Dynamical Maps, Cantor Spectra, and Localization for Fibonacci and Related Quasiperiodic Lattices

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The one-dimensional, discrete Schrödinger equation is studied when the potential is allowed to take on two values, V_A and V_B, which are arranged according to a generalized Fibonacci sequence. The problem is reduced to a dynamical map for the traces of the transfer matrices which are given recursively by $M_{l+1}=M_{l-1}M_l^n$, where n is a positive integer. A related class of sequences whose transfer matrices obey the recursion formula $M_{l+1}=M_{l-1}^nM_l$ is also investigated.

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The one-dimensional Schrödinger equation has stimulated a considerable amount of work based on both numerical calculations and renormalization-group techniques to illustrate the scaling properties of the electron states and eigenvalue spectrum.[1-10] Our understanding of this problem has indeed inspired further exploratory work by theorists and experimentalists on systems whose nonperiodicity is simulated by the requirement that a material parameter follow the Fibonacci sequence with the *golden mean*.[11-18] The work of Kohmoto, Kadanoff, and Tang[3] and Ostlund *et al.*[2] is generally credited with reflecting the quasiperiodicity of the system under investigation in a dynamical map approach.[17] For the quasiperiodic Schrödinger equation, it has been demonstrated that the wave functions are *critical* and are neither localized nor extended in a standard way.[7,9]

So far dynamical-systems techniques have been applied to only one example of a general sequence which obeys an inflation scheme for the building blocks forming a binary string. In this paper, we introduce and examine two classes of dynamical systems for the traces of the transfer matrices of a binary string, thus generalizing the Fibonacci sequence. We obtain closed-form expressions for the dynamical maps and their invariant manifolds. According to the numerical calculations, one of the maps has a large set of initial conditions for which the corresponding orbits are bounded.

We now describe how to construct the first class of quasiperiodic sequences by exploiting the algorithm for generating a continued fraction (CF).[19] Let $[b_0,b_1,b_2,\ldots]$ denote a simple CF where the b_n denote integers. If this CF is broken off after l terms, we have a rotational approximation A_l/B_l where A_l and B_l are coprime integers which obey the recursion relations $A_l=b_lA_{l-1}+A_{l-2}$, $B_l=b_lB_{l-1}+B_{l-2}$ with $A_0=b_0$, $A_{-1}=1$, and $B_0=1$, $B_{-1}=0$. If b_l is l independent, we have $B_l=A_{l-1}$. If $b_l=1$, the CF has the golden-mean value of $g=(1+5^{1/2})/2$ and we obtain the well-known recursion formula for Fibonacci numbers. The corresponding Fibonacci sequence with the golden mean consisting of building blocks A and B is generated as $S_1=\{A\}$, $S_2=\{BA\}$, $S_3=\{ABA\},\ldots,$ where each term is the *sum* of its predecessors. When $b_l=2$, we obtain the *silver mean* $s=1+2^{1/2}$ and the sequence $S_1=\{A\}$, $S_2=\{BA\}$, $S_3=\{ABABA\},\ldots,$ where each term of the string is constructed by our putting together two replicas of the term immediately preceding it with its predecessor, and left-right ordering is preserved. These two examples belong to a general class of nonperiodic but subtle sequences which never quite repeat but obey the recursion relation

$$S_{l+1}=S_{l-1}S_l^n, \tag{1}$$

where $l\geq 2$ and n is a positive integer. We could now apply the recursion relation in Eq. (1) to a model system such as a superlattice and examine the plasmon spectrum or the *concentration* of light within a multilayer system.[13,18] In order to illustrate the mathematical and physical properties of this class of sequences by dynamical-systems techniques, we choose to deal with the simplest model for electronic properties of a one-dimensional quasicrystal. This is the one-dimensional version of an almost-periodic (discrete) Schrödinger equation,

$$\begin{pmatrix}\psi_{l+1}\\ \psi_l\end{pmatrix}=M(l)\begin{pmatrix}\psi_l\\ \psi_{l-1}\end{pmatrix}, \tag{2}$$

where ψ_l denotes the wave function at the lth lattice site, $M(l)$ is a transfer matrix defined by

$$M(l)=\begin{pmatrix}E-V_l & -1\\ 1 & 0\end{pmatrix}, \tag{3}$$

and the potential V_l takes two values V_A and V_B. Since the generalized Fibonacci sequence is constructed by Eq. (1), then $M_l\equiv M(F_l)M(F_l-1)\ldots M(2)M(1)$, where F_l is a Fibonacci number, obeys $M_{l+1}=M_{l-1}M_l^n$.

