One-dimensional k-component Fibonacci structures

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A one-dimensional k-component Fibonacci structure, with k different intervals, is the natural extension of the standard Fibonacci structure with two intervals. We prove that the structures with $k \leq 5$ are quasiperiodic, and the projection method can be applied to deal with the pattern and indexing problem of its x-ray-diffraction spectrum. For $k > 5$, the resulting structures are no longer quasiperiodic, but they are still ordering. The analytically obtained results have been compared to experimental results for Ta-Al three-component Fibonacci superlattice structures and to numerical calculations.

I. INTRODUCTION

In recent years there has been an abundance of theoretical and experimental work in one-dimensional (1D) quasiperiodic systems.[1–8] From the theoretician's point of view, there is interest because although quasicrystals are perfectly ordered, the Bloch theorem is inapplicable to them since there is no translational symmetry. This problem represents, in some respects, an intermediate case between periodic and disodered solids. For the 1D case, known as the Fibonacci chain, it has been proved that the energy spectrum is a singular continuous Cantor set, i.e., neither continuous nor pointlike, and the eigenstates are believed to be critical, i.e., neither localized nor extended. On the experimental side, advances in thin film techniques have made it possible to prepare artificially 1D quasiperiodic superlattices. Because the fabrication of quasiperiodic superlattices is easier than the growth of large single-phase quasicrystals, and due to the fact that the characteristic intervals and the growth sequence can be intentionally chosen, quasiperiodic superlattices play a very important role in the study of the physical properties of quasicrystals.

In 1985, Merlin *et al.* reported the first realization of Fibonacci superlattices.[5] The Fibonacci sequence is obtained by repeated application of the substitution rules $A \rightarrow AB$ and $B \rightarrow A$, in which the ratio of the two incommensurate intervals A and B, d_A/d_B, is equal to the golden mean $\tau = (\sqrt{5}+1)/2$. The x-ray diffraction and Raman spectra presented the self-similarity. Since then, many experiments on quasiperiodic superlattices have been reported.[6–9] However, to our knowledge, most of these have been based on the Fibonacci sequence and only very few experiments have been performed on non-Fibonacci structures. For example, Thue-Morse superlattices,[10] which can be generated by the substitution rule $A \rightarrow AB$ and $B \rightarrow BA$, belong to the class of structures based on automatic sequences. Their behavior is, in some respects, intermediate between quasiperiodicity and randomness. Birch *et al.*[11] reported a class of quasiperiodic superlattice structures which can be generated by the inflation rule $A \rightarrow A^mB$ and $B \rightarrow A$. All of the above-mentioned structures include only two intervals of length d_A and d_B.

In the present work, the standard Fibonacci structure with two intervals has been generalized to k-component Fibonacci structure with k intervals. This structure has many advantages: it can be periodic ($k = 1$), quasiperiodic ($k \leq 5$), or only ordering ($k > 5$).

II. SUBSTITUTION RULES AND ALGEBRAIC NUMBER THEORY

Let us suppose that we have a set of k elements $(A_1, A_2, \ldots, A_k)$. Let T be substitution,

$$TA_1 = A_1A_k, TA_k = A_{k-1}, \ldots, TA_i = A_{i-1}, \ldots, TA_2 = A_1.$$

Let $C_n = T^nA_1$. Thus

$$\begin{aligned} C_0 &= A_1, \\ C_1 &= A_1A_k, \\ C_2 &= A_1A_kA_{k-1}, \\ &\cdots \\ C_k &= A_1A_kA_{k-1}\ldots A_3A_2, \end{aligned}$$

and in general $C_n = C_{n-1} + C_{n-k}$. Let A_i be a tile (interval) of length d_i. Then the k-component Fibonacci tiling is obtained as $\lim_{n\to\infty} C_n$ by choosing the origin appropriately.

A question arises of whether the tilings obtained above are quasiperiodic for all k's. The Bombier-Taylor theorem gives a sufficient condition for absence of quasiperiodicity:[12,13] if the characteristic polynomial of the substitution rule has only one root λ_0 of absolute value greater than one, i.e., λ_0 is a Pisot number, then the tiling is quasiperiodic and can be generated by a cut-and-project method. Otherwise, the tiling is not quasiperiodic.

