DETERMINING QUASICRYSTAL STRUCTURES ON SUBSTITUTION TILINGS

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Abstract. Quasicrystals are characterized by the diffraction patterns which consist of pure bright peaks. Substitution tilings are commonly used to obtain geometrical models for quasicrystals. We consider certain substitution tilings and show how to determine a quasicrystalline structure for the substitution tilings computationally. In order to do this, it is important to have the Meyer property on the substitution tilings. We use the recent result of Lee-Solomyak in [18] which determines the Meyer property on the substitution tilings from the expansion maps.

Keywords: Quasicrystals, Pure point diffraction, Self-affine tilings, Overlap coincidence, Meyer sets, Algorithm.

1. Introduction

For the study of geometric structures of quasicrystals, substitutions are commonly used to create mathematical models. Many known examples such as the Penrose tiling and the Robinson tiling can be created by this method. Mathematically quasicrystals are characterized as the structures of models whose diffraction patterns consist purely of Bragg peaks without diffuse background. The diffraction is described by the diffraction measure of the point sets representing the models and the diffraction measure is a Fourier transformation of an autocorrelation of a Dirac measure defined on the point sets.

Let \( \Lambda = (\Lambda_i)_{i \leq m} \) be a multi-colour point set in \( \mathbb{R}^d \). We consider a measure of the form \( \nu = \sum_{i \leq m} a_i \delta_{\Lambda_i} \), where \( \delta_{\Lambda_i} = \sum_{x \in \Lambda_i} \delta_x \) and \( a_i \in \mathbb{C} \). The autocorrelation of \( \nu \) is

\[
\gamma(\nu) = \lim_{n \to \infty} \frac{1}{\text{Vol}(B_n)} [\nu|_{B_n} * \bar{\nu}|_{B_n}],
\]

where \( \nu|_{B_n} \) is a measure of \( \nu \) restricted on the ball \( B_n \) of radius \( n \) and \( \bar{\nu} \) is the measure, defined by \( \bar{\nu}(f) = \nu(f) \), where \( f \) is a continuous function with compact support and \( \bar{f}(x) = f(-x) \). The diffraction measure of \( \nu \) is the Fourier transform \( \hat{\gamma}(\nu) \) of the autocorrelation (see [10]). When the diffraction measure \( \hat{\gamma}(\nu) \) is a pure point measure, we say that \( \Lambda \) has pure point diffraction spectrum and so the structures of quasicrystals.

There are many criteria in literature which characterize the structures of quasicrystals. One of the criteria is that the pure point diffractivity of \( \Lambda \) is equivalent to pure point dynamical spectral property of \( \Lambda \) [8, 20, 15, 11, 3, 19]. Another criterion is that regular model sets are pure point

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diffractive [10, 21, 4, 13]. A third criterion is ‘almost periodicity’, which says that if a uniformly
discrete set Λ admits an autocorrelation, then Λ is pure point diffractive if and only if for all ϵ > 0,
the set
\[ \{ t \in \mathbb{R}^d : \text{density}(\Lambda \setminus (\Lambda - t + B_\epsilon)) \leq \epsilon \} \]
is relatively dense (see [22, 4, 11]). When we restrict to the setting of substitution tilings or point
sets, the equivalent criterion to the almost periodicity can be described by the notion of overlap
coincidence [22, 13]. This overlap coincidence plays an important role on getting the computational
algorithm to determine the pure point diffractivity on the substitution tilings. The detail justification
about the algorithm and the main theorem can be found in [1]. We provide a few examples in the
last section some of which are not mentioned there.

