near the band edges have been derived.[16] Similar results have been derived for spin and phonon models built on quasiperiodic lattices. (An important difference between one-dimensional, and higher-dimensional quasicrystals is evident here; it has been shown that many models of a two-dimensional quasicrystal have spectra of nonzero measure.[9]) One way to progress further on this question of the dynamic properties of quasiperiodic systems would be to try to calculate the Green's functions for some appropriate model. Given a method for calculating one- and two-particle Green's functions, many quantities of great physical interest would become accessible: the density of states (DOS), the static and dynamic structure factors for phonon models, the conductivity of electronic models, and so on. For the particular case of the Fibonacci lattice, much progress has already been made in this direction by renormalization-group techniques.[9,16,17]

The point of this article then is threefold:

(i) To calculate the one-particle Green's functions analytically for a one-dimensional quasi-periodic model.

(ii) To analyze a model more general than the Fibonacci chain. While there is some evidence to suggest

that the Fibonacci chain displays many generic properties of one-dimensional quasiperiodic systems,[18] it is clearly important to study a variety of these models, if we wish to draw general conclusions about real quasicrystals from our results. The results derived in this article apply to a large class of two-tile quasilattices generated by inflation rules.

(iii) To show how we can derive analytic expressions for the densities of states and dynamic structure factors of our models from our expressions for the Green's functions. The dynamic structure factor is one of the most interesting, nontrivial functions derivable from the Green's functions, yielding as it does, much information about the nature of the normal modes of vibration of the quasicrystal, without our ever actually having to solve the eigenvalue problem. And, of course, it can also describe inelastic neutron scattering from our crystal.

In Sec. II we describe our quasilattices, and the methods for their generation. In Sec. III we summarize the principal results of the continued-fraction method for calculating the Green's functions and density of states for a general one-dimensional lattice. In Sec. IV we apply these results to the calculation of the densities of states of quasiperiodic systems. In Sec. V we derive a general formula for the dynamic structure function of a one-dimensional system and in Sec. VI we apply this to the quasiperiodic system. In Sec. VII we present some analysis and discussion of our results, and our conclusions.

II. CONSTRUCTION OF ONE-DIMENSIONAL QUASILATTICES

The quasilattices which we will be studying are all one-dimensional, two-tile lattices generated by inflation rules. A simple and general method for producing such lattices has been proposed by Lu, Odagaki, and Birman.[19] In the case of a two-tile lattice, their method may be summarized as follows. The tiles are represented by the letters A and B and lattices by strings of letters. The "addition" of two strings of letters, $S_1 + S_2$ (which is noncommutative) is equivalent to their concatenation $S_1|S_2$, with S_1 given first. The "multiplication" of a string S by an integer n means the repetition n times of the string S. To create a lattice, we take the vector $\mathbf{x} = (A, B)$, and operate upon it repeatedly with a 2 × 2 matrix of integers, M:

$$\mathbf{x}' = M\mathbf{x}. \qquad (1)$$

We then take either one of the elements of the resulting vector as our lattice, or the concatenation of both of them. In this article we will take the first element of the vector. As shown by Lu, Odagaki, and Birman, when the matrix M is nonsingular, this produces a lattice which is in general quasiperiodic in the limit where the matrix is applied an infinite number of times. Furthermore, it is a simple matter to show that, if the matrix M is given as

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}, \qquad (2)$$

then the transfer-matrix method is exactly equivalent to the repeated application of the inflation rules

$$A \to m_{11}A + m_{12}B \quad \text{and} \quad B \to m_{21}A + m_{22}B, \qquad (3)$$

starting from a single letter A. It is upon inflation rules of exactly this kind that the real-space renormalization-group methods of Ashraff, Luck, and Stinchcombe[9,16,17] are based, which have yielded many interesting results concerning the Fibonacci chain. We, however, will not be exploiting these methods here.

Quasiperiodic lattices can also be generated by projection from higher-dimensional periodic lattices, and many two-tile one-dimensional ones can be produced by projection from a two-dimensional rectangular lattice, as described, for example, by Elser.[20] The majority of the lattices generated by the matrix method cannot also be produced by projection in this manner, but three classes of lattices which can be given by Holzer.[18] These are the ones produced by the matrices

$$\begin{pmatrix} n & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & n-1 \\ 1 & n \end{pmatrix}, \quad \begin{pmatrix} n & 1 \\ n-1 & 1 \end{pmatrix}. \qquad (4)$$

All three classes include forms of the Fibonacci chain as a special case when $n = 1$. The first matrix gives the so-called precious-mean (PM) class of quasilattices, which are generated by projection from a square lattice with a projection line elevated at an angle $\tan^{-1} \tau_n$ to the horizontal, where τ_n is the larger root of the quadratic equation

$$\tau_n^2 - n\tau_n - 1 = 0. \qquad (5)$$

If the length of the longer (A-type) tile is l_A and that of the shorter one l_B, then the positions of the sites on the PM lattices are given by

$$l_m = m\alpha + (l_B - l_A)\left\{\frac{m}{1 + \tau_n^{-1}}\right\}. \qquad (6)$$

where

$$\alpha = \frac{l_A\tau_n + l_B}{\tau_n + 1} \qquad (7)$$

is the mean lattice parameter, and $\{x\}$ means the fractional part of x. The length of the mth link is then given by

$$d_m = \alpha + (l_B - l_A)f\left(\frac{m}{1 + \tau_n^{-1}}\right), \qquad (8)$$

where the periodic function $f(x)$ is given by

$$f(x) = \left\{x + \frac{1}{1 + \tau_n^{-1}}\right\} - \{x\}. \qquad (9)$$

A similar expression can be constructed for any other set

of variables (e.g., hopping coefficients) which vary along the lattice with the pattern of A's and B's in the chain.

In this paper we will use the PM lattices to illustrate many of our results about general quasiperiodic systems, since we can obtain results about these lattices by other analytic methods, as demonstrated in Sec. VII, and these then give us a check on the Green's-function method.

III. THE GREEN'S FUNCTIONS FOR A ONE-DIMENSIONAL MODEL

The retarded site-site Green's functions

$$G_{mn}(t) = \frac{2\pi}{i\hbar}\Theta(t)\left\langle\{a_m(t), a_n^\dagger(0)\}\right\rangle. \tag{10}$$

for a tight-binding model in one-dimension satisfying the Hamiltonian

$$H = \sum_i \varepsilon_i a_i^\dagger a_i + \sum_{i\neq j} V_{ij} a_i^\dagger a_j, \tag{11}$$

obey the equation of motion

$$i\hbar\frac{dG_{mn}}{dt} = 2\pi\delta(t)\delta_{mn} + \sum_j(\delta_{mj}\varepsilon_j + V_{mj})G_{jn}. \tag{12}$$

V_{ij} is, in general, a Hermitian matrix but we can, without loss of generality, assume it to be real. Fourier transforming and taking the case of a model with nearest-neighbor hopping interactions only,

$$V_{i,i+1} = V_{i+1,i} = V_i, \tag{13}$$

we find

$$(E - \varepsilon_m)G_{mn}(E) = \delta_{mn} + V_{m-1}G_{m-1,n} + V_mG_{m+1,n}. \tag{14}$$

