Inflation versus projection sets:  
The role of the window in averaging and diffraction

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Abstract
Tilings based on the cut and project method are key model systems for the description of aperiodic solids. Typically, quantities of interest in crystallography involve averaging over large patches, and are well defined only in the infinite-volume limit. In particular, this is the case for autocorrelation and diffraction measures. For cut and project systems, the averaging can conveniently be transferred to internal space, which means dealing with the corresponding windows. We illustrate this by the example of averaged shelling numbers for the Fibonacci tiling and review the standard approach to the diffraction for this example. Further, we discuss recent developments for inflation-symmetric cut and project structures, which are based on an internal counterpart of the renormalisation cocycle. Finally, we briefly review the notion of hyperuniformity, which has recently gained popularity, and its application to aperiodic structures.

Keywords: Quasicrystals; projection method; inflation rules; averaging; autocorrelation; diffraction; hyperuniformity

1. Introduction

The discovery of quasicrystals in the early 1980s not only led to a reconsideration of the fundamental concept of a crystal (see [32] and references therein), but also highlighted the need for a mathematically robust treatment of the diffraction of systems that exhibit aperiodic order. The foundations for a rigorous approach were laid by Hof [33]. In particular, the measure-theoretic approach via the autocorrelation and diffraction measures allows for a mathematically rigorous discussion and separation of the different spectral components, the pure point, singular continuous and absolutely continuous part; see [15] for background and examples, and [16] Sec. 9 for a systematic exposition. For general background on the theory of aperiodic order, we refer to [42, 3, 15] and references therein.

Within a few years, it was established that regular model sets [38] (systems obtained by projection from higher-dimensional lattices via cut and project mechanisms with ‘nice’ windows) have pure point diffraction [46, 44]. We refer to [16] for details and examples, and to [6] for an instructive application of the cut and project approach to an experimentally observed structure with twelvefold symmetry. The result on the pure point nature of diffraction holds for rather general setups, including cut and project schemes with non-Euclidean internal spaces. It has recently been generalised to weak model sets of extremal densities [21, 15], for which the window may even entirely consist of boundary, that is, has no interior; see also [49, 50] for recent work on pure point spectra.

While systems based on a cut and project scheme are generally well understood, this is less so for systems originating from substitution or inflation rules, which constitute another popular method of generating systems with aperiodic order; see [10, 30] and references therein for details. There has been recent progress particularly on substitutions of constant length; see [36, 23, 24, 5, 11, 26].

There are familiar examples of inflation-based structures for all spectral types, such as the Fibonacci chain for a pure-point diffractive system, the Thue–Morse chain for a system with purely singular continuous diffraction, and the binary Rudin–Shapiro chain as the paradigm of a system with absolutely continuous diffraction; see [42, 8, 4] for details. When one equips the Rudin–Shapiro chain with balanced weights (±1), it becomes homometric with the binary Bernoulli chain with random weights ±1 [14]. It is easy to construct inflation-based systems which combine any of these spectral components in their diffraction; see [10] for examples. As of today, the celebrated Pisot substitution conjecture (which stipulates that an irreducible Pisot substitution has pure point spectrum) remains open; see [2] for a review of the state of affairs.

While diffraction was the first property to be analysed in detail, many other questions from traditional crystallography and lattice theory require an extension to their aperiodic counterparts [22]. In particular, classic counting problems based on lattices, when
reformulated for point sets in aperiodic tilings, need both a conceptual reformulation and new tools to tackle them. The key observation is the necessity to employ averaging concepts, and then tools from dynamical systems and ergodic theory [13] [18] [13]. If one is in the favourable situation of point sets that emerge from either the projection formalism or an inflation procedure, many of these averaged quantities are well defined and can actually be calculated; see [13] and references therein. Despite some progress, many questions in this context remain open.

Let us sketch how this introductory review is organised. Our guiding example in this exposition is the classic, self-similar Fibonacci tiling of the real line. Its descriptions as an inflation set and as a cut and project set are reviewed in Section 2. As a simple example of the role of the window in averaging, we discuss the averaged shelling for this system in Section 3. This is followed by a brief review of the standard approach to diffraction in Section 4, where we exploit the description of the Fibonacci point set as a cut and project set and the general results for the diffraction of regular model sets.

In Section 5, we introduce the recently developed internal cocycle approach. For systems which possess both an inflation and a projection interpretation, such as the Fibonacci tiling, the inflation cocycle can be lifted to internal space. This makes it possible to efficiently compute the diffraction of certain cut and project systems with complicated windows, such as windows with fractal boundaries which are commonly found in inflation structures. We explore this with planar examples, which are based on the Fibonacci substitution, in Section 6.

Finally, in Section 7, we discuss the use of ‘hyperuniformity’ as a measure of order in Fibonacci systems. This amounts to an investigation of the asymptotic behaviour of the total diffraction intensity near the origin. It turns out that this can distinguish between generic and inflation-invariant choices for the window in the cut and project scheme.