2. Preliminary

2.1. Tilings. We begin with a set of types (or colours) \{1, \ldots, m\}, which we fix once and for all. A
tile in \(\mathbb{R}^d\) is defined as a pair \(T = (A, i)\) where \(A = \text{supp}(T)\) (the support of \(T\)) is a compact set in \(\mathbb{R}^d\),
which is the closure of its interior, and \(i = l(T) \in \{1, \ldots, m\}\) is the type of \(T\). We say that a set \(P\) of
tiles is a patch if the number of tiles in \(P\) is finite and the tiles of \(P\) have mutually disjoint interiors. We
say that two patches \(P_1\) and \(P_2\) are translationally equivalent if \(P_2 = g + P_1\) for some \(g \in \mathbb{R}^d\). A tiling of
\(\mathbb{R}^d\) is a set \(T\) of tiles such that \(\mathbb{R}^d = \bigcup\{\text{supp}(T) : T \in T\}\) and distinct tiles have disjoint interiors. We
always assume that any two \(T\)-tiles with the same colour are translationally equivalent (hence there
are finitely many \(T\)-tiles up to translations). Let \(\Xi(T) := \{x \in \mathbb{R}^d : T = x + T' \text{ for some } T, T' \in T\}\). We
say that \(T\) has finite local complexity (FLC) if for each radius \(R > 0\) there are only finitely many
equivalent classes of patches whose support lies in some ball of radius \(R\). We say that \(T\) is repetitive
if for every compact set \(K \subset \mathbb{R}^d\), \(\{t \in \mathbb{R}^d : T \cap K = (t + T) \cap K\}\) is relatively dense.

2.2. Substitutions.

2.2.1. Example of a substitution tiling. The Fibonacci substitution tiling is defined by the following
substitution rule

\[
\begin{array}{ccc}
0 & \tau & \rightarrow \\
A_1 & A_2 & \text{and} \\
0 & 1 & \rightarrow \\
A_2 & A_1 & \text{respectively}.
\end{array}
\]

where \(\tau^2 - \tau - 1 = 0\). The tiles \(A_1\) and \(A_2\) satisfy the following tile-equations
\[
\tau A_1 = A_1 \cup (A_2 + \tau) \quad \text{and} \quad \tau A_2 = A_1
\]
Continuously iterating the tiles and subdividing them, we can construct a tiling.

2.2.2. Substitutions on tilings. We say that a linear map \(Q : \mathbb{R}^d \to \mathbb{R}^d\) is expansive if all its eigenvalues
lie outside the closed unit disk in \(\mathbb{C}\).

Definition 2.1. Let \(A = \{T_1, \ldots, T_m\}\) be a finite set of tiles in \(\mathbb{R}^d\) such that \(T_i = (A_i, i)\); we will
call them prototiles. Denote by \(\mathcal{P}_A\) the set of non empty patches. We say that \(\Omega : A \to \mathcal{P}_A\) is a
tile-substitution (or simply substitution) with an expansive map $Q$ if there exist finite sets $D_{ij} \subset \mathbb{R}^d$ for $i,j \leq m$ such that

\begin{equation}
\Omega(T_j) = \{ u + T_i : u \in D_{ij}, \ i = 1, \ldots, m \}
\end{equation}

with

\begin{equation}
Q A_j = \bigcup_{i=1}^{m} (D_{ij} + A_i) \quad \text{for } j \leq m.
\end{equation}

Here all sets in the right-hand side must have disjoint interiors; it is possible for some of the $D_{ij}$ to be empty.

We say that $\mathcal{T}$ is a substitution tiling if $\mathcal{T}$ is a tiling and $\Omega(\mathcal{T}) = \mathcal{T}$ with some substitution $\Omega$. We say that substitution tiling is primitive if the corresponding substitution matrix $S$, with $S_{ij} = \sharp(D_{ij})$, is primitive, i.e. $S^\ell$ is a positive matrix for some $\ell \in \mathbb{Z}_+$. A repetitive primitive substitution tiling with FLC is called a self-affine tiling. Let $\Lambda_{\mathcal{T}} = (\Lambda_i)_{i \leq m}$ be the multi-colour point set representing $\mathcal{T}$. For any self-affine tiling which satisfies (2.2), we define an $m \times m$ array $\Phi$ for which each entry is $\Phi_{ij}$,

$$\Phi_{ij} = \{ f : x \mapsto Qx + d : d \in D_{ij} \}$$

and call $\Phi$ a matrix function system (MFS) for the substitution $\Omega$. We compose

$$\Phi \circ \Phi = ((\Phi \circ \Phi)_{ij}),$$

where

$$\Phi \circ \Phi = \bigcup_{k=1}^{m} \Phi_{ik} \circ \Phi_{kj} \quad \text{and} \quad \Phi_{ik} \circ \Phi_{kj} \ := \left\{ \begin{array}{ll} g \circ f : & g \in \Phi_{ik}, f \in \Phi_{kj} \\ \emptyset & \text{if } \Phi_{ik} = \emptyset \text{ or } \Phi_{kj} = \emptyset. \end{array} \right.$$ We write $\Phi^2$ for $\Phi \circ \Phi$ and similarly $\Phi^n$ for $n$-fold composition of $\Phi$ for $n \in \mathbb{Z}_+$. We write $\Phi^n(x)$ for $(\Phi^n_{ij}(x))_{i \leq m}$ where $x \in \Lambda_j$ and $n \in \mathbb{Z}_+$.