In our case, the substitution matrix M of T is

$$M = \begin{pmatrix} 1 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix}_{k\times k} . \tag{1}$$

Then the characteristic polynomial of M is

$$P_k(\lambda) = \lambda^k - \lambda^{k-1} - 1. \tag{2}$$

The set of all distinct eigenvalues of M is called the spectrum of M and is denoted by $\sigma(M)$,

$$\rho(M) = \max_{\lambda_j\in\sigma(M)} |\lambda_j| \tag{3}$$

is called the spectral radius of M. We have the following results (the proofs are given in the Appendix).

(1) Each eigenvalue of M is simple.

(2) For $k \geq 2$ there is always a unique positive eigenvalue $\lambda_0 = \rho(M) \in \sigma(M)$ and $1 < \lambda_0 < 2$. λ_0 is the leading eigenvalue of M.

(3) $\sigma(M) \subset R$, where R is the region enclosed by the curves $ABCDEOA$ and $AHMGNFEO_1A$ in Fig. 1.

(4) If $\lambda_j \in \sigma(M)$ lies on the curve $ABCDEFGMA$ in Fig. 1, then $\lambda_j = e^{\pm i\frac{\pi}{3}}$. In addition $\lambda_j = e^{\pm i\frac{\pi}{3}}$ is the only pair of eigenvalues with modulus equal to one if and only if $k \equiv 5 \pmod 6$ (namely, $k = 5, 11, 17, \ldots$).

(5) If k is odd, then λ_0 is the unique real eigenvalue of M. If k is even, then M has exactly two real eigenvalues λ_0, λ_1, where $\lambda_1 < 0$, $1/\lambda_0 < |\lambda_1| < 1$.

(6) The number of pairs of nonreal roots of modulus greater than 1 is $[k/6]$, where $[.]$ denotes the integer part.

From these results it follows that λ_0 is a Pisot number for $2 \leq k \leq 5$, and that the corresponding tiling is quasiperiodic; for $k > 5$, λ_0 is not a Pisot number and the tiling is no longer quasiperiodic, but it is still ordering since substitution rules imply ordering; for $k = 1$, the tiling is periodic.

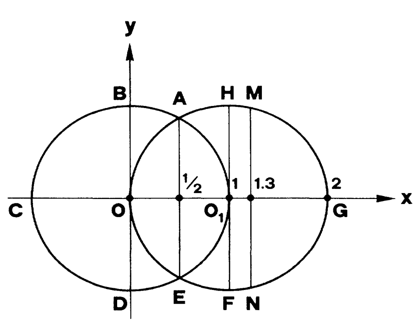

FIG. 1. The region of the spectrum of M.

III. PROJECTION METHOD AND DIFFRACTION SPECTRUM

A low-dimensional quasiperiodic structure may be considered as the projection of high-dimensional periodic structure.[14,15] Therefore , when $k \leq 5$, the k-component Fibonacci lattice can be obtaind by a projection method. For this reason, supposing that $|A_i|_n$ represents the number of A_i in $C_n^{(k)}$, a set of ration is defined from this sequence, $\eta_i = \lim_{n\to\infty}(|A_i|_n/|A_1|_n)$. The set of η_i satisfies the following equation:

$$\begin{aligned} &\eta_k^k + \eta_k = 1, \\ &1 : \eta_k = \eta_k : \eta_{k-1} = \cdots = \eta_3 : \eta_2. \end{aligned} \tag{4}$$

It is easy to prove that all these ratios are irrational numbers between zero and one, except $\eta_1 = 1$. η_k is just the reciprocal of the leading eigenvalue of the matrix M, $\eta_k = 1/\lambda_0$. For example, when $k = 3$,

$$\begin{aligned} \eta_3 &= \sqrt[3]{1/2 + 1/2\sqrt{31/27}} + \sqrt[3]{1/2 - 1/2\sqrt{31/27}}, \\ \eta_2 &= -2/3 + \sqrt[3]{29/54 + 1/2\sqrt{31/27}} \\ &\quad + \sqrt[3]{29/54 - 1/2\sqrt{31/27}}, \\ \eta_1 &= 1. \end{aligned} \tag{5}$$

Now, consider a K-dimensional regular periodic lattice with unit lattice vector $(e_1, e_2, \ldots, e_k)$. Let $X : \{x_1, x_2, \ldots, x_k\}$ be a coordinate system constructed from any lattice point O (which will be the origin) and a basis $\{e_1, e_2, \ldots, e_k\}$. Let $X' : \{x_1', x_2', \ldots, x_k'\}$ be another orthogonal coordinate system constructed from O with a basis $\{e_1', e_2', \ldots, e_k'\}$. The two coordinate systems X and X' are related by $X = AX'$, i.e.,