Similarly, we can show that the displacement-displacement Green's functions

$$G_{mn}(t) = \frac{2\pi}{i\hbar}\Theta(t)\left\langle[u_m(t), u_n(0)]\right\rangle. \tag{15}$$

for a harmonic phonon model in one dimension obeying the Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i,j}\frac{k_{ij}}{2}(u_i - u_j)^2,$$
$$= \sum_i \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i,j}\Phi_{ij}u_iu_j \tag{16}$$

satisfy the equation of motion

$$m\frac{d^2G_{mn}}{dt^2} = -2\pi\delta(t)\delta_{mn} - \sum_j\Phi_{mj}G_{jn}(t). \tag{17}$$

Specializing again to systems with nearest-neighbor interactions only and Fourier transforming, we arrive at an equation of motion exactly the same as Eq. (14), except for the replacements

$$E \to m\omega^2, \quad \varepsilon_i \to k_{i,i-1} + k_{i,i+1}, \quad V_i \to -k_{i,i+1}. \tag{18}$$

Throughout much of what follows, we will use the notation and nomenclature of Eq. (14) and the electronic problem, but our results are equally applicable to the problem of phonon dynamics.

In order to study the solutions of the equations of motion for a quasiperiodic system, we use the approach favored by most workers—that of "periodic approximation." That is, we study the infinite chain consisting of the periodic repetition of an arbitrarily high-order approximant to the true quasilattice. This approximant is formed by iteration of Eq. (1) a finite number of times m. The quasiperiodic chain itself is regarded as the limit of this chain as $m \to \infty$.

The method we use to find the Green's functions, which is due to Lovesey,[21] is in fact very general, being applicable to any system in which the coefficients are periodic along the lattice. First, to simplify the equations a little, let us introduce the notation $\Omega_n = E - \varepsilon_n$ (or $\Omega_n = m\omega^2 - k_{n,n-1} - k_{n,n+1}$ for the phonon case). Then our equations of motion look like this:

$$\Omega_mG_{mn} = \delta_{mn} + V_{m-1}G_{m-1,n} + V_mG_{m+1,n}. \tag{19}$$

We define the two sets of quantities

$$\lambda_m = \frac{G_{m+1,n}}{G_{mn}}, \quad m \geq n, \tag{20}$$

$$\mu_m = \frac{G_{m+1,n}}{G_{mn}}, \quad m < n. \tag{21}$$

which, as it turns out, are independent of n and periodic in their indices, with the same period as the coefficients in the equations of motion. If we can find the values of these ratios, then we can calculate all the Green's functions for, as is easily shown,

$$\frac{1}{G_{mm}} = V_m\left(\mu_m - \lambda_m\right). \tag{22}$$

Once we have the diagonal Green's functions, we can get all the others by using the defining equations (20) and (21). Thus these ratios neatly parametrize the whole infinite set of functions G_{mn} in only $2N$ quantities, where N is the periodicity of the lattice.

The ratios are evaluated by a procedure involving continued fractions. In brief, we can show that λ_0 and μ_0 are the two solutions of the quadratic equation

$$p_N\lambda_0^2 + (p_{N+1} - q_N)\lambda_0 - q_{N+1} = 0, \tag{23}$$

where the sets of numbers $\{p_m\}, \{q_m\}$ both satisfy the same three-term recurrence relation:

$$V_mp_{m+1} + \Omega_mp_m + V_{m-1}p_{m-1} = 0, \tag{24}$$

$$V_mq_{m+1} + \Omega_mq_m + V_{m-1}q_{m-1} = 0, \tag{24}$$

with the initial conditions

$$p_1 = q_0 = 1, \quad p_0 = q_1 = 0. \tag{25}$$

A useful alternative definition of $\{p_m\}, \{q_m\}$, familiar from the transfer-matrix method of Aubry and André,[22] is

$$S_m = \begin{pmatrix} p_{m+1} & q_{m+1} \\ p_m & q_m \end{pmatrix} = \prod_{i=1}^{m} M_i \qquad (26)$$

with

$$M_i = \begin{pmatrix} -\Omega_i/V_i & -V_{i-1}/V_i \\ 1 & 0 \end{pmatrix}. \qquad (27)$$

Setting $m = 0$ in Eq. (22), we get

$$
\begin{aligned}
\frac{1}{G_{00}} &= V_0(\mu_0 - \lambda_0) \\
&= \pm V_0 \frac{\sqrt{(p_{N+1} - q_N)^2 + 4 p_N q_{N+1}}}{p_N} \\
&= \pm V_0 \frac{\sqrt{\xi_N^2 - 4 D_N}}{p_N},
\end{aligned} \qquad (28)
$$

where ξ_N and D_N are the trace and the determinant respectively, of the matrix S_N. As it turns out, however, $D_N = 1$ on account of the periodicity of the coefficients V_i, and so this formula further simplifies to read

$$G_{00} = \pm \frac{1}{V_0} \frac{p_N}{\sqrt{\xi_N^2 - 4}}. \qquad (29)$$

The meaning of the $\pm$ in this formula is considered below.

The argument which leads to Eq. (23) can be applied to any pair of variables λ_m, μ_m, to derive a quadratic equation of which they are the two solutions. However, this turns out to be unnecessary since we can show that

$$\lambda_m = -\frac{p_{m+1}\lambda_0 - q_{m+1}}{p_m\lambda_0 - q_m}, \qquad (30)$$

with a similar expression holding for μ_m, and this immediately gives us all the other Green's functions. We will see below how these results lead to expressions for the density of states and the dynamic structure factor, but first there are a number of observations that we should make about the Green's functions.

First, there is the question of the ambiguous sign in Eq. (29). This arises because Lovesey's method does not distinguish between the advanced and retarded Green's functions for the problem. In order to identify the retarded Green's function, we must introduce a small positive imaginary part into the energy—$E \rightarrow z = E + i\eta$—and then solve for G_{mn}. If we use this procedure, the continued-fraction method converges to a unique limit which is always one or other of the solutions to our quadratic equation when $\eta \rightarrow 0^+$, and this gives us a procedure for choosing the sign. The other solution to the quadratic gives the advanced Green's function for the problem. A formal procedure based on these principles for choosing the sign in Eq. (29) has been given by Lovesey and Westhead.[23]

Second, note that when λ_0, μ_0 (and therefore G_{00}) are real, all the other λ_m, μ_m are also real [by Eq. (30)], and so therefore are all the G_{mn}. And when λ_0, μ_0 are complex, so are all the other λ's and μ's. When the G_{mn} are

all real, the density of states (per site), given by

$$\rho(E) = \frac{1}{N} \sum_{m=1}^{N} \operatorname{Im} G_{mm}(E) \qquad (31)$$

and the structure factor, given by Eq. (46), are zero. So, as far as these quantities are concerned, the only interesting case is that of imaginary G_{00}. For this case ("within the allowed energy bands") since every pair of numbers λ_m, μ_m are complex, and are solutions to the same quadratic equation, we know that

$$\mu_m = \lambda_m^*. \qquad (32)$$

Thus the density of states and the structure factor, in fact, only depend on N (complex) quantities.

