ONE-DIMENSIONAL QUASI-CRYSTALS AND SEQUENCES OF ONES AND ZEROS

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We derive the relationship between one-dimensional quasi-crystals and sequences of ones and zeros introduced by de Bruijn. Properties of these sequences are used to derive explicit expressions for the positions of the quasi-crystal atoms, for nearest neighbor distances, and a classification in which all identical but shifted quasi-crystals are classified into a single class.

In an alloy of Al and Mn, Shechtman, Blech, Gratias and Cahn [1] discovered a crystal-like structure with an icosahedral diffraction pattern. Levine and Steinhardt [2] soon after introduced a model structure which gives rise to a similar diffraction pattern. Geometric projection methods of constructing such crystal-like structures, called quasi-crystals, have been given by Kramer and Neri [3], Elser [4], Zia and Dallas [5], and Duneau and Katz [6].

Geometric projection methods to construct one-dimensional quasi-crystals consider a two-dimensional square lattice of points with sides of the square of unit length. In addition to an orthogonal X, Y coordinate system, see fig. 1, a second rotated X', Y' coordinate system is introduced. The angle of rotation θ is such that $\tan\theta$ is irrational. In the "cell" method of constructing one-dimensional quasi-crystals [4], a line A, see fig. 1, is drawn parallel to the X' axis and displaced a distance d along the Y' axis. The line is assumed not to intersect any lattice point. The lower left-hand corner of each square cut by this line is projected onto line A. The array of projected points constitutes a one-dimensional quasi-crystal with two

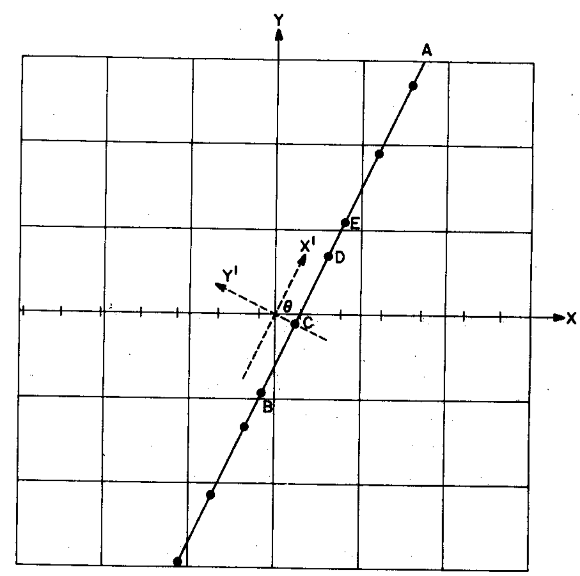

Fig. 1. Circles on line A represent atoms of a one-dimensional quasi-crystal. Hash marks on the X-axis represent the projections of the intersections of line A with the horizontal lattice lines.

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basic lengths, of lengths cos θ and sin θ.

De Bruijn [7] has defined the following sequences of ones and zeros:

$$P_\gamma(z) = \lceil \gamma + (z+1)/\alpha \rceil - \lceil \gamma + z/\alpha \rceil, \quad (1)$$

$$Q_\gamma(z) = \lfloor \gamma + (z+1)/\alpha \rfloor - \lfloor \gamma + z/\alpha \rfloor, \quad (2)$$

where γ and $\alpha > 1$ are real numbers. $\lfloor x \rfloor$, called the floor of x, is the largest integer less than or equal to x, i.e. the integer part of x. $\lceil x \rceil$, called the roof of x is the smallest integer greater than or equal to x. The sequence P_γ takes its ones on the set

$$\{\lfloor \alpha(n-\gamma) \rfloor \mid n \in \mathbb{Z}\}, \quad (3a)$$

and its zeros on the set

$$\{\lceil (n+\gamma)\alpha/(\alpha-1) \rceil - 1 \mid n \in \mathbb{Z}\}. \quad (3b)$$