2. The Fibonacci tiling revisited

Let us start with a paradigm of aperiodic order in one dimension, the classic Fibonacci tiling. It can be defined via the primitive two-letter inflation rule

\[ \varrho: \ a \mapsto ab, \ b \mapsto a, \]

where \(a\) and \(b\) represent tiles (or intervals) of length \(\tau = \frac{1}{2}(1 + \sqrt{5})\) and 1, respectively. The corresponding incidence matrix is given by

\[ M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \]

which has Perron–Frobenius eigenvalue \(\tau\). Its left and right eigenvectors read

\[ (1) \quad |v\rangle = \frac{\tau + 2}{\sqrt{5}} (\tau, 1) \quad \text{and} \quad |v\rangle = (\tau^{-1}, \tau^{-2})^T, \]

where we employ Dirac’s intuitive ‘bra-c-ket’ notation, which makes it easy to distinguish row and column vectors. We normalise the right eigenvector \(|v\rangle\) such that \(\langle 1 | v \rangle = 1\), which means that its entries are the relative frequencies of the tiles. For later convenience, we normalise the left eigenvector \(|u\rangle\) by setting \(\langle u | v \rangle = 1\), rather than using the vector of natural tile lengths itself. With this normalisation, we have

\[ (2) \quad \lim_{n \to \infty} \tau^{-n} M^n = \frac{\tau + 2}{\sqrt{5}} \begin{pmatrix} 1 & \tau^{-1} \\ \tau^{-1} & \tau^{-2} \end{pmatrix} = |v\rangle \langle u| =: P, \]

where \(P = P^2\) is a symmetric projector of rank 1 with spectrum \(\{1, 0\}\).

Starting from the legal seed \(b|a\), where the vertical bar denotes the origin, and iterating the square of the inflation rule \(\varrho\), generates a tiling of the real line that is invariant under \( \varrho^2\); see [16, Ex. 4.6] for details and why it does not matter which of the two fixed points of \( \varrho^2\) one chooses. Let us use the left endpoints of each interval as control points and denote the set of these points by \(A_a\) and \(A_b\), respectively. Clearly, since \(0 \in A_a\) and all tiles have either length \(\tau\) or length 1, all coordinates are integer linear combinations of these two tile lengths, and we have

\[ A_{a,b} \subset \mathbb{Z}[\tau] = \{ m + n \tau : m, n \in \mathbb{Z} \}. \]

While the incidence matrix \(M\) only contains information about the number of tiles under inflation, but not about their positions, the latter information can be encoded by introducing the displacement matrix

\[ (4) \quad T = \begin{pmatrix} \{0\} & \{\tau\} \\ \{\tau\} & \varnothing \end{pmatrix}, \]

where \(\varnothing\) denotes the empty set. Note that \(T\) is the geometric counterpart of the instruction matrices that are used in the symbolic context [13]. The matrix elements of \(T\) are sets that specify the relative displacement for all tiles under inflation. For instance, the two entries in the first column correspond to a long tile with relative shift 0 and a small tile with shift \(\tau\) originating from inflating a long tile. Clearly, the inflation matrix \(M\) is recovered if one takes the elementwise cardinality of \(T\), noting that the empty set has cardinality 0.

The inflation rule \(\varrho\) induces an iteration on pairs of point sets, namely

\[ (5) \quad A_{a,(n+1)} = \tau A_a^{(n)} \cup \tau A_b^{(n)}, \quad A_b^{(n+1)} = \tau A_a^{(n)} + \tau, \]
The windows \( W_a \) and \( W_b \) are the cross-sections of the yellow and green strips, respectively.

with suitable initial conditions \( \Lambda_{a,b}^{(0)} \). When one starts with the left endpoints of a legal seed, this iteration precisely reproduces the endpoints of the corresponding, successive inflation steps. In this case, the unique solution to the above choice of \( \Lambda_{a,b} \) is \( \Lambda_{a,b} = \{ 0 \} \) and \( \Lambda_{a,b}^{(0)} = \{ -1 \} \).

The point sets \( \Lambda_{a,b} \) also have an interpretation as a cut and project set. Here, we use the natural (Minkowski) embedding of the module \( \mathbb{Z}[\tau] \) in the plane \( \mathbb{R}^2 \), by associating to each \( x = m + n\tau \in \mathbb{Z}[\tau] \) its image \( x^* = m+n\tau^* = m+n(1-\tau) \) under algebraic conjugation (which maps \( \sqrt{5} \) to \( -\sqrt{5} \)). This gives
\[
\mathcal{L} = \left\{ (x,x^*) : x \in \mathbb{Z}[\tau] \right\}
\]
\[
= \left\{ (m+n\tau, m+n\tau^*) : m,n \in \mathbb{Z} \right\}
\]
\[
= \left\{ (m(1,1)+n(\tau,\tau^*)) : m,n \in \mathbb{Z} \right\},
\]
which is a planar lattice with basis vectors \((1,1)\) and \((\tau,\tau^*)\); see \([13,6]\) for details and further examples. Here, we refer to the two one-dimensional subspaces of \( \mathbb{R}^2 = \mathbb{R} \times \mathbb{R} \) as the \textit{physical} and the \textit{internal} space, respectively. The physical space hosts our point sets \( \Lambda_{a,b} \), while the windows are subsets of the internal space, with the \( \ast \)-map providing the relevant link between the two spaces.