The energy spectrum E is obtained by our looking for energies whose corresponding wave functions do not grow as the number of lattice sites is inflated through the generalized Fibonacci numbers. This means that the eigenvalues of M_l must be complex with unit magnitude, as $l \to \infty$.[4] This condition for E to be in the energy spectrum is transferred to the trace which must satisfy $|\mathrm{Tr} M_l| < 2$, since M_l has unit determinant. The matrix recursion relation for M_l leads to a discrete dynamical system with the traces as elements. We now examine the two cases corresponding to $n=2$ and $n=3$ in some detail. If we define $x_l = \frac{1}{2}\,\mathrm{Tr} M_l$, calculation shows that the generalized Fibonacci sequence with the silver mean, i.e., $n=2$, has a recursion relation for x_l that is given by the following pair of equations:

$$x_{l+1} = 4x_l t_{l+1} - x_{l-1}, \tag{4a}$$

$$t_{l+1} = x_{l-1}x_l - t_l, \tag{4b}$$

with the initial conditions for the dynamical system given by

$$x_1 = \tfrac{1}{2}\,\mathrm{Tr} M_A, \quad x_2 = \tfrac{1}{2}\,\mathrm{Tr}(M_B M_A),$$
$$t_3 = x_1(x_2 - \tfrac{1}{2}) - \tfrac{1}{4}(V_A - V_B). \tag{5}$$

Here M_A and M_B are the matrices in Eq. (3) with $V_n = V_A$ and V_B, respectively. If we define a three-dimensional vector by $\mathbf{r}_l \equiv (x_l, y_l, z_l) = (x_l, x_{l+1}, t_{l+2})$, Eq. (4) can be written as a nonlinear dynamical map

$$\mathbf{r}_{l+1} = T_s(\mathbf{r}_l)$$
$$= (y_l, 4y_l z_l - x_l, y_l(4y_l z_l - x_l) - z_l). \tag{6}$$

T_s in Eq. (6) has an invariant given by

$$I_s = x_l^2 + y_l^2 + 4z_l^2 - 4x_l y_l z_l - 1$$
$$= \tfrac{1}{8}\,\mathrm{Tr}[M_l, M_{l-1}]^2. \tag{7}$$

These remarkable results show that the points obtained from Eq. (6) by successive iterations are actually confined on the same two-dimensional manifold (for a given value of I_s) as the dynamical system for the Fibonacci sequence with the golden mean.[7] As a matter of fact, for the initial conditions in Eq. (5), we find that I_s is given by $(V_A - V_B)^2/4$. Almost all orbits on the manifold (see Fig. 1 of Ref. 17) escape to infinity along one of the four parts which extend from the middle portion. The rate of escape of these orbits is greater than for those unbounded orbits for the map with the golden mean. The scale transformation in Eq. (6) has a two-cycle orbit $A(0,0,a/2) \to B(0,0,-a/2) \to A$ where $a \equiv (I_x + 1)^{1/2}$ and a four-cycle orbit $C(0,a,0) \to D(a,0,0) \to E(0,-a,0) \to F(-a,0,0) \to C$. The wave functions governed by these orbits are self-similar and therefore intermediate between a localized and extended state. Linearization of T_s^2 and T_s^4 about their fixed points yields scaling exponents for the energy spectrum. There are three major bands: The central part scales with an eigenvalue of T^4 and the two outer regions scale with an eigenvalue of T^2.