### 2.3. Overlaps.

Overlap and overlap coincidence are originally defined with tiles in substitution tilings [22]. For computational reason, we define overlaps with the corresponding representative points of tiles here. A triple $(u,y,v)$, with $u + T_i, v + T_j \in \mathcal{T}$ and $y \in \Xi(\mathcal{T})$, is called an overlap (or real overlap) if

\begin{equation}
(u + A_i - y)^c \cap (v + A_j)^c \neq \emptyset,
\end{equation}

where $A_i = \text{supp}(T_i)$ and $A_j = \text{supp}(T_j)$. We define $(u + A_i - y) \cap (v + A_j)$ the support of an overlap $(u,y,v)$ and denote it by $\text{supp}(u,y,v)$. We say that two overlaps $(u,y,v)$ and $(u',y',v')$ are equivalent if there exists $g \in \mathbb{R}^d$ such that $u - y = g + u' - y'$ and $v = g + v'$, where $u + T_i, u' + T_i \in \mathcal{T}$ and $v + T_j, v' + T_j \in \mathcal{T}$ for some $1 \leq i,j \leq m$. Denote by $[(u,y,v)]$ the equivalence class of an overlap. An overlap $(u,y,v)$ is a coincidence if

$$u - y = v \quad \text{and} \quad u + T_i, v + T_i \in \mathcal{T} \quad \text{for some } i \leq m.$$

For an overlap $\mathcal{O} = (u,y,v)$ in $\mathcal{T}$, we define $k$-th inflated overlap

$$\Phi^k \mathcal{O} = \{ (u',Q^k y,v') : u' \in \Phi^k(u), v' \in \Phi^k(v), \text{ and } (u',Q^k y,v') \text{ is an overlap} \}.$$

**Definition 2.2.** We say that a self-affine tiling $\mathcal{T}$ admits an overlap coincidence if there exists $\ell \in \mathbb{Z}_+$ such that for each overlap $\mathcal{O}$ in $\mathcal{T}$, $\Phi^\ell \mathcal{O}$ contains a coincidence.
We say that a discrete point set \( \Xi \) is a Meyer set if \( \Xi \) is relatively dense and \( \Xi - \Xi \) is uniformly discrete. For \( \alpha \in \Xi(T) \), define
\[
E_{\alpha} := \{(u, Q^n \alpha, v) : (u, Q^n \alpha, v) \text{ is overlap in } T \text{ and } n \in \mathbb{N} \}.
\]

**Theorem 2.3.** [16, 13] Let \( T \) be a self-affine tiling in \( \mathbb{R}^d \) such that \( \Xi(T) \) is a Meyer set. Then the following are equivalent:

(i) \( \Lambda_T \) is pure point diffractive.
(ii) \( T \) admits an overlap coincidence.
(iii) There exists \( \ell \in \mathbb{Z}^+ \) such that for any overlap \( O \) in \( E_{\alpha} \), \( \Phi^\ell O \) contains a coincidence.

In actual computation, it is not easy to determine whether a given triple is an overlap, since the interior intersection is hard to determine. So we introduce a notion of potential overlaps. From (2.3), for any overlap \((u, y, v)\) in \( T \) it is easy to observe that
\[
|u - y - v| \leq R := 2 \cdot \max\{\text{diam}(A_i) : i \leq m\},
\]
where \( \text{diam}(A) \) is the diameter of \( A \).