For a particular energy to fall within the allowed bands, we require that the square root appearing in Eq. (29) have a negative argument. That is, we require that

$$|\xi_N| < 2. \qquad (33)$$

This criterion was first deduced by other means by Kohmoto, Kadanoff, and Tang,[13] and by Ostlund and Pandit.[14]

Our next goal is the calculation of the density of states for our model. For this we require all the diagonal Green's functions G_{mm}. As we have argued, we need only find their values within the allowed bands, where Eq. (32) applies, since the density of states is (by definition) zero outside them. From Eqs. (22), (23), and (30), we get

$$G_{mm} = \pm \frac{1}{V_0} \frac{p_m^2 q_{N+1} + p_m q_m (q_N - p_{N+1}) - q_m^2 p_N}{\sqrt{\xi_N^2 - 4}}. \qquad (34)$$

Now we substitute this into Eq. (31) and perform the sum. As demonstrated by Lovesey,[21] this can be done in closed form using the Christoffel-Darboux formula, which is proved in any text covering the general properties of orthogonal polynomials (see, for example, Rainville[24]). The result is

$$\rho(E) = \frac{V_0}{N} \left| \frac{d\xi_N/dE}{\sqrt{\xi_N^2 - 4}} \right|. \qquad (35)$$

IV. DENSITY OF STATES
FOR A QUASIPERIODIC CHAIN

We now wish to evaluate Eq. (35) for periodic approximations to the quasiperiodic system. In the past, researchers have investigated systems (principally Fibonacci lattices) which are characterized by transfer matrices of the form

$$M_i = \begin{pmatrix} x_i & -1 \\ 1 & 0 \end{pmatrix}, \qquad (36)$$

where x_i takes on one of two values x_A, x_B according to

the sequence of A's and B's in the quasiperiodic chain.[25] For systems of this kind, one can use the matrix formula, Eq. (1), directly to give the transfer matrix S_k of the kth periodic approximation to the quasicrystal. S_k is given recursively by

$$S_{k+1} = T_k^{m_{12}} S_k^{m_{11}},$$

$$T_{k+1} = T_k^{m_{22}} S_k^{m_{21}}, \qquad (37)$$

with the initial conditions

$$S_0 = \begin{pmatrix} x_A & -1 \\ 1 & 0 \end{pmatrix}, \quad T_0 = \begin{pmatrix} x_B & -1 \\ 1 & 0 \end{pmatrix}. \qquad (38)$$

However, for systems characterized by more complicated matrices of the form (27), this method breaks down, because each matrix depends on variables V_i and V_{i+1} on two consecutive links of the chain, so that one cannot associate one particular matrix with an A-type link, and one with a B-type link. And in general one must also assume that the coefficient $\Omega_i = E - \varepsilon_i$ depends on the types of the links to either side of the ith site, because the phonon problem requires it [see Eq. (18)]. For the Fibonacci chain, even this is not a problem, since every periodic approximant starts with an A-type link. It takes only a moment to convince oneself that if this is the case, then one can still define matrices S_0, T_0 so that Eq. (37) is correct. For the more complicated chains, however, we must go through some maneuvers first to convert the problem into one for which the matrices obey Eq. (37).

Consider the chain generated by repeated application of the matrix

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}, \qquad (39)$$

to the primitive vector (A, B). It is clear that, as long as m_{11} and m_{21} are both nonzero, every periodic approximant to this chain will start with an A-type link, and so Eq. (37) will be applicable. Also, if two or more elements of the matrix are zero, the chain generated will be a periodic one, in which case its Green's functions are easily calculated directly from the equation of motion, and we do not need all this apparatus of quadratics and transfer matrices. Thus the only cases requiring more careful consideration are ones in which one or the other of m_{11} and m_{21} is zero and all the other matrix elements are nonzero. For such a case, consider the chain generated by repeated application of the matrix

$$M = \begin{pmatrix} m_{22} & m_{21} \\ m_{12} & m_{11} \end{pmatrix}, \qquad (40)$$

to the primitive vector (B, A). The reader should convince him or herself that this produces exactly the same chain as we had before, except that it is inverted. This chain must, of course, have exactly the same physical properties as the original. So we may, if we wish, calculate the density of states for this chain instead, knowing

that it will be the same as that of our original chain. However, since m_{22} and m_{12} are both nonzero by hypothesis, every periodic approximation to this chain begins with a B-type link, and therefore Eq. (37) is valid once more (except for the obvious modifications which have to be made in rearranging the m's and swapping the initial conditions).

In what follows, we study only chains in which every periodic approximation starts with an A-type link. We lose no generality by doing this since the A's and B's are after all only labels for certain values of the coefficients, and we are free to swap these labels around as we choose. For these chains, the relations (37) hold, and the only question is what the appropriate initial conditions are. Our assumption that each periodic approximant starts with an A-type link is not correct for the very first stage in the process where the second element of our vector is just the letter B. So we must do one iteration of the inflation rules by hand to get to an appropriate starting point.
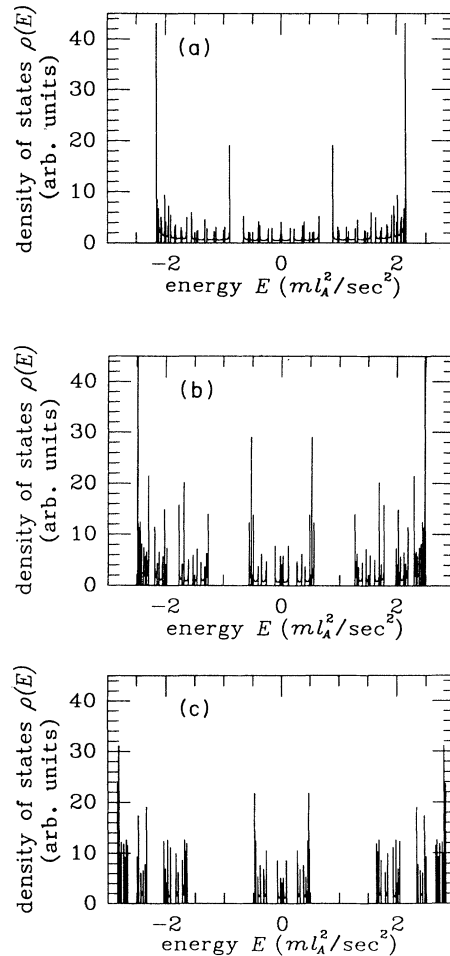

FIG. 1. Densities of states (DOS) for the one-dimensional tight-binding model on a Fibonacci chain, calculated from Eq. (35) with $\varepsilon_i = 0$ for all i, $V_A = 1$, and (a) $V_B = 1.2$, (b) $V_B = 1.6$, and (c) $V_B = 2.0$.
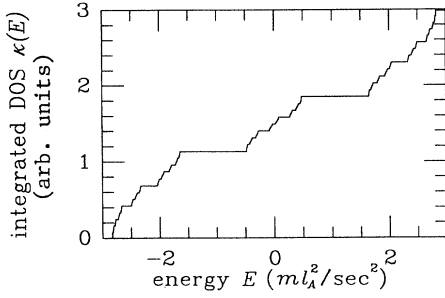
FIG. 2. Integrated density of states for the one-dimensional tight-binding model on a Fibonacci chain with $\varepsilon_i = 0$ for all i, $V_A = 1$, and $V_B = 2.0$. Calculated by numerically integrating the data from Fig. 1(c).