The sequence Q_γ takes its ones on the set

$$\{\lceil \alpha(n-\gamma) \rceil - 1 \mid n \in \mathbb{Z}\}, \quad (4a)$$

and its zeros on the set

$$\{\lfloor (n+\gamma)\alpha/(\alpha-1) \rfloor \mid n \in \mathbb{Z}\}. \quad (4b)$$

One-dimensional quasi-crystals are related to these sequences via the following two theorems:

Theorem 1. A mapping exists between the sequences of ones and zeros of $P_\gamma(z)$ with

$$\gamma = -d/\sin\theta \quad (5a)$$

and

$$\alpha = \tan\theta, \quad (5b)$$

and the one-dimensional quasi-crystal constructed with a line A, see fig. 1, rotated by an angle θ and displaced a distance d: To each zero of $P_\gamma(z)$ there corresponds a segment of length sin θ, and to each one there correspond two segments, one of length sin θ followed by one of length cos θ.

Proof. Let $x_\gamma(z)$ denote the projection of the intersection of line A with a lattice line at $Y = z$ onto the X axis. $x_\gamma(z) = \gamma + z/\alpha$ where γ and α are defined in eqs. (5a) and (5b). To a pair of consecutive points $x_\gamma(z)$ and $x_\gamma(z+1)$ which fall between the same vertical lattice lines there corresponds a segment of length sin θ. To a pair which fall on opposite sides of a vertical lattice line there correspond two consecutive segments of length sin θ and cos θ. For example, see fig. 1, to the pair of points $x_\gamma(0) = \gamma$ and $x_\gamma(1) = \gamma + 1/\alpha$ corresponds the segment BC, to the pair of points $x_\gamma(1) = \gamma + 1/\alpha$ and $x_\gamma(2) = \gamma + 2/\alpha$, the segments CD and DE. Finally, from eq. (1), the value of $P_\gamma(z)$ is zero if $x_\gamma(z)$ and $x_\gamma(z+1)$ fall between the same vertical lattice lines, and is one if on opposite sides of a vertical lattice line.

A second relationship gives a one-to-one correspondence between a sequence of ones and zeros and the sequence of segments of lengths sin θ and cos θ of the one-dimensional quasi-crystal:

Theorem 2. The sequence of ones and zeros $Q_{\gamma^*}(z)$, where

$$Q_{\gamma^*}(z) = \lfloor \gamma^* + (z+1)/\alpha^* \rfloor - \lfloor \gamma^* + z/\alpha^* \rfloor \quad (6)$$

and

$$\alpha^* = 1 + \alpha^{-1}, \quad (7a)$$

$$-\alpha^*\gamma^* = \gamma + \lceil \gamma \rceil + 1, \quad (7b)$$

with γ and α defined in eqs. (5a) and (5b), is in a one-to-one correspondence with the sequence of segments of a one-dimensional quasi-crystal: Each one corresponds to a segment of length sin θ, and each zero to a segment of length cos θ.

Proof. We transform the sequence $P_\gamma(z)$ of theorem 1 by replacing each zero by one and each one by ten, i.e. $0 \to 1$ and $1 \to 10$. In this new sequence, each one corresponds to a segment of the one-dimensional quasi-crystal of length sin θ and each zero to a segment of length cos θ. In the new sequence we indicate the places of the ones: To $P_\gamma(n)$ there corresponds a group 1 or 10 starting at index M. M is twice the number of ones among $P_\gamma(0)$, $P_\gamma(1), \ldots, P_\gamma(n-1)$, plus the number of zeros among $P_\gamma(0)$, $P_\gamma(1), \ldots, P_\gamma(n-1)$. Using eq. (1), we have $M = \lceil \gamma + n/\alpha \rceil - \lceil \gamma \rceil + n$. Consequently, the new sequence has ones at

$$\{\lceil \gamma + n/\alpha \rceil - \lceil \gamma \rceil + n \mid n \in \mathbb{Z}\},$$

which can be written as

$$\{\lceil\alpha^*(n-\gamma^*)\rceil - 1 \mid n \in \mathbf{Z}\}, \tag{8}$$

with α^* and γ^* defined by eqs. (7a) and (7b). On comparing eq. (8) with eq. (4a) we have that the new sequence is given by (2) with γ and α replaced by γ^* and α^*.