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{pmatrix} = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{k1} \\ a_{12} & a_{22} & \cdots & a_{k2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & a_{2k} & \cdots & a_{kk} \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ \vdots \\ x_k' \end{pmatrix}, \tag{6}$$

where $a_{ij} = e_i' \cdot e_j$ $(i, j = 1, 2, \ldots, k)$ are the orientation cosines of axis X_i'. If we choose the axis X_k' as the projecting line, its orientation cosines satisfy

$$a_{k1} : a_{k2} : \cdots : a_{kk} = 1 : \eta_2 : \cdots : \eta_k, \tag{7}$$

then, there will be no other points on this line since all the η_i (except η_1) are not rational. Take the set of points which lie within a certain distance, w, from the hypersurface and project them onto the line. The projected set of points will clearly be arranged aperiodically.

The k-dimensional periodic lattice of points may be represented by the function

$$U(x_1, x_2, \ldots, x_k) = (1/2\pi)^k \sum \delta(x_1 - n_1)\delta(x_2 - n_2) \cdots \delta(x_k - n_k), \tag{8}$$

where the sum is all the integers n_i ($i = 1, 2, \ldots, k$), and the projection function is

$$R(x_1', x_2', \ldots, x_{k-1}') = \begin{cases} 1 & \text{if } |x_i'| \le w_i \ (i = 1, 2, \ldots, k-1), \\ 0 & \text{otherwise,} \end{cases} \tag{9}$$

thus, the function

$$Q(x_k') = \int \cdots \int R(x_1', x_2', \ldots, x_{k-1}') U(x_1', x_2', \ldots, x_k') dx_1' dx_2' \ldots dx_{k-1}' \tag{10}$$

where $U(x_1', x_2', \ldots, x_k') \equiv U(\sum a_{i1}x_i', \sum a_{i2}x_i', \ldots, \sum a_{ik}x_i')$ is the sum of points of the k-component Fibonacci lattice. If a string of atoms were placed at these lattice points, the intensity of the diffraction pattern is related simply to the Fourier transform of $Q(x_k')$. Using $S(p_1, p_2, \ldots, p_{k-1})$ and $M(x_k', P_1, p_2, \ldots, p_{k-1})$ as the transformation of R and U, respectively, and according to the convolution law, we have

$$Q(x_k') = \int \cdots \int S(p_1, p_2, \ldots, p_{k-1}) M(x_k', p_1, p_2, \ldots, p_{k-1}) dp_1 dp_2 \cdots dp_{k-1}. \tag{11}$$

The Fourier transformation $F(q)$ of $Q(x_k')$ is

$$F(q) = \int \cdots \int S(-p_1, -P_2, \ldots, -p_{k-1}) V(q, p_1, p_2, \cdots, p_{k-1}) dp_1 dp_2 \cdots dp_{k-1}, \tag{12}$$

where

$$V(q, p_1, p_2, \ldots, p_{k-1}) = \sum \delta[p_1 - 2\pi p_1(n_1, n_2, \ldots, n_k)]\delta[p_2 - 2\pi p_2(n_1, n_2, \ldots, n_k)] \cdots \times \delta[p_{k-1} - 2\pi_{k-1}(n_1, n_2, \ldots, n_k)]\delta[q - 2\pi q(n_1, n_2, \ldots, n_k)],$$

$$S(p_1, p_2, \ldots, p_{k-1}) = \prod_{i=1}^{k-1} 2w_i \sin p_i w_i / p_i w_i.$$

Therefore, we have

$$F(q) = \sum S[p_1(n_1, n_2, \ldots, n_k), p_2(n_1, n_2, \ldots, n_{k-1}), \ldots, p_{k-1}(n_1, n_2, \ldots, n_{k-1})]\delta[q - q(n_1, n_2, \ldots, n_k)], \tag{13}$$

where

$$p_1(n_1, n_2, \ldots, n_k) = \begin{vmatrix} n_1 & a_{21} & \cdots & a_{k1} \\ n_2 & a_{22} & \cdots & a_{k2} \\ \vdots & \vdots & \ddots & \vdots \\ n_k & a_{2k} & \cdots & a_{kk} \end{vmatrix}, \tag{14}$$

$$p_2(n_1, n_2, \ldots, n_k) = \begin{vmatrix} a_{11} & n_1 & \cdots & a_{k1} \\ a_{12} & n_2 & \cdots & a_{k2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & n_k & \cdots & a_{kk} \end{vmatrix}, \tag{15}$$