Let us illustrate the principle with the example of the PM chains. For these chains one iteration of the inflation rules gives us

$$M\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A^n B \\ A \end{pmatrix}. \tag{41}$$

Let us denote by Ω_α the value of Ω_i for a site with A-type links to either side of it, by Ω_β that for a site with a B-type link following it, and by Ω_γ that for a site preceded by a B-type link. (In this particular example there are no sites sandwiched between two B-type links.) Then

the appropriate initial conditions are

$$S_1 = M_\gamma M_\beta M_\alpha^{n-1},$$

$$T_1 = M_\alpha, \tag{42}$$

where

$$M_\alpha = \begin{pmatrix} -\Omega_\alpha/V_A & -1 \\ 1 & 0 \end{pmatrix},$$

$$M_\beta = \begin{pmatrix} -\Omega_\beta/V_B & -V_A/V_B \\ 1 & 0 \end{pmatrix}, \tag{43}$$

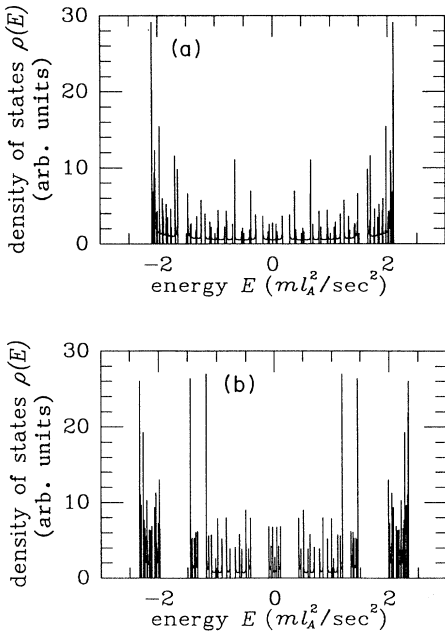$$M_\gamma = \begin{pmatrix} -\Omega_\gamma/V_A & -V_B/V_A \\ 1 & 0 \end{pmatrix}.$$

FIG. 3. Densities of states for the one-dimensional tight-binding model on an $n = 3$ PM lattice, calculated from Eq. (35) with $\varepsilon_i = 0$ for all i, $V_A = 1$ and (a) $V_B = 1.2$ and (b) $V_B = 1.6$.
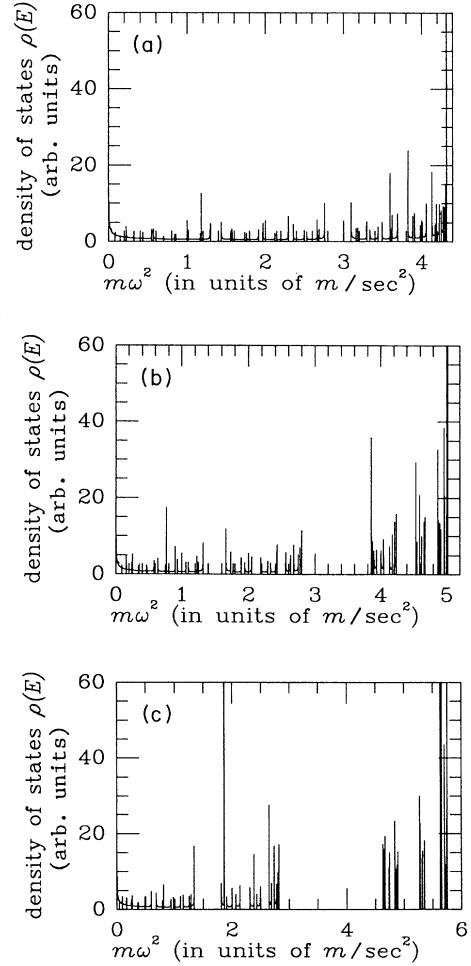
FIG. 4. Densities of states for the one-dimensional harmonic phonon model on a Fibonacci chain, calculated from Eq. (35) with $k_A = 1$, and (a) $k_B = 1.2$, (b) $k_B = 1.6$, and (c) $k_B = 2.0$.

In order to evaluate the density of states we need both the trace of the transfer matrix for the entire system, and the derivative of that trace with respect to energy. The simplest way to get the derivative exactly is just to differentiate both Eq. (37) and the initial conditions, to give a recursion relation for the derivatives of the transfer matrices. We then simply substitute the results into Eq. (35). (This is to be contrasted with the trace recursion methods of Kohmoto, Kadanoff, and Tang,[13] in which the entire transfer matrix is never calculated; only the trace is.) We have done this for the examples of the PM lattices with $n = 1$ and $n = 3$ for both the electron and the phonon problems. The results are shown in Figs. 1–6. The $n = 1$ case is just the Fibonacci chain, for which both the density of states[16] $\rho(E)$ (albeit for a slightly
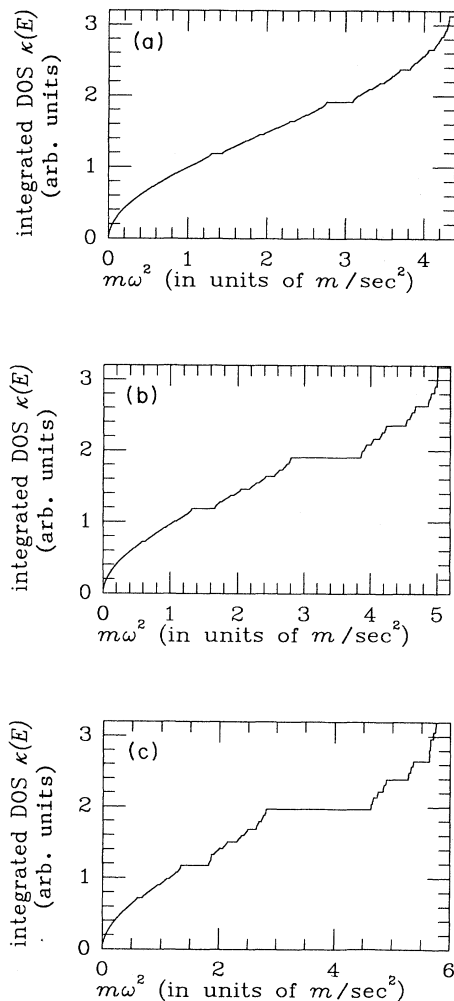
FIG. 5. Integrated densities of states for the one-dimensional harmonic phonon model on a Fibonacci chain with $k_A = 1$, and (a) $k_B = 1.2$, (b) $k_B = 1.6$, and (c) $k_B = 2.0$. Calculated by numerically integrating the data from Fig. 4. Compare with curves appearing in Fig. 7.
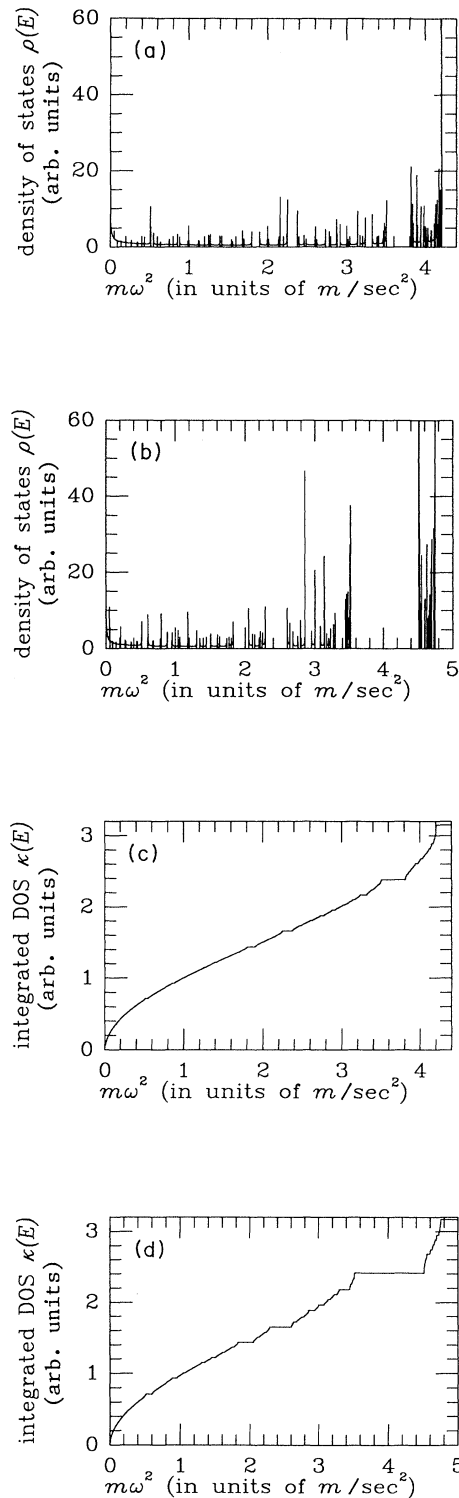
FIG. 6. Densities of states and integrated densities of states for the one-dimensional harmonic phonon model on an $n = 3$ PM lattice, calculated from Eq. (35) with $k_A = 1$. (a) DOS with $k_B = 1.2$, (b) DOS with $k_B = 1.6$, (c) IDOS with $k_B = 1.2$ and (d) IDOS with $k_B = 1.6$. Compare curves of IDOS with curves appearing in Fig. 8.