The point sets \( \Lambda_{a,b} \) are given by the projection of two strips of the lattice \( \mathcal{L} \); compare Figure 1. The strips are defined by their cross-sections, usually called \textit{windows}, which are the half-open intervals \( W_a = [\tau - 2, \tau - 1) \) and \( W_b = [-1, \tau - 2) \). With \( L = \mathbb{Z}[\tau] \), the projection of \( \mathcal{L} \) into physical space, the point sets are thus given by
\[
\Lambda_{a,b} = \left\{ x \in \mathbb{R} : x^* \in W_{a,b} \right\}.
\]

The windows \( W_{a,b} \), or more precisely their closures, can be obtained as the unique solutions of a contractive iterated function system that arises from the \( \ast \)-image of \((5)\).

\[
W_a = \sigma W_a \cup \sigma W_b, \quad W_b = \sigma W_a + \sigma,
\]
where \( \sigma = \tau^* = 1 - \tau \) satisfies \( |\sigma| < 1 \). One key property, which can be employed to show that these point sets are pure point diffractive, is the fact that the \( \ast \)-images of the point sets \( \Lambda_{a,b} \) are \textit{uniformly distributed} in the windows \( W_{a,b} \), which makes it possible to translate the computation of \textit{average quantities} in physical space to computations in internal space.

### 3. Shelling

Let us discuss a simple example of an averaged quantity, the averaged shelling function for the Fibonacci point set; see \([13]\) for the concept and various applications to aperiodic systems. For a point set, the \textit{shelling} problem asks for the number \( n(r) \) of points that lie on shells of radius \( r \), taken with respect to a fixed centre. For an aperiodic point set, this generally depends on the choice of the centre. The \textit{averaged shelling} numbers \( a(r) \) are obtained by taking the average over all choices of centres, where we limit ourselves to centres that are themselves in the point set. Clearly, since we are dealing with a one-dimensional point set, any shell can have at most two points, so \( n(r) \in \{0, 1, 2\} \) for all \( r \in \mathbb{R} \), with \( n(r) = 0 \) if \( r \notin \mathbb{Z}[\tau] \), as well as \( n(0) = a(0) = 1 \). Clearly, this also implies that \( a(r) \in \{0, 2\} \) for all \( r \in \mathbb{R} \), with \( a(r) = 0 \) whenever \( r \notin \mathbb{Z}[\tau] \).

Consider a point \( x \in \Lambda \) and \( r = m+n\tau \in \mathbb{Z}[\tau] \). To compute \( n(r) \), we have to check whether \( x \pm r \) are also in the point set \( \Lambda \). From the model set description, we know that \( x^* \in W \), and checking whether \( x \pm r \) are in \( \Lambda \) is equivalent to checking whether \( x^* \pm r^* \in W \). While it is possible to perform this computation for any given value of \( x \) and \( r \), there is no simple closed formula for these coefficients.

To obtain the averaged shelling number, we have to consider all \( x \in \Lambda \) as centres, each with the same weight, which means averaging over all \( x^* \in W \). Define \( \nu(r) = \nu(-r) \) as the relative frequency to find a point in \( \Lambda \) at \( x \) as well as at \( x+r \), so \( a(0) = \nu(0) = 1 \) and \( a(r) = 2\nu(r) \) for \( r > 0 \), to account for the points on both sides. Now, for \( r \in \mathbb{Z}[\tau] \), the frequency \( \nu(r) \) of having both \( x^* \in W \) and \( x^* + r^* \in W \) can be calculated as the overlap length between the window \( W \) and the shifted window \( W - r^* \), divided by the length of \( W \), which is \( |W| = \tau \). This is correct because the uniform distribution of points in the window \([16,39]\) implies that the frequency of any configuration is proportional to the length of the corresponding sub-window. Clearly, the length of the overlap between these two intervals is 0 whenever \( |r^*| > \tau \), and decreases linearly with \( |r^*| \), so we get
\[
\nu(r) = \frac{|W \cap (W - r^*)|}{|W|} = \begin{cases} 1 - \frac{|r^*|}{\tau}, & \text{if } r \in \mathbb{Z}[\tau] \text{ and } |r^*| \leq \tau, \\ 0, & \text{otherwise.} \end{cases}
\]
behind this observation is the total discontinuity of the Fibonacci point set as a function of \( \nu \)

te find two points at a distance \( r \) (respectively normalised).

Fibonacci point set are given by the Dirac comb corresponding to the diffraction of this point set. Clearly, correlations are much easier handled in internal space, where we can calculate them via volumes of intersections of windows, as we shall see shortly.

4. Standard approach to diffraction

Here, we start with a brief summary of the derivation of the diffraction spectrum for the Fibonacci point set \( A = A_1 \cup A_0 \), considered as a cut and project set \( A = \{ x \in L : x^* \in W \} \) with \( W = W_a \cup W_b \). Assume that we place point scatterers of unit scattering strength at all points \( x \in A \), and consider the corresponding Dirac comb

\[
\omega = \delta_A := \sum_{x \in A} \delta_{x^*}.
\]

We associate to \( \omega \) the autocorrelation \( \gamma = \omega \otimes \bar{\omega} \), where \( \bar{\omega} \) is the ‘flipped-over’ (reflected) version of \( \omega \) and \( \otimes \) denotes volume-averaged (or Eberlein) convolution [16, Sec. 8.8]. The diffraction measure \( \hat{\gamma} \) is the Fourier transform of the autocorrelation.