$\cdots$

$$p_{k-1}(n_1, n_2, \ldots, n_k) = \begin{vmatrix} a_{11} & \cdots & n_1 & a_{k1} \\ a_{12} & \cdots & n_2 & a_{k2} \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & \cdots & n_k & a_{kk} \end{vmatrix}, \tag{16}$$

$$q(n_1, n_2, \ldots, n_k) = \begin{vmatrix} a_{11} & \cdots & a_{k-1,1} & n_1 \\ a_{12} & \cdots & a_{k-1,2} & n_2 \\ \vdots & \vdots & \ddots & \vdots \\ a_{1k} & \cdots & a_{k-1,k} & n_k \end{vmatrix}. \tag{17}$$

Considering Eqs. (17) and $|A| = 1$, $q(n_1, n_2, \ldots, n_k)$ can be rewritten as

$$q(n_1, n_2, \ldots, n_k) = 2\pi D^{-1} \sum_{i=1}^{k} n_i \eta_i, \tag{18}$$

where

$$D = \sum_{i=1}^{k} \eta_i d_i \tag{19}$$

and η_i (i runs from 1 to k) are integers, D is an average lattice parameter. The Fourier transform of the k-($k \le 5$)component Fibonacci lattice consists of δ-function peaks at $q(n_1, n_2, \ldots, n_k)$. The strongest peaks correspond to $p_i w_i \cong 0$. It is easy to prove that the strongest peaks are for

$$n_1 : n_2 : \cdots : n_k \cong 1 : \eta_2 : \cdots : \eta_k, \tag{20}$$

this condition leads to the series of $(n_1, n_2, \ldots, n_k)$ which are the so-called general Fibonacci numbers $(a_n, a_{n-k+1}, a_{n-k+2}, \ldots, a_{n-1})$. All of these $\{a_i\}$ belong to the sequence described as $a_i = a_{i-1} + a_{i-k}$ with $a_1 = a_2 = \cdots = a_{k-1} = 0$ and $a_k = 1$. Then the strongest peaks satisfy

$$q(a_{n+k}, a_{n+1}, \ldots, a_{n+k-1}) = q(a_{n+k-1}, a_n, \ldots, a_{n+k-2}) + q(a_n, a_{n-k+1}, \cdots, a_{n-1}), \tag{21}$$

which reflects the self-similarity of its diffraction spectrum.

IV. EXPERIMENT AND NUMERICAL CACULATION

In order to test the above-mentioned results, a three-component Fibonacci Ta/Al superlattice was grown epitaxially on glass substrates by dual-target magnetron sputtering. The parameters of the structure were chosen so that the Ta slabs, with the same thickness, were separated by three different slabs of Al. In a typical sample, the building blocks A_1, A_2, and A_3 consisted of (12.7 Å Ta + 36.44 Å Al), (12.7 Å Ta + 9.89 Å Al) and (12.7 Å Ta + 21.11 Å Al), respectively. d_2/d_1 and d_3/d_1 were approximately η_2 and η_3, respectively, the average lattice parameter was $D = d_1 + \eta_2 d_2 + \eta_3 d_3 = 82.72$ Å. The sample consisted of 16 generations. The total thickness was about 1.56 μm. A more detailed description of the sample preparation is given in Ref. 16.

X-ray scattering measurements were performed on the sample. A 12 kW Rigaku rotating anode x-ray source [a Cu anode in the high brilliance 0.2×2 mm^2 spot mode and a symmetric graphite (002) monochromator] was used. The scattering vector was nomal to the surface.

Figures 2 and 3 show the θ-2θ scan of x-ray diffraction in the low and high angle regions, respectively. In the low angle region, at least 14 satellite peaks were found. In the high angle region, the main diffraction peak was found. It corresponds to the reflection from the bcc Ta(110) and fcc Al(111) planes, which have an equal interlayer spacing of 0.2338 nm. On both sides of the main Bragg reflection, many satellite peaks were found. All the satellites can be indexed as $[n_1, n_2, n_3]$. The experimental values of q from x-ray diffractions are in excellent agreement with above calculated from Eq. (18). The self-similarity relation (21) is satisfied.