different model) and the integrated density of states[25] (DOS) $\kappa(E)$ have been calculated by other means. A numerical integration of our data is included for comparison with the published plots. The agreement is excellent.

Expression (35) can be integrated explicitly. The result is

$$\kappa(E) = \int_0^E \rho(E')dE' = \frac{V_0}{N}\cos^{-1}[\tfrac{1}{2}\xi_N(E)], \qquad (44)$$

to within a constant. Unfortunately, this expression is useless in the limit as $N \to \infty$ because the multivalued nature of the inverse cosine function means that $\kappa(E)$ becomes completely arbitrary. Nonetheless, it is comforting to see it here because in the periodic case at least, the curve of $\kappa(E)$ against E should be the same as the dispersion curve of k against E for excitations varying harmonically in space. And it has been argued elsewhere[26] that the integrated density of states should take the place of the wave vector k in the calculation of the dynamic properties of a quasiperiodic system where the wave vector itself is no longer a good quantum number for labeling the states. We will see in Sec. VII how this replacement appears in the calculation of the dynamic structure factor.

V. DYNAMIC STRUCTURE FACTOR

We now turn to the calculation of the dynamic structure factor for our phonon model. This is given in terms of the displacement-displacement Green's functions by

$$S(q,\omega) = \lim_{L\to\infty}\left(\frac{1}{L}\,\mathrm{Im}\sum_{mn}e^{iq(r_m-r_n)}G_{mn}(\omega)\right). \qquad (45)$$

where the sums run over L sites. Given that G_{mn} is symmetric [which we can see by taking Eqs. (13) and (14) together], this is also equal to

$$S(q,\omega) = \lim_{L\to\infty}\left(\frac{1}{L}\sum_{mn}\cos q(r_m-r_n)\,\mathrm{Im}\,G_{mn}(\omega)\right), \qquad (46)$$

and so $S(q,\omega)$ vanishes when the G_{mn} are all real, i.e., outside the allowed bands. Within the bands, we evaluate the sum in Eq. (45) as follows.

Consider first the $G_{mn}(\omega)$ for $m \geq n$. Given that we already know G_{00} from Eq. (29), we can write

$$G_{mn} = \beta_m\beta_n^* G_{00}, \quad m \geq n, \qquad (47)$$

where

$$\beta_m = \begin{cases} \displaystyle\prod_{i=1}^m \lambda_{i-1}, & m > 0 \\[2ex] 1, & m = 0 \\[2ex] \displaystyle\prod_{i=-1}^m \lambda_i^{-1}, & m < 0. \end{cases} \qquad (48)$$

Similarly, if $m \leq n$, then

$$G_{mn} = \beta_m^*\beta_n G_{00}, \quad m \leq n. \qquad (49)$$

Substituting these expressions into (45), we get

$$\begin{aligned}
\mathrm{Im}\sum_{mn}e^{iq(r_m-r_n)}G_{mn} &= \mathrm{Re}\left(\sum_{m>n}e^{iq(r_m-r_n)}\beta_m\beta_n^* + \sum_m|\beta_m|^2 + \sum_{m<n}e^{iq(r_m-r_n)}\beta_m^*\beta_n\right)\mathrm{Im}\,G_{00}, \\
&= \sum_{m,n}e^{iq(r_m-r_n)}(\beta_m\beta_n^* + \beta_m^*\beta_n)\,\mathrm{Im}\,G_{00}, \\
&= \left(\left|\sum_m e^{iqr_m}\beta_m\right|^2 + \left|\sum_m e^{iqr_m}\beta_m^*\right|^2\right)\mathrm{Im}\,G_{00}, \qquad (50)
\end{aligned}$$

where we have made use of the fact that G_{00} is purely imaginary within the allowed bands. The sums appearing here can be simplified by making use of the relations

$$\beta_{pN+m} = \beta_N^p\beta_m, \quad r_{pN+m} = pr_N + r_m, \qquad (51)$$

which derive, once again, from the periodicity of the variables $\{\lambda_m\}$. We get

$$\sum_m e^{iqr_m}\beta_m = \sum_p e^{iqpr_N}\beta_N^p\sum_{m=0}^{N-1}e^{iqr_m}\beta_m. \qquad (52)$$

The first of the sums on the right-hand side can be evaluated exactly, using the result that

$$\sum_{m=-\infty}^{\infty}e^{imx} = 2\pi\sum_{k=-\infty}^{\infty}\delta(x-2\pi k), \qquad (53)$$

giving δ functions at a sparse set of points along the q axis, and zero elsewhere. If we write $\beta_N = e^{i\phi}$,[27] then the positions of these δ functions are given by

$$q = \frac{2\pi l - \phi}{D}, \qquad (54)$$

where l is an integer, and $D = r_N - r_0$, which is the repeat length of the lattice. At these points we can calculate the "heights" of the δ functions and get

$$S(q,\omega) = \frac{2\pi\delta(0)}{N^2} \left| \sum_{m=0}^{N-1} e^{iqr_m} \beta_m \right|^2 \mathrm{Im}\, G_{00}. \qquad (55)$$