The incommensurate system whose building blocks are generated by the recursion relation in Eq. (1) when $n=3$ has a mean value for the Fibonacci numbers F_{l+1}/F_l which approaches a *bronze mean* $\beta = (3 + 13^{1/2})/2$. The dynamical map for this case is given by

$$x_{l+1} = 2x_l t_{l+1} - g_{l+1}, \tag{8a}$$

$$g_{l+1} = 2x_{l-1}x_l - t_l, \tag{8b}$$

$$t_{l+1} = 2x_l g_{l+1} - x_{l-1}, \tag{8c}$$

where x_1 and x_2 have the same values as for the silver-mean map and $g_3 = 2x_1x_2 - x_1 + (V_B - V_A)/2$. By the definition of a three-dimensional vector $\mathbf{r}_l = (x_l, x_{l-1}, g_{l+1})$, Eqs. (8) are alternatively expressed as $\mathbf{r}_l = T_\beta(\mathbf{r}_l)$ where T_β is a nonlinear map given explicitly by

$$x_{l+1} = (4x_l^2 - 1)z_l - 2x_l y_l, \quad y_{l+1} = x_l,$$
$$z_{l+1} = 2x_l(x_{l+1} - z_l) + y_l. \tag{9}$$

The map in Eq. (9) has a conserved quantity given by Eq. (7) with $z_l \to z_l/2$. Thus the class of Fibonacci sequences in Eq. (1) have the same invariant for $n = 1$, 2, and 3 and we believe that this is true for all values of n. Our numerical calculations also show that almost all orbits for T_β are strictly escaping. The rate of escape increases with the index n. We were able to identify a six-cycle and two-cycle orbit for the map T_β. Our conclusions are that the quasiperiodic sequences in Eq. (1) would not easily show the *critical* effects in the proposed experiments since there appear to be so few bounded or-

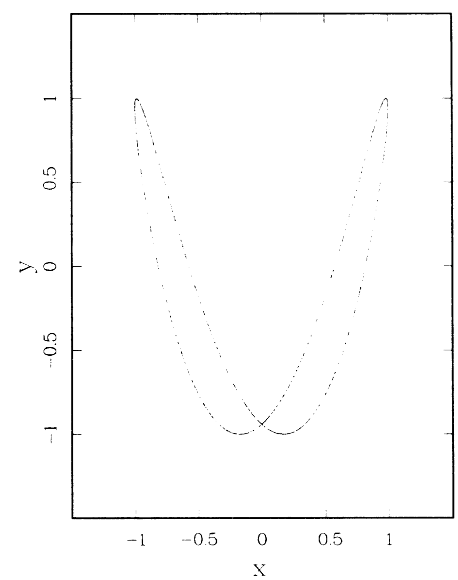

FIG. 1. An aperiodic orbit for the copper-mean map in Eq. (11) when $\gamma = y_1 - 2x_1$ for an initial point with $x_1 = y_1 = 1599/1699$. When the rounding error is made sufficiently small, all points on the orbit lie on a *closed* curve. Otherwise, some of the points obtained during the course of iteration would not be found on this curve.

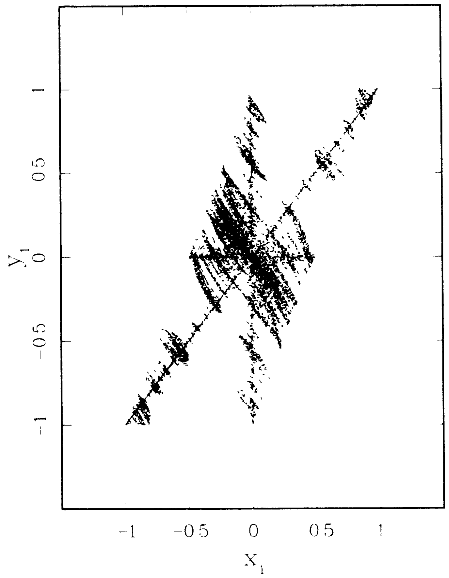

FIG. 2. The set of initial points with coordinates (x_1,y_1) which yield bounded (cyclic or aperiodic) orbits for the map in Eq. (11) with $\gamma=y_1-2x_1$. For the mesh size chosen, there are 16806 points in this diagram which do not escape after 2000 iterations.

bits.