Numerical calculations of x-ray-diffraction spectra from k-component Fibonacci lattices have been carried out for $k = 3, 5, 6, 7, 8, 9$, and 277 to test the transition between the quasiperiodic and the nonquasiperiodic region. We supposed a set of identical 2D atom planes arranged in k-component Fibonacci sequence. The av-

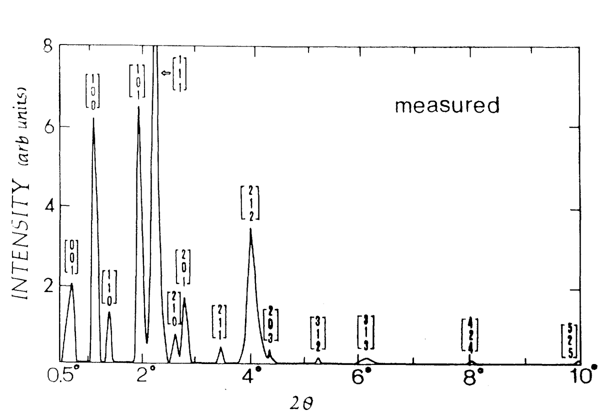

FIG. 2. The θ-2θ scan of x-ray diffraction in the low angle region for the $3CF$ Ta/Al superlattice.

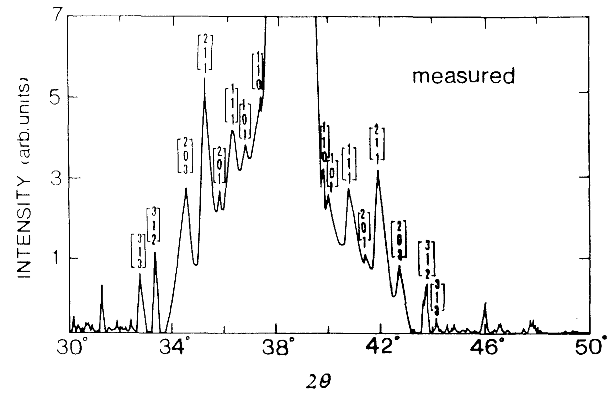

FIG. 3. The θ-2θ scan of x-ray diffraction in the high angle region for the $3CF$ Ta/Al superlattice.

erage atomic scattering factor of each atom plane was taken as one and the scattering vector was kept nomal to the atom planes. With these assumptions the x-ray-diffraction intensity is given by

$$I \propto \frac{1+\cos^2 2\theta}{\sin\theta \sin 2\theta} \sum_{j=1}^{m} \exp(i4\pi z_j \sin\theta/\lambda), \tag{22}$$

where z_j is position of ith plane, and m is the total number of atom planes. In the case of $k = 3$, our model consists of 15 generations and a total thickness of 7000 Å. The peaks can be indexed as $[n_1, n_2, n_3]$ (see Fig. 4). This result is the typical diffraction spectrum of a quasiperiodic structure and it is in very good agreement with the above discussion. For $k = 5$, we obtained a similar result. In the cases of $k = 6, 7, 8, 9$, although some peaks can be found in the diffraction spectra, those peaks cannot be indexed by the projection method. As k increases, the diffraction spectra get more and more complex. For $k = 277$, $\eta_{277} \cong 0.985$, $d_1 = 106.6$ Å, and a total thickness of 21.8 μm or so, the simulated result is very complex (see Fig. 5). Comparing with Fig. 4, one can easily find that the self-similarity in this spectrum has almost disappeared.

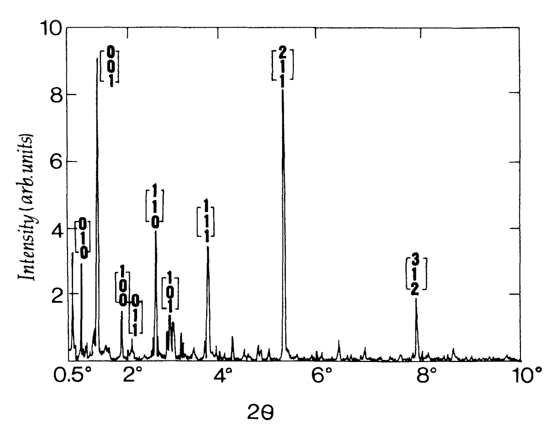

FIG. 4. The simulation of x-ray-diffraction intensity ($k = 3$). Note that

$q(a_{n+3}, a_{n+1}, a_{n+2}) = q(a_{n+2}, a_n, a_{n+1}) + q(a_n, a_{n-2}, a_{n_1})$.