(For convenience, we have divided by an extra factor of N here to give the structure factor *per site* which converges to a well-defined limit as $N \to \infty$.) Similar manipulations demonstrate that the other term in Eq. (50) is zero everywhere except at the points

$$q = \frac{2\pi l + \phi}{D}, \qquad (56)$$

where it is

$$S(q,\omega) = \frac{2\pi\delta(0)}{N^2} \left| \sum_{m=0}^{N-1} e^{iqr_m} \beta_m^* \right|^2 \mathrm{Im}\, G_{00}. \qquad (57)$$

The values of the β_m are easily found by substituting Eq. (30) into Eq. (48). For $m \geq 0$ we get

$$\beta_m = (-1)^m (q_m - p_m \lambda_0), \qquad (58)$$

where λ_0 is given by Eq. (23). Since the $\{p_m\}$, $\{q_m\}$ are all real, β_m^* is simply

$$\beta_m^* = (-1)^m (q_m - p_m \lambda_0^*). \qquad (59)$$

The finite sums in Eqs. (55) and (57) can be evaluated by a computer for any given set of coefficients ε_i, V_i, and are sufficiently easily calculated that lattices with large periods can be investigated without squandering large amounts of computer time. However, for lattices generated by inflation rules of the type given in Eq. (3) there is a more efficient way to perform these sums.

VI. DYNAMIC STRUCTURE FACTOR FOR A QUASICRYSTAL

To evaluate Eqs. (55) and (57) for a quasicrystal generated by the matrix method of Lu, Odagaki, and Bir-

man, we consider two different finite approximants to our quasiperiodic lattice—those given by the top and bottom components of the vector $\mathbf{x}'$ defined in Eq. (1). Quantities defined on the second of these will be denoted by primed variables, e.g., $\{p_m'\}$, $\{q_m'\}$, N'. $\{p_m'\}$, $\{q_m'\}$ are components of the transfer matrices T_k introduced in Eq. (37). Now we define four quantities, Σ_p, Σ_q, Σ_p', Σ_q' by

$$\Sigma_p = \sum_{m=0}^{N-1} (-1)^m e^{iqr_m} p_m, \quad \Sigma_q = \sum_{m=0}^{N-1} (-1)^m e^{iqr_m} q_m,$$
$$(60)$$
$$\Sigma_p' = \sum_{m=0}^{N'-1} (-1)^m e^{iqr_m} p_m', \quad \Sigma_q' = \sum_{m=0}^{N'-1} (-1)^m e^{iqr_m} q_m'.$$

Note that N', the period of the second approximation, is not necessarily the same as N, the period of the first. The structure factor is nonzero at the points

$$q = \frac{2\pi l \pm \phi}{D}, \qquad (61)$$

where it takes the values

$$S(q,\omega) = \begin{cases} \dfrac{2\pi\delta(0)}{N^2} |\Sigma_q - \Sigma_p \lambda_0|^2 \mathrm{Im}\, G_{00}, & + \text{ sign} \\[3mm] \dfrac{2\pi\delta(0)}{N^2} |\Sigma_q - \Sigma_p \lambda_0^*|^2 \mathrm{Im}\, G_{00}, & - \text{ sign}. \end{cases}$$
$$(62)$$

We can now develop recursion relations for the Σ variables which mirror the recursion used to build up the chain. Consider Σ_p. We denote by $\Sigma_p^{(k)}$ the value of this variable for the kth periodic approximation to the quasiperiodic chain, and by N_k the number of sites in one period of this approximation. We can write $\Sigma_p^{(k+1)}$ as

$$\Sigma_p^{(k+1)} = \sum_{m=0}^{N_{k+1}-1} (-1)^m e^{iqr_m} p_m^{(k+1)}$$

$$= \sum_{j=0}^{m_{11}-1} \sum_{m=0}^{N_k-1} (-1)^{jN_k+m} \exp(iqr_{jN_k+m}) p_{jN_k+m}^{(k+1)}$$

$$+ \sum_{j=0}^{m_{12}-1} \sum_{m=0}^{N_k-1'} (-1)^{m_{11}N_k + jN_k' + m} \exp(iqr_{m_{11}N_k + jN_k' + m}) p_{m_{11}N_k + jN_k' + m}^{(k+1)}. \qquad (63)$$

Because Eqs. (24) are homogeneous we can write $p_{jN_k+m}^{(k+1)}$ as a linear combination $ap_m^{(k)} + bq_m^{(k)}$. Setting m equal to 0 and 1 successively and applying Eqs. (25), we can find a and b. The result is that

$$p_{jN_k+m}^{(k+1)} = p_{jN_k+1}^{(k+1)} p_m^{(k)} + p_{jN_k}^{(k+1)} q_m^{(k)}. \qquad (64)$$

Similarly,

$$p^{(k+1)}_{m_{11}N_k+jN'_k+m} = p^{(k+1)}_{m_{11}N_k+jN'_k+1}p'^{(k)}_m + p^{(k+1)}_{m_{11}N_k+jN'_k}q'^{(k)}_m.$$ (65)

Substituting these into Eq. (63) we find

$$\Sigma^{(k+1)}_p = \sum_{j=0}^{m_{11}-1}(-1)^{jN_k}\exp(iqjr_{N_k})\left(p^{(k+1)}_{jN_k+1}\Sigma^{(k)}_p + p^{(k+1)}_{jN_k}\Sigma^{(k)}_q\right)$$

$$+ \sum_{j=0}^{m_{12}-1}(-1)^{m_{11}N_k+jN'_k}\exp[iq(m_{11}r_{N_k}+jr_{N'_k})]\left(p^{(k+1)}_{m_{11}N_k+jN'_k+1}\Sigma'^{(k)}_p + p^{(k+1)}_{m_{11}N_k+jN'_k}\Sigma'^{(k)}_q\right).$$ (66)

And similar relations can be derived for $\Sigma^{(k+1)}_q$ and the primed variables. This expression may appear at first difficult, and far more trouble than the simple sum appearing in Eqs. (60). Note, however, that it requires a knowledge of the variables $\{p_m\}, \{q_m\}$ only at certain special points. In fact these p's and q's are the very ones that appear as the elements of the matrices calculated at successive stages in the iteration of Eq. (37). These matrix elements have only to be calculated once at any given energy, and then from Eq. (66) and those like it we can calculate the dynamic structure factor at any wave vector we please. Thus we can use these formulas to calculate the Σ variables iteratively, much faster than it is possible to calculate the sums appearing in their definition, and in this way we can study very large lattices.

As a simple example of this procedure, let us examine the Fibonacci chain once more. For this case, the iterative equations for Σ_p, Σ_q simplify to just two:

$$\Sigma^{(k+1)}_p = \Sigma^{(k)}_p + (-1)^{N_k}e^{iqr_{N_k}}$$
$$\times\left(p_{N_k+1}\Sigma^{(k-1)}_p + p_{N_k}\Sigma^{(k-1)}_q\right),$$

$$\Sigma^{(k+1)}_q = \Sigma^{(k)}_q + (-1)^{N_k}e^{iqr_{N_k}}$$
$$\times\left(q_{N_k+1}\Sigma^{(k-1)}_p + q_{N_k}\Sigma^{(k-1)}_q\right),$$ (67)

where the numbers N_k are now the Fibonacci numbers. The values of N_k and r_{N_k} need only be evaluated once ever. Thus the calculation of the structure factor at a range of different wave vectors for a particular energy essentially only involves the iteration of the two equations above.