From the general diffraction theory for cut and project sets with well-behaved windows, we know that the diffraction measure of this system is a pure point measure, so consists of Bragg peaks only. These Bragg peaks are located on the projection of the entire dual lattice

\[
L^* = \frac{1}{\sqrt{\tau}} \left\{ m(\tau - 1, \tau) + n(1, -1) : m, n \in \mathbb{Z} \right\}
\]
to the physical space (the first coordinate), which is \( L^* = \frac{1}{\sqrt{\tau}} \mathbb{Z}[\tau] \). We call this set the Fourier module of the Fibonacci point set; it coincides with the dynamical spectrum (in additive notation) in the mathematical literature. Note that \( \frac{1}{\sqrt{\tau}} = (2\tau - 1)/5 \), so \( L^* \subset \mathbb{Q}[\tau] \), which means that the \( \ast \)-map is well defined for all \( k \in L^* \). The Fourier module is a dense subset of \( \mathbb{R} \), which means that the diffraction consists of Bragg peaks on a dense set in space, where the intensities are locally summable.

The diffraction measure is thus the countable sum

\[
\hat{\gamma} = \sum_{k \in L^*} |A(k)|^2 \delta_k
\]

where the diffraction amplitudes, or Fourier–Bohr (FB) coefficients, are given by the general formula

\[
(9) \quad A(k) = \frac{\text{dens}(A)}{\text{vol}(W)} \hat{\gamma}_W(-k^*) = \frac{\text{dens}(A)}{\text{vol}(W)} \hat{\gamma}_W(k^*)
\]

for all \( k \in L^* \), and vanish otherwise. Here, \( 1_W \) denotes the characteristic function of the window \( W \), defined by

\[
1_W(x) = \begin{cases} 1, & \text{if } x \in W, \\ 0, & \text{otherwise}, \end{cases}
\]

and \( \hat{g} \) and \( \check{g} \) denote the Fourier transform and inverse Fourier transform of an \( L^1 \)-function \( g \), respectively. With \( \text{dens}(A) = (\tau + 2)/5 \) and \( \text{vol}(W) = \tau \), Eq. (9) evaluates to

\[
A(k) = \frac{1}{\sqrt{\tau}} \int_{-1}^{\tau} e^{2\pi ik^*y} \, dy = \frac{\tau}{\sqrt{\tau}} e^{\pi i k^*(\tau - 2)} \text{sinc}(\pi \tau k^*)
\]

where \( \text{sinc}(x) = \sin(x)/x \). Hence, the diffraction intensities are

\[
(10) \quad I(k) = |A(k)|^2 = \left( \frac{\tau}{\sqrt{\tau}} \text{sinc}(\pi \tau k^*) \right)^2
\]

for all \( k \in L^* \), and 0 otherwise. This is illustrated in Figure 3.

The corresponding autocorrelation measure \( \gamma \) can be expressed in terms of the (dimensionless) pair correlation coefficients

\[
\nu(r) := \frac{\text{dens}(A \cap (A - r))}{\text{dens}(A)} = \nu(-r),
\]

which are positive for all \( r \in A - A \subset \mathbb{Z}[\tau] \) and vanish for all other distances \( r \). These are precisely the coefficients we defined in Eq. (5) to compute the shelling numbers. The link between the two expressions is provided by the \( \ast \)-map and the uniform distribution of \( A^* \) in the window \( W \). In terms of these pair correlation coefficients, the autocorrelation measure is

\[
\gamma = \text{dens}(A) \sum_{r \in A - A} \nu(r) \delta_r,
\]
which is a pure point measure supported on the difference set \( A - A \).

More generally, we may associate two different, in general complex, scattering strengths \( u_a \) and \( u_b \) to the points in \( A_a \) and \( A_b \), respectively, and consider the weighted Dirac comb \( \omega = u_a \delta_{A_a} + u_b \delta_{A_b} \). In this case, the diffraction intensity for all wavevectors \( k \in L^\circ \) is given by the superposition

\[
I(k) = |u_a A_a(k) + u_b A_b(k)|^2
\]

of the corresponding FB amplitudes

\[
A_{a,b}(k) = \frac{\text{dens}(A_{a,b})}{\text{vol}(W_{a,b})} \hat{1}_{W_{a,b}}(-k^*)
= \frac{\text{dens}(A)}{\text{vol}(W)} \hat{1}_{W_{a,b}}(-k^*) = \frac{1}{\sqrt{5}} \hat{1}_{W_{a,b}}(-k^*) .
\]

The corresponding autocorrelation measure can once more be expressed in terms of pair correlation functions, now distinguishing points in \( A_a \) and \( A_b \),

\[
\nu_{\alpha\beta}(r) := \frac{\text{dens}(A_{\alpha}\cap(A_{\beta} - r))}{\text{dens}(A)} = \nu_{\beta\alpha}(-r).
\]

These coefficients are positive for all \( r \in A_{\beta} - A_{\alpha} \) and vanish otherwise, and in particular satisfy the relation \( \sum_{\alpha,\beta \in \{a,b\}} \nu_{\alpha\beta}(r) = \nu(r) \).