An algebraic expression for the coordinates of the one-dimensional quasi-crystal atoms follows from theorem 2:

Theorem 3. The positions x' of the atoms of a one-dimensional quasi-crystal are given by

$$x'(z) = z\cos\theta + (\lfloor\gamma^* + z/\alpha^*\rfloor - \lfloor\gamma^*\rfloor) \times (\sin\theta - \cos\theta) \tag{9}$$

for all $z \in \mathbf{Z}$.

Proof. We choose the origin at the atom, indexed by $z = 0$, on the left of the segment corresponding to $Q_{\gamma^*}(0)$. The position $x'(z)$ of the zth atom is at the right of the segment corresponding to $Q_{\gamma^*}(z-1)$. $x'(z)$ is equal to $\sin\theta$ times the number of ones among $Q_{\gamma^*}(0), Q_{\gamma^*}(1), \dots, Q_{\gamma^*}(z-1)$, plus $\cos\theta$ times the number of zeros among $Q_{\gamma^*}(0), Q_{\gamma^*}(1), \dots, Q_{\gamma^*}(z-1)$. Using eq. (6), theorem 3 follows.

From theorem 3 we have that the nearest neighbor distances of the zth quasi-crystal atom are given by

$$\cos\theta + Q_{\gamma^*}(N)(\sin\theta - \cos\theta)$$

for $N = z$ and $z + 1$.

Sequences $P_\gamma(z)$ (and $Q_\gamma(z)$) can be classified into equivalence classes: We define two sequences $P_\gamma(z)$ and $P_{\gamma'}(z)$ to belong to the same class, and said to be equivalent, if for all z and integer N:

$$P_{\gamma'}(z) = P_\gamma(z+N). \tag{10}$$

Two equivalent sequences are then identical but shifted sequences of ones and zeros. The following theorem holds for both sequences $P_\gamma(z)$ and $Q_\gamma(z)$:

Theorem 4. Sequences $P_{\gamma+M+N/\alpha}(z)$ and $P_\gamma(z)$, where M and N are integers, are equivalent.

The proof follows by substituting $\gamma + M + N/\alpha$ for γ into eq. (1)

$$\begin{aligned} P_{\gamma+M+N/\alpha}(z) &= \lceil\gamma + M + N/\alpha + (z+1)/\alpha\rceil \\ &\quad - \lceil\gamma + M + N/\alpha + z/\alpha\rceil \\ &= \lceil\gamma + (z+N+1)/\alpha\rceil \\ &\quad - \lceil\gamma + (z+N)/\alpha\rceil \\ &= P_\gamma(z+N), \end{aligned}$$

and using the definition of equivalent sequences, eq. (10).

Two one-dimensional quasi-crystals are said to be equivalent if the corresponding sequences $P_\gamma(z)$ (and $Q_{\gamma^*}(z)$) are equivalent. Two equivalent one-dimensional quasi-crystals are identical but shifted sequences of lengths $\sin\theta$ and $\cos\theta$. In terms of the parameters θ and d of the projection method of constructing one-dimensional quasi-crystals we have:

Theorem 5. One-dimensional quasi-crystals constructed with angle θ and displacements $d + M\cos\theta + N\sin\theta$, where M and N are arbitrary integers, are equivalent one-dimensional quasi-crystals.

Proof. Let $P_\gamma(z)$ denote the sequence which by theorem 1 corresponds to the one-dimensional quasi-crystal constructed with the angle θ and displacement d. From eqs. (5a) and (5b) it follows that corresponding to the one-dimensional quasi-crystals constructed with angle θ and displacements $d + M\cos\theta + N\sin\theta$ are the sequences $P_{\gamma+M+N/\alpha}(z)$. Since by theorem 4 these sequences are equivalent, it follows that the corresponding one-dimensional quasi-crystals are also equivalent.

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