The initial conditions come from Eq. (42). They are

$$\Sigma^{(1)}_p = -e^{iql_A}, \quad \Sigma^{(2)}_p = -e^{iql_A} + e^{iq(l_A+l_B)}\frac{\Omega_\beta}{k_B},$$

$$\Sigma^{(1)}_q = 0, \quad \Sigma^{(2)}_q = -e^{iq(l_A+l_B)}\frac{k_A}{k_B}.$$ (68)

The results from the evaluation of the dynamic structure factor for the Fibonacci chain and the $n = 3$ PM lattice are shown in Figs. 7 and 8. In both cases the results are for lattices with a repeat length of 500 links.

In these plots all points at which the heights of the δ functions are over a certain threshold are marked with black dots. (Surface plots of these functions turn out to yield almost no information to the eye because the functions are so spiky.) All the plots are of generically the same form. They consist of sets of identical curves, displaced from one another along the q axis, with intensities varying from curve to curve and also within each curve with wave vector. This kind of behavior was first seen in the calculations of Ashraff and Stinchcombe.[17] As $q \to 0$ all the plots display the so-called "effective-medium" behavior; i.e., the intensities of all the curves tend to zero, except for one, the curve which passes through the origin. In the limit of small wave vector, this curve tends to the periodic-crystal result $m\omega^2 \sim q^2$. The results for the Fibonacci chain agree favorably with previous calculations of the same quantity by a decimation method.[17]

VII. DISCUSSION

Let us turn first to the results for the spectra of the electron and phonon systems. These show a complicated system of bands of varying sizes up to a certain maximum energy (or frequency). The larger the band gaps grow, the more V_B differs from V_A. If we denote by m the order of the finite approximant which is repeated to build up our lattice (see Sec. III), then from our results it appears that each time we increase m, the bands in our spectra develop additional band gaps within them, in the manner of a Cantor-set construction. In the case of the Fibonacci chain, we already know this to be exactly the case, with the spectrum of the true quasicrystal having zero measure.[13,15]

For the case of the PM lattices, much light can be shed on these observations by treating the density-of-states problem using degenerate perturbation theory. This gives us, to first order in the small quantity $(V_B - V_A)/\overline{V}$, the sizes and positions of the band gaps. A full account of this calculation is given elsewhere,[28] but for comparison with the results given in this paper, we will reiterate our results briefly here.

We work as usual with the electron model, since we know that by the replacements (18) we can convert the results into results for the phonon model. We then write the Hamiltonian, Eq. (11), as $H = H_0 + H_1$, where
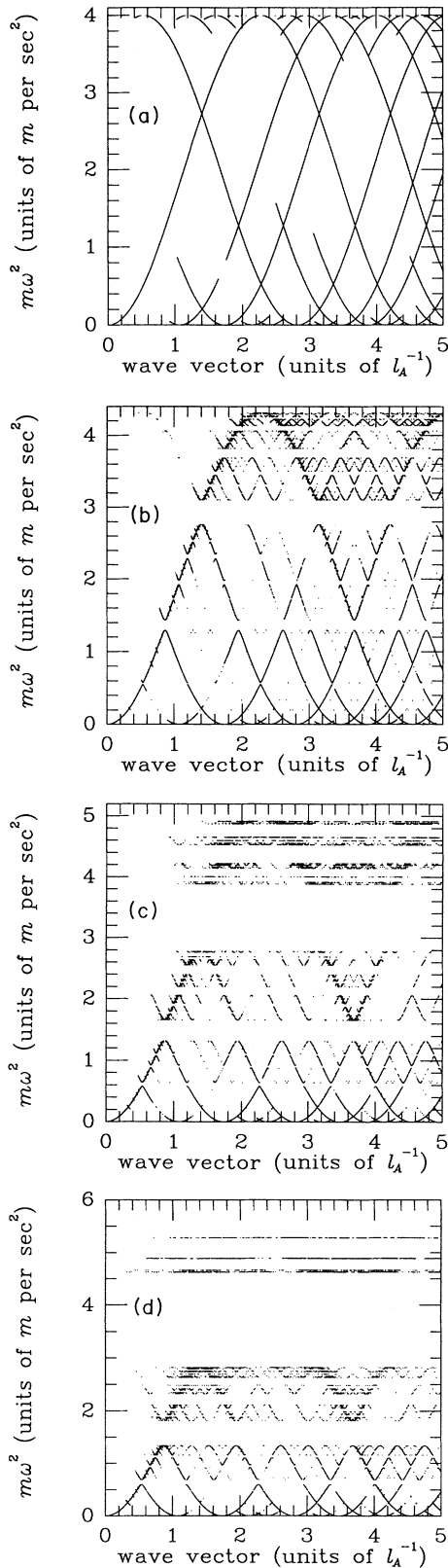
FIG. 7. Dynamic structure function for the harmonic phonon model on the Fibonacci chain, calculated from Eqs. (62) and (67) with $d_A = \tau_1$, $d_B = 1$, $k_A = 1$, and (a) $k_B = 1.0$, (b) $k_B = 1.2$, (c) $k_B = 1.6$, and (d) $k_B = 2.0$.

$$H_0 = \sum_i \overline{\varepsilon} a_i^\dagger a_i + \overline{V}(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i),$$

$$H_1 = \sum_i \delta_i a_i^\dagger a_i + \Delta_i (a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i),$$

(69)

with

$$\delta_i = \varepsilon_i - \overline{\varepsilon}, \quad \Delta_i = V_i - \overline{V}.$$

(70)

where $\overline{\varepsilon}$ and $\overline{V}$ are the site-averaged values of ε and V. Δ_i and δ_i are given in closed form by equations similar to Eq. (8). The eigenstates of H_0 are easily written down, and treating H_1 as a perturbation on these, we find that for the electron model band gaps appear at all energies satisfying

$$E_l = \pm 2\overline{V} \cos\left(\frac{\pi l}{1 + \tau_n^{-1}}\right), \quad l \text{ integer},$$

(71)

whose size, to a first approximation, is given by

$$\Delta E_l = \frac{2(V_B - V_A)}{\pi l} \left|\sin\left(\frac{\pi l}{1 + \tau_n^{-1}}\right)\right|.$$

(72)