The relation (11) between the FB coefficients and the Fourier transform of the compact windows holds for any regular model set, which is a cut and project set with some ‘niceness’ constraint on the window; see [16, Thm. 9.4] for details. While this works well for many of the nice examples with polygonal windows, it becomes practically impossible to compute the FB coefficients in this way if the windows are compact sets with fractal boundaries. Such windows naturally arise for cut and project sets which also possess an inflation symmetry. Indeed, some of the structure models of icosahedral quasicrystals, see [51] for an example, feature experimentally determined windows whose shapes may indicate first steps of a fractal construction on the boundary.

Let us therefore explain a different approach that will permit an efficient computation of the diffraction also for such, more complicated, situations.

5. Renormalisation and internal cocycle

Let us reconsider our motivating example, the Fibonacci point sets \( A_{a,b} \) of Eq. (5). We will use both their inflation structure and their description as cut and project sets. Here, we make use of the iteration (3) and the corresponding relation (7) for the windows (or, more precisely, the closure of the windows). This inflation structure induces the following relation between the characteristic functions of the windows,

\[
(12) \quad 1_{W_a} = 1_{\sigma W_a \cup \sigma W_b} \quad \text{and} \quad 1_{W_b} = 1_{\sigma W_a + \sigma},
\]

where we again set \( \sigma = \tau^* = 1 - \tau \). Since the (closed) windows only share at most boundary points, we observe that \( 1_{\sigma W_a \cup \sigma W_b} = 1_{\sigma W_a} + 1_{\sigma W_b} \) holds as an equality of \( L^1 \)-functions. Now, we can apply the Fourier transform, where it will turn out to be more convenient to work with the inverse Fourier transform from the start. Applying the transform yields the relations

\[
(13) \quad \hat{1}_{W_a} = \hat{1}_{\sigma W_a} + \hat{1}_{\sigma W_b} \quad \text{and} \quad \hat{1}_{W_b} = \hat{1}_{\sigma W_a + \sigma} .
\]

Note that, by an elementary change of variable calculation, one has

\[
(14) \quad \hat{1}_{\alpha K + \beta}(y) = |\alpha| e^{2\pi i \beta y} \hat{1}_K(\alpha y)
\]

for arbitrary \( \alpha, \beta \in \mathbb{R} \) with \( \alpha \neq 0 \) and any compact set \( K \subset \mathbb{R} \).

Defining \( h_{a,b} := \hat{1}_{W_{a,b}} \) and using Eq. (14), we can rewrite Eq. (13) as

\[
(15) \quad \begin{pmatrix} h_a \\ h_b \end{pmatrix}(y) = |\sigma| B(y) \begin{pmatrix} h_a \\ h_b \end{pmatrix}(\sigma y)
\]

with the matrix

\[
(16) \quad B(y) := \begin{pmatrix} 1 & 1 \\ e^{2\pi i \sigma y} & 0 \end{pmatrix} .
\]

The matrix \( B \) is obtained by first taking the \( * \)-map of the set–valued displacement matrix \( T \) of Eq. (1) and then its inverse Fourier transform. For this reason, \( B \) is called the internal Fourier matrix [15], to distinguish it from the Fourier matrix of the renormalisation approach in physical space [9, 8]; see [23, 26] for various extensions with more flexibility in the choice of the interval lengths.

Going back to using Dirac notation, we introduce \( |h\rangle = (h_a, h_b)^T \), which satisfies \( |h(0)\rangle = \tau |v\rangle \) with the right eigenvector \( |v\rangle \) of the substitution matrix.
$M$ from Eq. (2). Applying the iteration \( (15) \) \( n \) times then gives
\[
|h(y)| = |\sigma^n B^{(n)}(y)|h(\sigma^ny))
\]
where
\[
B^{(n)}(y) := B(y)B(\sigma y)\cdots B(\sigma^{n-1}y).
\]
In particular, these matrices satisfy \( B^{(1)} = B \) and \( B^{(n)}(0) = M^n \) for all \( n \in \mathbb{N} \), where \( M \) is the substitution matrix from Eq. (11), as well as the relations
\[
B^{(n+m)}(y) = B^{(n)}(y)B^{(m)}(\sigma^n y)
\]
for any \( m, n \in \mathbb{N} \). Note that \( B^{(n)}(y) \) defines a matrix cocycle, called the internal cocycle, which is related to the usual inflation cocycle (in physical space) by an application of the \( * \)-map to the displacement matrices of the powers of the inflation rule; compare [11,18] and see [25,26] for a similar approach. Note also that \( |\sigma| < 1 \), which means that \( \sigma^n \) approaches 0 exponentially fast as \( n \to \infty \). We can exploit this exponential convergence to efficiently compute the diffraction amplitudes, which are essentially the elements of the vector \( |h\rangle \).

Considering the limit as \( n \to \infty \) in Eq. (17), one can show that
\[
|h(y)| = C(y)|h(0)|
\]
with
\[
C(y) := \lim_{n \to \infty} |\sigma|^n B^{(n)}(y),
\]
which exists pointwise for every \( y \in \mathbb{R} \). In fact, one has compact convergence, which implies that \( C(y) \) is continuous [18, Thm. 4.6 and Cor. 4.7], Clearly, since \( B^{(n)}(0) = M^n \), we have \( C(0) = P \) with the projector \( P = |v\rangle\langle u| \) from Eq. (3).