The quasiperiodicity was then generated by the construction of a separate class of sequences given recursively by

$$S_{l+1}=S_{l-1}^n S_l, \tag{10}$$

where $n=2,3,\ldots$, so as to see whether this rearrangement of the generalized Fibonacci series would improve the number of bounded orbits for a chosen value of n. For the sequence in (10), the number of building blocks is f_l where $f_{l+1}=nf_{l-1}+f_l$. When $n=2$, we obtain $f_{l+1}/f_l\to 2$ as $l\to\infty$. We refer to this ratio as the *copper mean.* The recursion relation for half the trace of the transfer matrices given recursively by $M_{l+1}=M_{l-1}^2 M_l$ has been evaluated for two sets of initial conditions. For a system of A's and B's with $S_1=\{B\}$, $S_2=\{A\}$, $S_3=\{BBA\},\ldots$, we obtain

$$x_{l+1}=2(2x_{l-1}^2-1)x_l+\gamma, \tag{11}$$

where $\gamma=x_2-2x_1$. For the sequence beginning with $S_1=\{B\}$, $S_2=\{BA\}$, $S_3=\{BBBA\},\ldots$, the map is also given by Eq. (11) except that $\gamma=-1$. The map in Eq. (11) has been studied numerically for various values of x_1 and x_2. A more detailed study of the map with regards to the stability of the fixed points and the possible existence of attractors is worthwhile undertaking. These results will be published elsewhere. Our conclusions for the present study are as follows.

The map in Eq. (11) is two dimensional with

$$(x_{l+1},y_{l+1})=(y_l,4x_l^2y_l-2y_l+\gamma).$$

The initial points (x_1,y_1) for which the orbits of the map are bounded are very large in number. This is in sharp contrast to the class of sequences in Eq. (1) where the closed (periodic) orbits are isolated and appear to be only few in number. An example of a bounded orbit for Eq. (11) is shown in Fig. 1. Figure 2 shows those initial values for which the orbits are bounded. Furthermore, each bounded orbit of Eq. (11) has a unique initial point when γ is energy dependent. The map for which $\gamma=-1$ also has a dense set of initial points which yield bounded orbits. As the index n increases for the class of sequences in Eq. (10), we anticipate that the unshaded regions in Fig. 2 corresponding to escape orbits become smaller in area. These results suggest that the *concentration* of light in layered structures would be more easily observable when the quasiperiodicity is simulated by Eq. (10). Our analysis shows that the sequences in Eqs. (1) and (10) are the *reverse* of each other and this observation is the main result of this paper.[20]

When $\gamma=x_2-2x_1$, the map in Eq. (11) has a two-cycle orbit given by $(\frac{1}{4},-1)\to(-1,\frac{1}{4})$. However, the corresponding matrices are four-cycle. The map also has a three-cycle orbit given by $(\frac{1}{2},-\frac{1}{4})\to(-\frac{1}{4},-1)\to(-1,\frac{1}{2})$ and the corresponding matrices are six-cycle. The feature that makes the map in Eq. (11) interesting is that there appears to be at least one periodic orbit for every cycle.

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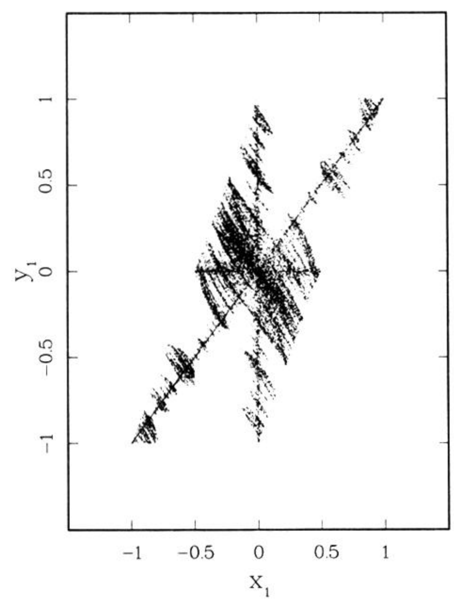
[20]Calculations have shown that the off-diagonal version of the quasiperiodic Schrödinger equation which is given by

$$t_{l+1}\psi_{l+1}+t_l\psi_{l-1}=E\psi_l$$

has the same trace map as the diagonal version in Eq. (3) when the hopping matrix elements $\{t_l\}$ have two values t_A and t_B which obey the Fibonacci sequence with the golden, silver, bronze, and copper means, respectively.



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