We say that a triple \((u, y, v)\), with \( u + T_i, v + T_j \in T \) for some \( i, j \leq m \) and \( y \in \Xi(T) \), is called a potential overlap if \( |u - y - v| \leq R \). Similarly to the \( k \)-th iterated overlap, for each potential overlap \( O = (u, y, v) \) in \( T \), we define \( k \)-th inflated potential overlap
\[
\Phi^k O = \{(u', Q^k y, v') : u' \in \Phi^k(u), v' \in \Phi^k(v), \text{ and } (u', Q^k y, v') \text{ is a potential overlap}\}
\]
and the equivalence class of \( \Phi^k O \)
\[
[\Phi^k O] = \{[O'] : O' \in \Phi^k O\}.
\]

It is proved in [22, 16] that the number of equivalence classes of overlaps for a tiling which has the Meyer property is finite. And it is shown in [17] that substitution tiling with pure point diffraction spectrum necessarily have the Meyer property. So to obtain overlap coincidence, we assume the Meyer property of \( \Xi(T) \). The next theorem gives a criterion on \( Q \) for the Meyer property.

A set of algebraic integers \( \Theta = \{\theta_1, \cdots, \theta_r\} \) is a Pisot family if for any \( 1 \leq j \leq r \), every Galois conjugate \( \gamma \) of \( \theta_j \) with \( |\gamma| \geq 1 \) is contained in \( \Theta \).

**Theorem 2.4.** [18] Let \( T \) be a self-affine tiling in \( \mathbb{R}^d \) with a diagonalizable expansion map \( Q \). Suppose that all the eigenvalues of \( Q \) are algebraic conjugates with the same multiplicity. Then \( \Xi(T) \) is a Meyer set if and only if the set of all the eigenvalues of \( Q \) is a Pisot family.

Under Pisot family condition on \( Q \), it is easy to show the Meyer property in practice. The main new result of the above theorem is showing the partial converse.

Let \( \xi \in \mathbb{R}^d \) be a fixed point under the substitution such that \( \xi \in \Phi(\xi) \). When there is no confusion, we will identify \( \xi \) with a coloured point \((\xi, i)\) in \( \Lambda_T \) with \( \xi \in \mathbb{R}^d \). We find a basis of \( \mathbb{R}^d \)
\[
B = \{\alpha_1, \ldots, \alpha_d\} \subset \Xi(T).
\]

For any \( \alpha \in B \) and any \( M \in \mathbb{Z}_{\geq 0} \), define
\[
G_{\alpha, M} := \bigcup_{0 \leq n \leq M} \{[(y, Q^n \alpha, z)] : y, z \in \Phi^{N+k+n}(\xi) \text{ and } (y, Q^n \alpha, z) \text{ is a potential overlap}\},
\]

\[1^1\text{It is possible to take a smaller } R. \text{ See [1] for details.}\]
\[ \mathcal{G}_\alpha := \bigcup_{M \in \mathbb{Z}_{\geq 0}} \mathcal{G}_{\alpha,M} \text{ and } \mathcal{G} = \bigcup_{\alpha \in \mathcal{B}} \mathcal{G}_\alpha \]

From the Meyer property of \( \Xi(T) \), there exists \( M \in \mathbb{Z}_{\geq 0} \) such that \( \mathcal{G}_{\alpha,M} = \mathcal{G}_{\alpha,M+1} \) (refer [1] to find \( M \)).

**Lemma 2.5.** Let \( \alpha \in \mathcal{B} \). If \( \mathcal{G}_{\alpha,M} = \mathcal{G}_{\alpha,M+1} \) for some \( M = (M_\alpha) \in \mathbb{Z}_{\geq 0} \), then
\[ \mathcal{G}_{\alpha,M} = \mathcal{G}_\alpha. \]

Let \( \mathcal{G}_{\text{coin}} \) be the set of all equivalence classes of overlaps in \( T \) which lead to coincidence after \( \sharp \mathcal{G} \)-iterations and \( \mathcal{G}_{\text{res}} := \mathcal{G} \setminus \mathcal{G}_{\text{coin}} \). Draw a graph whose vertices are elements in \( \mathcal{G} \) and edges from a potential overlap \( O \) to \( O' \) are \( k \)-multiple if the inflated potential overlap \( \Phi O \) contains \( k \)-copies of \( O' \) for some \( k \in \mathbb{Z}_+ \). For simplicity, we use the same name \( \mathcal{G} \) for the graph. Similarly \( \mathcal{G}_{\text{coin}} \) and \( \mathcal{G}_{\text{res}} \) stand for the induced graphs of \( \mathcal{G} \) for the corresponding set. For any graph \( \mathcal{G} \), we denote by \( \rho(\mathcal{G}) \) the spectral radius of the graph \( \mathcal{G} \).