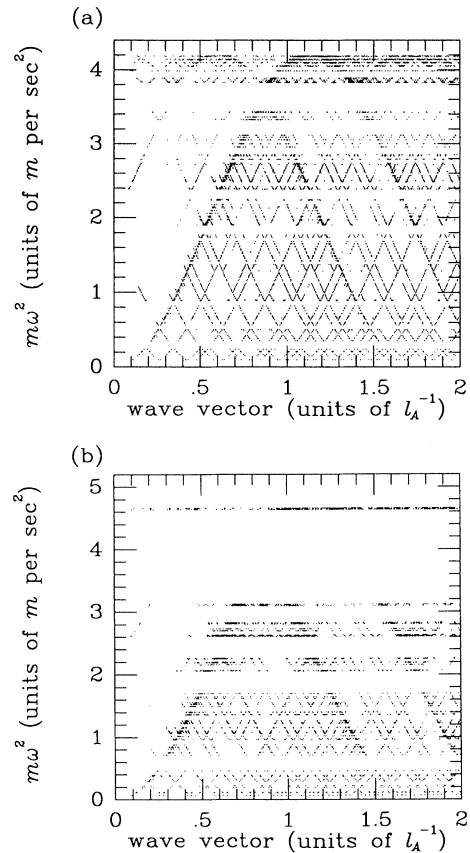And for the phonon model we have gaps at

FIG. 8. Dynamic structure function for the harmonic phonon model on the $n = 3$ PM lattice, calculated from Eqs. (62) and (67) with $d_A = \tau_3$, $d_B = 1$, $k_A = 1$, and (a) $k_B = 1.2$ and (b) $k_B = 1.6$.

$$m\omega_{lm}^2 = 2\overline{k}\left[1 + (-1)^m \cos\left(\frac{\pi l}{1 + \tau_n^{-1}}\right)\right],$$

$$l, m \text{ integers,} \quad (73)$$

whose size is

$$\Delta\omega_{lm}^2 = \frac{2(k_B - k_A)\omega_{lm}^2}{\pi \overline{l}\overline{k}}\left|\sin\left(\frac{\pi l}{1 + \tau_n^{-1}}\right)\right|. \quad (74)$$

These results agree well with Figs. 1(a), 3(a), 4(a), and 6(a), but, predictably, less well with the other results, for which our so-called small parameter is actually ~ 1.

Notice that the last expression, for the size of the band gaps in the phonon model, depends on ω_{lm} so that the sizes of the gaps become smaller as $\omega \to 0$. In this limit then, we would expect the integrated density-of-states curve to tend to the inverse cosine of the unperturbed system, behavior which is evident in Figs. 5, 6(c), and 6(d). Notice also that the maximum frequency at which a band gap can appear is $4\overline{k}$, which is also the maximum frequency of any propagating mode in the unperturbed system, and that at this frequency the size of the gap is zero. This means that the maximum allowed frequency for the perturbed system should also be $4\overline{k}$. This behavior[29] is also evident in Figs. 4–6.

Turning now to the analysis of the results for the dynamic structure function, we can learn something of the reason for the characteristic "satellite curves" form of Figs. 7 and 8, by a direct evaluation of Eq. (45) from first principles. In the case of a periodic lattice this can be done simply by Fourier transforming the site annihilation operators and writing them in terms of the phonon operators a_k. By analogy, we can label each phonon mode in the quasicrystal by some label κ and then expand the a_m as linear combinations of the annihilation operators for these phonons. As it turns out, the appropriate label for the states in this case is the integrated density of states. For the particular case of the PM lattices, we can write the expansion in terms of the function $\chi_\kappa(x)$ defined by

$$a_m = e^{i\kappa m}\chi_\kappa\left(\frac{m}{1 + \tau_n^{-1}}\right)a_\kappa,$$

$$(75)$$

$$\chi_\kappa(x + 1) = \chi_\kappa(x), \quad \text{for all } x.$$

It can now be shown[28] that the dynamic structure function takes the form

$$S(q, \omega) = 2\pi\delta(0)\sum_{j,k}|g_{\nu j}(q)|^2\delta(\omega - \omega(\nu)), \quad (76)$$

where

$$\nu = -q\alpha + \frac{2\pi j}{1 + \tau_n^{-1}} + 2\pi k, \quad (77)$$

and the numbers $g_{\kappa j}(q)$ are the coefficients in the Fourier expansion of the periodic function

$$g_\kappa(x, q) = \chi_\kappa(x)\exp\left[-iq(l_A - l_B)\{x\}\right]. \quad (78)$$

This gives a set of curves, all copies of the curve $\omega(\kappa)$ at

a dense set of positions along the q axis, with intensities given by the coefficients $g_{\kappa j}(q)$ in the Fourier expansion of $\chi_\kappa(x)\exp\left[-iq(l_A - l_B)\{x\}\right]$. Note that, since $g_{\kappa j}(q)$ is dependent on q as well as on j, the intensity of each curve varies with q, as well as each curve having a different intensity from its neighbors.

The positions of the curves relative to one another are dependent solely on the geometry of the quasicrystal, and the shape of each curve is dependent solely on the phonon dynamics. Apart from providing an explanation of the appearance of the plots of $S(q, \omega)$ we can also see that if we are interested in investigating particular detailed properties of the structure functions, then we need only look at the curve $\omega(\kappa)$, which saves us from worrying about the complication of the geometry. As an example, since we have already shown that the IDOS curve becomes cosinusoidal as $\omega \to 0$, the apparent effective-medium behavior of $S(q, \omega)$ near the origin is in fact genuine, and traveling waves of very small wave vector will propagate in a quasiperiodic system exactly as if in a classical elastic medium.

The coefficients $g_{\kappa j}(q)$ are, in general, not easy to calculate, but there is one case in which they can be worked out exactly, and that is when $k_A = k_B$. In this case, $\chi_\kappa(x)$ is a constant, independent of both κ and x, which for convenience we will set equal to one. Then

$$g_\kappa(x, q) = \exp\left[-iq(l_A - l_B)\{x\}\right]. \quad (79)$$

Fourier transforming, we find that

$$|g_{\kappa j}(q)|^2 = \left(\frac{\sin[\pi j - \frac{1}{2}q(l_A - l_B)]}{\pi j - \frac{1}{2}q(l_A - l_B)}\right)^2. \quad (80)$$

For the particular case of the Fibonacci chain, this result is equivalent to the previous direct evaluation of the dynamic structure factor for $k_A = k_B$ by Ashraff and Stinchcombe,[17] and gives us a useful check on the Green's-function method. Elsewhere, we show how it can be extended to the $k_A \neq k_B$ case by perturbation theory.[28]

To conclude, we have calculated the site-site one-particle Green's functions for a large class of one-dimensional quasiperiodic systems, and using them, the densities of states and dynamic structure factors of these systems also. The densities of states all show a dense set of band gaps, whose size and position is in agreement with the perturbation-theory calculation of the same quantities. The structure factors take the form of repeated copies of the integrated density-of-states curve at a dense set of positions along the wave-vector axis. We have outlined arguments which explain why $S(q, \omega)$ should take this form, and to give the positions of the curves. Also, from the perturbation-theory treatment we can show that in the limit of small wave vector the structure factor tends to that of a classical elastic medium (the so-called effective-medium behavior).

There are many extensions to this work that immediately suggest themselves. Perhaps two of the most interesting are (i) the calculation of the conductivity for the

electronic system using the Green's functions and (ii) the calculation of the spectra of slightly disordered quasiperiodic systems.

In the longer term we would hope to see more calculations of the dynamic properties of higher-dimensional quasicrystals being performed. For comparison with experiment, a calculation of the dynamic structure factor for a three-dimensional quasicrystal, possibly taking account of the effects of slight disorder in the lattice, is an important goal.

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[29] I am grateful to Professor D. Sherrington for pointing out this result.