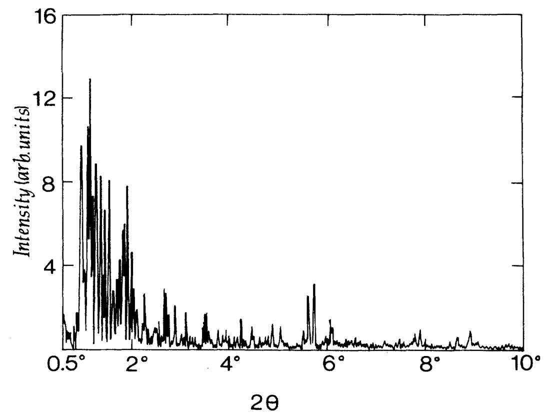

FIG. 5. The simulation of x-ray diffraction intensity ($k = 277$). The chaos-like spectrum is shown.

V. DISCUSSIONS

The 1D k-component Fibonacci structure can be obtained by defining k incommensurate intervals and ordering them in special substitution. It has been proved that, in the cases of $k \leq 5$, the structures are strict quasiperiodic, i.e., their Fourier transforms are a sum of weighted δ functions and the peaks are indexible using a finite set of base vectors. These structures can also be obtained by a projection method from k-dimensional hyperspace onto a line, whose orientation cosines satisfy Eq. (7). In this case the diffraction patterns are related to $(k-1)$ irrational numbers and the diffraction peak positions can be labeled by k integers. It is interesting to note that the periodic and standard Fibonacci structures can be thought of as the degenerate case for $k = 1$ and $k = 2$, respectively. In the case of $k > 5$, the structures are not strict quasiperiodic. We believe that they are still ordering and their behavior is intermediate between quasperiodicity and randomness. A sequence generated through substitution consisting of only k different intervals can always be obtained from the projection of the directed walk on a k-dimensional hypercubic lattice.[14] For $k > 5$, the directed walk seems to have unbounded fluctuations, i.e., the fluctuation of the positions of lattice points around their average lattice diverges as length of the chain increases. However, it is possible that their Fourier spectra are discrete. In physical terms, this means that the structure is quasiperiodic, but is not strict quasiperiodic and has no average lattice. Such as the cases of $k = 6, 7, 8, 9$, some discrete peaks can be found. As k increase, the diffraction spectra will get away from the discrete one. For example, $k = 277$, the simulated result is very complex, the spectrum is neither discrete nor continuance. We speculate that the spectrum may be approached to chaos. In a more precise way, the order in the sequence is best analyzed in terms of the fluctuation of the lifted structure in perp space.[13] However, a model with k incommensurate lengths is far more difficult to study than that with only one length or two arbitrary lengths. In spite of the difficulty, further theoretical and experimental investigations must be done to explain the transition between quasiperiodic and nonquasiperiodic.

Finally, these structures are of interest to understand the links between type of order and quasiperiodicity and to provide a model for fabrication of quasperiodic superlattices for use in a wide range of theoretical and experimental studies based on their unique properties.

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APPENDIX

The statements on the eigenvalues of the substitution matrix M are proven as follows.[17]

Proof 1. Consider the derivative

$$P_k'(\lambda) = k\lambda^{k-1} - (k-1)\lambda^{k-2} = \lambda^{k-2}[k\lambda - (k-1)]$$

of $P_k(\lambda)$. It is clear that the zero points 0, $(k-1)/k$ of $P_k'(\lambda)$ are not the zero points of $P_k(\lambda)$, so $[P_k(\lambda), P_k'(\lambda)] = 1$. Hence each eigenvalue of M is simple.

Proof 2. Note that M is non-negative and irreducible. By the Perron-Frobenius theorem (Ref. 17, pp. 536 and 537), we have that $\lambda_0 = \rho(M) \in \sigma(M)$ and $1 < \lambda_0 < 2$. Let $V(c_1, c_2, \ldots, c_n)$ denote the number of change of sign in the sequence $c_1, c_2, \ldots, c_n$ of real numbers. For the coefficients $1, -1, 0, \ldots, 0, -1$ of $P_k(\lambda)$, $V(1, -1, 0, \ldots, 0, -1) = 1$. Thus λ_0 is the unique positive root of $P_k(\lambda)$, by Descartes theorem. If $k \geq 3$, then $P_k(1)P_k(1.466) < 0$, and so $1 < \lambda_0 < 1.466$ for all $k \geq 3$.