**Theorem 2.6.** Let \( T \) be a self-affine tiling in \( \mathbb{R}^d \) such that \( \Xi(T) \) is a Meyer set. Then \( T \) admits an overlap coincidence if and only if \( \rho(\mathcal{G}_{\text{coin}}) > \rho(\mathcal{G}_{\text{res}}) \).

To show the ‘only if’ part, it is inevitable to estimate the contribution of potential overlaps whose tiles meet only at the boundaries. So a result on the Hausdorff dimension of the tile boundaries is shown on the way of proving the above theorem (see [1]).

Summarizing the results, we provide an algorithm to determine the pure point diffraction of a point set which represents a substitution tiling.

**Algorithm:** We assume that \( T \) is a self-affine tiling in \( \mathbb{R}^d \) with expansion map \( Q \) for which \( \Xi(T) \) is a Meyer set and \( T_i = (A_i, i), i \leq m \), are prototiles such that
\[ QA_j = \bigcup_{i \leq m} (D_{ij} + A_i) \text{ for } j \leq m. \]

- **Input:** \( \Phi \) is an \( m \times m \) matrix whose each entry is a set of functions from \( \mathbb{R}^d \) to \( \mathbb{R}^d \) such that \( \Phi = (\Phi_{ij}), \) where \( \Phi_{ij} = \{ f : x \rightarrow Qx + d, d \in D_{ij} \} \), i.e. \( \Phi \) is a MFS for \( T \).
- **Output:** True, if and only if \( \mathcal{A}_T \) is pure point diffraction.

(i) Find an initial point \( x \) such that \( x \in \Phi(x) \).
(ii) Find a basis \( \{ \alpha_1, \ldots, \alpha_d \} \subset \mathbb{R}^d \) such that \( \alpha_k \in \bigcup_{i \leq m}((\Phi^n(x))_i - (\Phi^n(x))_i) \) for some \( n \in \mathbb{Z}_+ \), for each \( 1 \leq k \leq d \).
(iii) For each \( 1 \leq k \leq d \), find all the potential overlaps \( \mathcal{G}_{\alpha_0,0} \) which occur from the translation \( \alpha_k \).
(iv) Find all the potential overlaps \( \mathcal{G} \) which occur from the translations \( Q^n \alpha_k \) with \( 1 \leq k \leq d \) and \( n \in \mathbb{Z}_+ \).
(v) Find all the potential overlaps \( \mathcal{G}_{\text{coin}} \) which lead to coincidences within \( \sharp \mathcal{G} \)-iterations.
(vi) If \( \rho(\mathcal{G}_{\text{coin}}) > \rho(\mathcal{G}_{\text{res}}) \) return true. Else, return false.
3. Computation with an algorithm

For one-dimension substitutions, it is not difficult to determine overlaps. For this case, we use overlaps directly to check overlap coincidence as it is shown in Example 3.1. In higher dimension, it is difficult to determine all the overlaps. So adopting the notion of potential overlaps, we determine the overlap coincidence. We implemented Mathematica programs which perform our algorithm to check the overlap coincidence for self-affine tilings. Readers can get the Mathematica programs in the website given in [2]. Below, we present two examples where the algorithm was applied, the fractal Penrose tiling in Example 3.2 and a fractal chair tiling in Example 3.3.

Example 3.1. There is a Pisot type substitution defined by \( a \rightarrow ab, b \rightarrow c, c \rightarrow a \) (see [6, 9]). The corresponding substitution matrix is \( M = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \). The PF-eigenvalue of \( M \) is \( \lambda \) for which \( \lambda^3 - \lambda^2 - 1 = 0 \) and a left eigenvector of \( M \) corresponding to \( \lambda \) is \( (\lambda^2, 1, \lambda) \). Let \( T_1(T_2, \text{ or } T_3) \) be the intervals of length \( \lambda^2(1, \text{ or } \lambda) \) starting from \( 0 \), respectively. We can construct a substitution tiling \( \mathcal{T} \) attaching these intervals to a bi-infinite fixed sequence as tiles. For any fixed repetitive substitution tiling \( \mathcal{T} \), it is enough to check overlap coincidence in one side of the tiling.