Using Eq. (18) with \( m = 1 \) and letting \( n \to \infty \), one obtains
\[
\tau C(y) = C(y)M,
\]
where \( \tau = \frac{\sigma}{\sigma+1} \). This relation implies that each row of \( C(y) \) is a multiple of the left eigenvector \( |u\rangle \) of the substitution matrix \( M \) from Eq. (2), which means that we can define a vector-valued function \( |c(y)\rangle \) such that
\[
C(y) = |c(y)\rangle\langle u|
\]
holds with \( |c(y)\rangle = (c_a(y), c_b(y))^T \), where we have \( |c(0)\rangle = |v\rangle \).

From Eqs. (19) and (21), we obtain
\[
|h(y)| = |c(y)\rangle\langle u|h(0)\rangle = \tau |c(y)\rangle
\]
and thus the inverse Fourier transforms of the windows, \( \hat{W}_{a,b} = h_{a,b} \), are encoded in the matrix \( C \).

For the Fibonacci case, we can calculate \( |c(y)\rangle \) by taking the Fourier transforms of the known windows \( W_{a,b} \) to obtain
\[
c_a(y) = \frac{e^{2\pi i(\tau-1)y} - e^{2\pi i(\tau-2)y}}{2\pi iy}.
\]
and
\[
c_b(y) = \frac{e^{2\pi i(\tau-2)y} - e^{-2\pi i(\tau-1)y}}{2\pi iy}.
\]
Note that these functions never vanish simultaneously, so \( C(y) \) is always a matrix of rank 1. However, taking the Fourier transform of the windows takes us essentially back to the standard approach.

The main benefit of the internal cocycle approach is that it applies in other situations, where no explicit calculation of the (inverse) Fourier transform of the windows is feasible. This is achieved by approximating \( C(y) \) by \( |\sigma|^n B^{(n)}(y) \) for a sufficiently large \( n \), such that \( |\sigma|^n y \) is small and \( C(y) \) is approximated sufficiently well. This works because the (closed) windows are compact sets, so that their (inverse) Fourier transforms are continuous functions. The convergence of this approximation is exponentially fast. We refer to [18] for further details and an illustration of the cocycle approach to more general inflation systems, and [19] for a planar example.

From the general formula (9) for regular model sets, the FB amplitudes are
\[
A_{a,b}(k) = \frac{h_{a,b}(k^*)}{\sqrt{5}} = \frac{\tau}{\sqrt{5}} c_{a,b}(k^*)
\]
for \( k \in L^\circ \). So, the relevant input is the knowledge of the Fourier module, which determines where the Bragg peaks are located. Then, one can approximate \( C \) by evaluating the matrix product in Eq. (20), for any chosen \( k \in L^\circ \), at \( y = k^* \) and with a sufficiently large \( n \). In what follows, numerical calculations and illustrations are based on this cocycle approach due to its superior speed and accuracy in the presence of complex windows.

6. Fractally bounded windows

The internal cocycle approach of Section 5 was first applied to a ternary inflation tiling with the smallest Pisot–Vijayaraghavan (PV) number (also known as the ‘plastic number’) as its inflation multiplier [19]. In the cut and project description, the internal space of this one-dimensional tiling is two-dimensional, and the windows are Rauzy fractals [12]. This means that the windows are still topologically regular, so the closure of their interior, but have a fractal boundary of zero Lebesgue measure. Consequently, the general diffraction result for model sets still applies, and the diffraction is given by the Fourier transform of the windows as described above. In turn, this means that the internal cocycle approach applies and can be used to compute the Fourier transforms and the diffraction intensities for such tilings; see [19] for details.

Here, we discuss examples of planar projection tilings with fractally bounded windows, which are
based on direct product variations (DPVs) of Fibonacci systems, as recently described in [7]. Clearly, if one considers a direct product structure based on the Fibonacci tiling, one obtains a tiling of the plane, called the square Fibonacci tiling. It is built from four prototiles, a large square of edge length $\tau$, a small square of edge length 1, and two rectangles with a long ($\tau$) and a short (1) edge; see Figure 4.

As a direct product of an inflation tiling, this two-dimensional square Fibonacci tiling also possesses an inflation rule, which takes the form

$$
\begin{array}{c}
0 & \rightarrow & 3 \\
1 & \rightarrow & 3 \\
2 & \rightarrow & 1 \\
3 & \rightarrow & 2
\end{array}
$$

where we labelled the small and large squares by 0 and 3, and the two rectangles by 1 and 2, respectively. A DPV is now obtained by modifying these rules while keeping the stone inflation character intact. Clearly, there are two possibilities to rearrange the images of the rectangles by swapping the two tiles, and a close inspection shows that there are altogether 12 ways of rearranging the image of the large square. This means that there are 48 distinct inflation rules in total, which all share these prototiles and the same inflation matrix.

Due to the direct product structure, the square Fibonacci tiling clearly possesses a cut and project description. The windows for the four prototiles are obtained as products of the original windows. The product structure thus extends to the diffraction measure, which is supported on the Fourier module

$$
L^\otimes \times L^\otimes,
$$

where $L^\otimes = \frac{1}{\sqrt{5}} Z[\tau]$ is the Fourier module of the one-dimensional Fibonacci tiling. The diffraction amplitudes are also given by products of those for the one-dimensional system, and thus easy to compute. An illustration of the diffraction pattern is shown in Figure 5. Here, Bragg peaks are represented by disks, centred at the position of the peak, with an area proportional to its intensity.