Proof 3. It is clear from Geršgorin's theorem (Ref. 17, p. 371) that

$$\sigma(M) \subset \{z \mid |z| \leq 1\} \cup \{z \mid |z-1| \leq 1\}.$$

But $|\lambda_j|^{k-1}|\lambda_j - 1| = 1$ for all $\lambda_j \in \sigma(M)$, so $\sigma(M) \cup S = \phi$, where S is the region enclosed by the curve $AOEO_1A$ in Fig. 1.

Proof 4. By Taussky's theorem (Ref. 17, p. 376), if $\lambda_j \in \sigma(M)$ lies on the curve $ABCDEFNGMHA$ of Fig. 1, then $\lambda_j = e^{\pm i\frac{\pi}{3}}$ is represented by A and E in Fig. 1.

Note that $\lambda_j = e^{\pm i\frac{\pi}{3}}$ implies $\lambda_j^6 = 1$. If $k \equiv 5(\text{mod}6)$, then $P_k(e^{\pm i\frac{\pi}{3}}) = 0$, so $\lambda_j \in \sigma(M)$. In addition, the following results are straightforward:

$$P_k(e^{i\frac{\pi}{3}}) = \begin{cases} e^{i\frac{\pi}{3}} - 1 - 1 \neq 0 & \text{when } k \equiv 1(\text{mod } 6), \\ e^{i\frac{2\pi}{3}} - e^{i\frac{\pi}{3}} - 1 \neq 0 & \text{when } k \equiv 2(\text{mod } 6), \\ -1 - e^{i\frac{2\pi}{3}} - 1 \neq 0 & \text{when } k \equiv 3(\text{mod } 6), \\ e^{i\frac{4\pi}{3}} - e^{i\pi} - 1 \neq 0 & \text{when } k \equiv 4(\text{mod } 6), \\ 1 - e^{i\frac{5\pi}{3}} - 1 \neq 0 & \text{when } k \equiv 0(\text{mod } 6). \end{cases}$$

But $P_k(e^{i\frac{\pi}{3}}) = 0$ if and only if $P_k(e^{-i\frac{\pi}{3}}) = 0$, so 4 has been proved.

Proof 5. We have seen in the proof above of 2 that λ_0 is the unique positive root of $P_k(\lambda)$, i.e., λ_0 is the unique positive eigenvalue of M.

Consider

$$P_k(-x) = \begin{cases} -x^k - x^{k-1} - 1, & \text{if } k \text{ is odd,} \\ x^k + x^{k-1} - 1, & \text{if } k \text{ is even.} \end{cases}$$

Note that $V(-1,-1,0,\ldots,0,-1) = 0$, $V(1,1,0,\ldots,0,-1) = 1$, we know that the number of negative eigenvalues of M is

$$n = \begin{cases} 0 & \text{if } k \text{ is odd,} \\ 1 & \text{if } k \text{ is even,} \end{cases}$$

by Descarte's theorem. Since $P_k(0) = -1 \neq 0$, we completed the proof 5.

Proof 6. Let the nonreal roots of $P_k(\lambda)$ be $\lambda = re^{i\theta}(r > 0, 0 < \theta < 2\pi)$. For the nonreal roots of modulus greater than 1, we have $r > 1$, $-\frac{\pi}{3} < \theta < \frac{\pi}{3}$ by proof 3. Since nonreal roots come by pairs of complex conjugate numbers, we only need to consider $0 < \theta < \frac{\pi}{3}$. By De Moivre's theorem, the equation $P_k(\lambda) = 0$ can be written in the form of a system of equations:

$$r^k \cos k\theta - r^{k-1}\cos(k-1)\theta - 1 = 0, \tag{A1}$$

$$r \sin k\theta = \sin(k-1)\theta, \tag{A2}$$

multiplying each side of Eq. (A1) by $\sin k\theta (\neq 0)$, then substituting (A2) into it, we obtain

$$r^{k-1}[\sin(k-1)\theta\cos k\theta - \sin k\theta\cos(k-1)\theta] - \sin k\theta = 0,$$

i.e,

$$\sin k\theta + r^{k-1}\sin\theta = 0. \tag{A3}$$

Hence, the system of Eqs. (A1) and (A2) is equivalent to that of (A2) and (A3).

Substituting (A2) into (A3), we obtain an equation on θ:

$$\sin k\theta + \left(\frac{\sin(k-1)\theta}{\sin k\theta}\right)^{k-1} \sin\theta = 0. \tag{A4}$$

Let

$$f(\theta) = \sin k\theta + \left(\frac{\sin(k-1)\theta}{\sin k\theta}\right)^{k-1} \sin\theta,$$

since $r > 1$, we consider two cases as follows.