\[
\begin{array}{cccccccccccc}
a & b & c & a & a & b & a & b & c & a & a & \cdots \\
0 & \lambda & \lambda^2 + 1 & 2\lambda^2 + \lambda + 1 & 3\lambda^2 + \lambda + 1 & 3\lambda^2 + \lambda + 2 & 4\lambda^2 + \lambda + 2 & 4\lambda^2 + 2\lambda + 3 & \cdots \\
\end{array}
\]

All overlaps are \([\lambda^2 - \lambda + T_1, 0 + T_1], [\lambda + T_1, 0 + T_1], [1 + T_1, 0 + T_1], [0 + T_2, 0 + T_1], [\lambda^2 - \lambda - 1 + T_2, 0 + T_1], [\lambda^2 - \lambda + T_2, 0 + T_1], [\lambda^2 - 1 + T_2, 0 + T_1], [1 + T_3, 0 + T_1], [\lambda^2 - \lambda + T_3, 0 + T_1], [0 + T_3, 0 + T_1], [-\lambda + 1 + T_3, 0 + T_1], [\lambda^2 - \lambda + 1 + T_3, 0 + T_1], [-\lambda^2 + 1 + T_3, 0 + T_2], [-\lambda + 1 + T_3, 0 + T_2], [-\lambda + 1 + T_3, 0 + T_2]. Every overlap admits coincidence when \( \Phi^{10} \) is applied to the pair of representative points of overlap tiles. For example, for an overlap \([\lambda^2 - \lambda + T_1, 0 + T_1] \), we look at

\[
\Phi^{10}\left(\begin{array}{c} \{\lambda^2 - \lambda\} \\ \emptyset \end{array}\right) \quad \text{and} \quad \Phi^{10}\left(\begin{array}{c} \{0\} \\ \emptyset \end{array}\right)
\]

Observe that \( \lambda^0 \in (\Phi^{10})_{11}(\lambda^2 - \lambda) \cap (\Phi^{10})_{11}(0) \). Thus \( \mathbf{A}_\mathcal{T} \) is pure point diffraction.

Example 3.2. Bandt-Gummelt in [7] gave two fractal Penrose tilings by fractal kites and darts having exact matching condition (see Figure 1 (a)). We confirm that these tilings admit overlap coincidence. Thus the tilings have pure point diffraction spectrum. The expanding matrix \( Q = \begin{pmatrix} t & 0 \\ 0 & t \end{pmatrix} \) where \( t^2 - t - 1 = 0 \) and the MFS \( \Phi \) is \( 20 \times 20 \) matrix such that \( \Phi = (F_{ij}) \) and \( F_{ij} = \{ f : f = Qx + d, d \in D_{ij} \} \). We give the digit set matrix \( (D_{ij}) \) in Figure 2, where \( w = \cos(\pi/5) + i\sin(\pi/5) \), \( t = \frac{1 + \sqrt{5}}{2} \), and \( c \in \mathbb{C} \) satisfies \( f(t^2i) = i \) with \( f(z) = \frac{2i}{t}w^4 + c \).
Example 3.3. Bandt found an aperiodic tiling by modifying the construction of crystallographic tiling [5]. He called it a fractal chair tiling. Note, to avoid confusion, that this tiling is not the fractal version of ordinary chair tiling in [12, 22, 14], not like Example 3.2. A single tile in the fractal chair tiling is a 3-reptile, i.e., it is subdivided into shrunk 3 similar copies, while the ordinary chair tile is a 4-reptile. The tile equations are given by

$$\lambda A_n = A_n \cup (A_n + \alpha^{n-1}) \cup (A_{n+1} + \alpha^n)$$

where $\lambda = -2\alpha^2 + \alpha$ and $\alpha^2 - \alpha + 1 = 0$ and $n$ of $A_n$ is a cyclic index modulo 6. The computation shows that the tiling does not admit overlap coincidence. So the point structure representing the tiling is not pure point diffractive, which means that there is continuous part in the diffraction pattern. Nonetheless the diffraction has a relatively dense set of Bragg peaks, since the tiling has the Meyer property (see [23, 17]). It would be interesting to know the reason why this tiling gives a structure which is not pure point diffractive and understand the continuous part of the diffraction spectrum more concretely. The figure is given in Figure 1(b).
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