It turns out that all 48 DPV inflation tilings are regular model sets, and hence are pure point diffractive; see [7, Thm. 5.2]. They all share the same Fourier module $L^\otimes \times L^\otimes$. This implies that the Bragg peaks are always located at the same positions. However, their intensities are determined by the Fourier transform of the windows, and it turns out that the windows of these DPVs can differ substantially.

In particular, 20 of these DPVs possess windows of Rauzy fractal type, of which there are three different types, called ‘castle’, ‘cross’ and ‘island’ in [7]. They have different fractal dimension of the window boundaries, which are approximately 1.875, 1.756 and 1.561, respectively. As the dimensions are all smaller than two, it is obvious that these boundaries have zero Lebesgue measure.

In what follows, we are going to illustrate some properties of these DPVs with three examples, one for each of these fractally bounded window types. The inflation rules for the three examples have the same images for the small square (tile 0) and both rectangles (tiles 1 and 2) as the square Fibonacci rule of Eq. 23, and thus only differ in the image of the large square (tile 3). For a discussion of the complete set of 48 DPVs, we refer to [7].

For the castle-type windows of Figure 6, we use the inflation

$$
\begin{array}{c}
3 & \rightarrow & 2 \\
0 & \rightarrow & 3 \\
1 & \rightarrow & 1
\end{array}
$$

for the large square. Note that this rule dissects the inflated large square such that there is a reflection symmetry along the main diagonal, which will be reflected in a symmetry of the tiling (which maps the...
The windows for the four types of tiles are distinguished by colour, namely red (0), yellow (1), green (2) and blue (3). The outer boxes mark the square $[-\tau, \tau]^2$, with the coordinate axes indicated as well.

squares onto themselves and interchanges the rectangles). This is also apparent for the windows in Figure 6. The windows for the large and small squares are mapped onto themselves under reflection at the main diagonal, while the windows for the rectangular tiles are interchanged. The diffraction pattern also respects this symmetry; an illustration is shown in Figure 7.

For the cross-type windows, the inflation of the large square is given by

\[
3 
\begin{array}{c|c|c}
2 & 1 \\
0 & 3 
\end{array}
\]

which, in contrast to the previous example, has no reflection symmetry. Consequently, neither the windows shown in Figure 8 nor the diffraction image illustrated in Figure 9 have any reflection symmetry.

\[
3 
\begin{array}{c|c|c}
0 & 3 \\
2 & 1 
\end{array}
\]

of the large square tile. The corresponding diffraction pattern is illustrated in Figure 11.

Comparing the diffraction patterns of Figures 7, 9 and 11 with those of the square Fibonacci tiling shown in Figure 5 we note that the strongest peaks remain pretty much the same, while the intensities of the weaker peaks show some intriguing behaviour. For the fractally-bounded windows, one generally sees more peaks, which is due to the larger spread of the window in internal space, and the slower asymptotic decay of the Fourier transform of the window. With limited resolution, some of the intensity distributions on these peaks could resemble continuous components, so might potentially be mistaken as such in experiments.
7. Diffraction and Hyperuniformity

The discovery of quasicrystals highlighted the lack of a clear definition of the concept of order. In crystallography, diffraction is the main tool to detect long-range order, and a pure point diffraction is generally associated to an ordered, (quasi)crystalline structure, while absolutely continuous diffraction is typically seen as an indication of random disorder (but see [29, 14, 27, 28] for examples of deterministic structures that show absolutely continuous diffraction). Here, we briefly discuss a related concept that has recently gained popularity.

From the original idea of using the degree of ‘(hyper)uniformity’ in density fluctuations in many-particle systems [52] to characterise their order, the scaling behaviour of the total diffraction intensity near the origin has emerged as a possible measure to capture long-distance correlations. As far as aperiodic structures are concerned, there are in fact a number of early, partly heuristic, results in the literature [35, 4, 31]. These have recently been reformulated and extended [20, 11] and rigorously established [17], using exact renormalisation relations for primitive inflation rules [8, 9, 36, 11, 20, 57].

For the investigation of scaling properties, we follow the existing literature and define

\[ Z(k) := \hat{\gamma}((0, k]), \]

which is a modified version of the distribution function of the diffraction measure. Here, \( Z(k) \) is the total diffraction intensity in the half-open interval \((0, k]\), and thus ignores the central peak. Due to the reflection symmetry of \( \hat{\gamma} \) with respect to the origin, this quantity can also be expressed as

\[ Z(k) = \frac{1}{2} \left( \hat{\gamma}([-k, k]) - \hat{\gamma}(\{0\}) \right). \]

The interest in the scaling of \( Z(k) \) as \( k \to 0 \) is motivated by the intuition that the small-\( k \) behaviour of the diffraction measure probes the long-wavelength fluctuations in the structure. As the latter is related to the variance in the distribution of patches, it can serve as an indicator for the degree of uniformity of the structure [52]. It is obvious that any periodic structure leads to \( Z(k) = 0 \) for all sufficiently small wave number \( k \).

Here, we review the result for variants of the one-dimensional Fibonacci model sets considered above, where we now allow for changes of the windows. For a general discussion of this approach and more examples of systems with different types of diffraction, we refer to [17] and references therein.