Case 1. $\sin(k-1)\theta < \sin k\theta < 0$. In this case,

$$(2n-1)\pi < k\theta < 2n\pi, \quad n \in N$$

and

$$\sin k\theta - \sin(k-1)\theta > 0 \quad \Longleftrightarrow$$

$$2\cos\frac{2k-1}{2}\theta \sin\frac{\theta}{2} > 0 \quad \Longleftrightarrow$$

$$2m\pi - \frac{\pi}{2} < \frac{2k-1}{2}\theta < 2m\pi + \frac{\pi}{2}, \quad m \in N,$$

i.e.,

$$\frac{2n-1}{k}\pi < \theta < \frac{2n}{k}\pi,$$

$$\frac{4m-1}{2k-1}\pi < \theta < \frac{4m+1}{2k-1}\pi, \quad n,m \in N.$$

Note that $\theta < \frac{\pi}{3}$, so $k > 6n$. When $n > m$ (n,m are integers, $n - m \geq 1$), we have

$$\frac{2n-1}{k} > \frac{4m+1}{2k-1},$$

but when $n < m$, we also have

$$\frac{2n}{k} < \frac{4m-1}{2k-1}.$$

Therefore, we must have $n = m$ and

$$\frac{4n-1}{2k-1}\pi < \theta < \frac{2n}{k}\pi. \tag{A5}$$

From this it follows that

$$2n\pi - \frac{\pi}{2} + \frac{4n-1}{2(2k-1)}\pi < k\theta < 2n\pi,$$

$$2n\pi - \frac{\pi}{2} - \frac{4n-1}{2(2k-1)}\pi < (k-1)\theta < 2n\pi - \frac{2n\pi}{k-1},$$

$$\begin{aligned} f\left(\frac{4n-1}{2k-1}\pi\right) &= -\cos\frac{4n-1}{2(2k-1)}\pi + \sin\frac{4n-1}{2k-1}\pi \\ &= -\cos\frac{4n-1}{2(2k-1)}\pi\left(1 - 2\sin\frac{4n-1}{2(2k-1)}\pi\right) \\ &< 0. \end{aligned}$$

(Note that $\frac{4n-1}{2k-1}\pi < \theta < \frac{\pi}{3} \Rightarrow \sin\frac{4n-1}{2(2k-1)}\pi < \frac{1}{2}$) and

$$f\left(\frac{2n\pi}{k} - 0\right) \to -0 + r\sin\frac{2n\pi}{k} > 0.$$

On the other hand, the derivative of $f(\theta)$ is

$$f'(\theta) = k\cos k\theta + r^{k-2}(k-1)r'_\theta \sin\theta + r^{k-1}\cos\theta,$$

where

$$\begin{aligned} r'_\theta &= \frac{(k-1)\cos(k-1)\theta\sin k\theta - k\cos k\theta\sin(k-1)\theta}{\sin^2 k\theta} \\ &= \frac{(k-1)\sin\theta - \cos k\theta\sin(k-1)\theta}{\sin^2 k\theta}. \end{aligned}$$

When θ satisfies (A5), we have

$$\cos k\theta > 0, \quad \sin(k-1)\theta < 0, \quad \sin\theta > 0, \quad \cos\theta > 0,$$

hence $r'_\theta > 0$, so $f(\theta)' > 0$, i.e., $f(\theta)$ is monotonic.

Consequently, for each $n = 0, 1, \ldots, [k/6] - 1$, there always exists a θ, which satisfies condition (A5), such that $f(\theta) = 0$. It is clear that the system of equations (A2) and (A4) is equivalent to that of (A1)and (A2).

Case 2. $\sin(k-1)\theta > \sin k\theta > 0$. Similar to case 1, we obtain

$$\frac{4n+1}{2k-1}\pi < \theta < \frac{2n+1}{k}\pi.$$

Clearly, $(k-1)\theta$ and $k\theta$ lie in the I or II quadrant. So that $f(\theta) > 0$, i.e., no solution of $P_k(\lambda) = 0$ exists in this case.

In summary, considering that the nonreal roots of $P_k(\lambda) = 0$ come by pairs of complex conjugate numbers, the number of pairs of nonreal roots of modulus greater than 1 is $[k/6]$. And they satisfy

$$\frac{4n-1}{2k-1}\pi < \theta < \frac{2n}{k}\pi, \quad n = 0, 1, \ldots, [k/6] - 1,$$

$$r = \frac{\sin(k-1)\theta}{\sin k\theta}.$$

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