Let us look at the diffraction for a cut and project set with the same setup as the Fibonacci tiling considered in Section 4, but with the window \( W \) replaced by an arbitrary finite interval of length \( s \). Note that these tilings, in general, do not possess an inflation symmetry. Nevertheless, the diffraction intensity is still of the form \( I(0) \), but now featuring the interval length \( s \), and is given by

\[ I(k) = I(0) (\text{sinc}(\pi sk^*))^2 \]

for all \( k \in L^\circ \). Now, consider a sequence of positions \( \tau^{-\ell}k \) with \( k \in L^\circ \) and \( \ell \in \mathbb{N}_0 \). Since we have \( \text{sinc}(x) = \sin(x)/x = \mathcal{O}(x^{-1}) \) as \( x \to \infty \), it follows that \( I(\tau^{-\ell}k) = \mathcal{O}(\tau^{-2\ell}) \) as \( \ell \to \infty \).

Consequently, the sum of intensities along the series of peaks,

\[ \Sigma(k) = \sum_{\ell=0}^{\infty} I(\tau^{-\ell}k), \]

satisfies the asymptotic behaviour

\[ \Sigma(\tau^{-\ell}k) \sim c(k) \tau^{-2\ell} \Sigma(k) \]
as $\ell \to \infty$, where it can be shown that $c(k) = \mathcal{O}(1)$ \cite{17}. Expressing $Z(k)$ in terms of these sums gives

$$Z(k) = \sum_{\kappa \in L_+} \Sigma(k),$$

which implies the asymptotic behaviour

$$Z(\tau^{-\ell}k) = \tau^{-2\ell} Z(k).$$

This leads to a scaling behaviour of the form $Z(k) = \mathcal{O}(k^2)$ as $k \to 0$.

This generic result remains true if we choose a window which corresponds to a tiling with inflation symmetry, which requires the window to be an interval of length $s \in \mathbb{Z}[\tau]$. This obviously holds for our original Fibonacci window $W$ of length $\tau$. However, one gets a stronger result for this case \cite{17,10}, as we shall now recall.

Choosing $s \in \mathbb{Z}[\tau]$ means $s = a + \beta \tau$ with $a, \beta \in \mathbb{Z}$. For $0 \neq k \in L_+$, let $k = \kappa/\sqrt{5}$ with $\kappa = m + \nu \tau$ for some $m, n \in \mathbb{Z}$, excluding $m = n = 0$. Applying the $\star$-map then gives

$$I(\tau^{-\ell}k) = I(0) \left( \sin \left( \frac{\pi \kappa^*}{\sqrt{5}} \right) \right)^2,$$

with $\ell \in \mathbb{N}_0$.

Now, denote by $f_n$ with $n \in \mathbb{Z}$ the Fibonacci numbers defined by $f_0 = 0$, $f_1 = 1$ and the recursion $f_{n+1} = f_n + f_{n-1}$. They satisfy the well-known formula

$$f_n = \frac{1}{\sqrt{5}} \left( \tau^n - (-1/\tau)^n \right) \quad (28)$$

for all $n \in \mathbb{Z}$. Using this relation, we obtain

$$\sin \left( \frac{\pi \kappa^*}{\sqrt{5}} \right)^2 = \sin \left( \frac{\pi |\kappa|}{\sqrt{5}} \right)^2 \quad (29)$$

$$= \frac{\pi^2 |\kappa|^2}{5} \tau^{-2\ell} + \mathcal{O}(\tau^{-6\ell})$$

as $\ell \to \infty$. Here, the first step follows by using Eq. \((28)\) to replace $\tau^\ell/\sqrt{5}$ and then reducing the argument via the relation

$$\sin(m\pi + x) = (-1)^m \sin(x),$$

which holds for all $m \in \mathbb{Z}$ and $x \in \mathbb{R}$. This is possible because all Fibonacci numbers are integers. The second step then uses the Taylor approximation $\sin(x) = x + \mathcal{O}(x^3)$ for small values of $x$.

Now, the same argument as above implies the asymptomatic behaviour

$$Z(\tau^{-\ell}k) \propto \tau^{-4\ell} Z(k),$$

and hence $Z(k) = \mathcal{O}(k^{4})$. This results means that, for inflation-invariant projection sets, the distribution function $Z(k)$ of the diffraction intensity vanishes like $k^4$ as $k \to 0$, while in the generic case we find a $k^2$-behaviour. This example illustrates that the behaviour of the diffraction intensity near $0$ can pick up non-trivial aspects of order in this system. This is illustrated for some cases in Figure \textbf{12}.

Let us briefly comment on the scaling behaviour for other prominent examples of aperiodic order discussed in \cite{17}. For noble means inflations, we observe the same $k^4$-scaling as for the Fibonacci tiling. The period doubling sequence, which is limit periodic, shows $k^2$-scaling, and a range of scaling exponents is accessible for substitutions of more than two letters. For the Thue–Morse sequence, which is the paradigm of an inflation structure with singular continuous diffraction, we do not obtain a power law, but an exponential scaling behaviour which decays faster than any power; see also \cite{12} for more on the scaling of the spectrum for this system. Finally, the Rudin–Shapiro sequence, which has absolutely continuous spectrum, shows a linear scaling behaviour, due to the constant density of its diffraction measure.
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