Periodic diffraction patterns for 1D quasicrystals

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Abstract

A simple model of 1D structure based on a Fibonacci sequence with variable atomic spacings is proposed. The model allows for observation of the continuous transition between periodic and non-periodic diffraction patterns. The diffraction patterns are calculated analytically both using "cut and project" and "average unit cell" methods, taking advantage of the physical space properties of the structure.

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1 Introduction

For nearly 100 years, the analysis of diffraction patterns of solids has been an essential tool for studying solids, since the diffraction pattern of a solid is essentially the (squared) Fourier transform of the set of atomic positions. Classical crystallography considered periodic structures, whose diffraction patterns consist entirely of sharp Bragg peaks. The Fourier transform of such a periodic set can be computed from the relevant unit cell. The discovery of quasicrystals showed that discrete diffraction patterns are associated not only with periodic structures but also with a large family of solids that have no discrete translation symmetry – quasicrystals. This fact was incorporated into a new definition of "crystal" proposed in 1992 by the Commission on Aperiodic Crystals established by the International Union of Crystallography: a crystal is defined to be any solid with an essentially discrete diffraction pattern.

Diffraction patterns for periodic and aperiodic crystals differ in substantial ways – for instance, the diffraction patterns of quasicrystals may exhibit "forbidden symmetry". It is therefore illuminating to consider a model that interpolates between periodic and aperiodic structures, and observe how the diffraction pattern changes.

We consider such a one-parameter family of structures in this paper. Specifically, we consider a fixed (Fibonacci) sequence of two types of "atoms", and vary the amount of space around each type of atom, while keeping the overall density fixed. The control parameter κ is the ratio of the two allowed distances between nearest neighbors. In all cases, the diffraction pattern is discrete, and the locations of the Bragg peaks are independent of κ. However, the *intensities* of the peaks are κ-dependent. When κ is rational, the intensities form a periodic pattern, while when κ is irrational, the diffraction pattern is aperiodic. We compute this diffraction pattern in two independent but equivalent ways: a) by recovering periodicity going to higher dimension (the "cut and project method" deeply discussed in many papers: [4, 7, 9, 12, 13, 14, 15, 16, 17, 18, 23]); b)using the concept of the reference lattice.

These results are in accordance with the ergodic theory of tiling spaces. It is known that the Bragg peaks of a tiling T occur at eigenvalues of the generator of translations on the hull of

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T (i.e., the space of all tilings in the same local isomorphism class as T) [8]. It is also known [21] that the hulls of modified Fibonacci chains with the same average spacing are topologically conjugate, hence that their generators of translations have the same spectral decomposition. The question of when and how such a modification affects the dynamical spectrum was addressed for one dimensional patterns in [5], and for higher dimensional patterns in [6]. (It should be noted that for a substitution tiling whose substitution matrix has two of more eigenvalues greater than 1, a generic change in tile length will destroy the Bragg peaks altogether, in sharp contrast to the behavior of modified Fibonacci chains, other Pisot substitutions, and other Sturmian sequences.)

Ergodic theory says nothing, however, about the intensities of the Bragg peaks. Although the spectrum of the generator of translations is complicated, for special values of the control parameter some of the peaks may have intensity zero, resulting in a simpler diffraction pattern. The calculations in this paper demonstrate that this does in fact happen.

2 The Modified Fibonacci Chain

The properties of Fibonacci sequences have already been thoroughly studied (see e.g., [22]). They are sequences of two elements A and B obtained from a substitution rule:

$$A \longrightarrow AB; \quad B \longrightarrow A. \tag{1}$$

Let $\vec{p}_m = (p_m^A, p_m^B)$ be the population vector, where p_m^X tells how many elements of type X are among the first m terms of the sequence. Of course, $p_m^A + p_m^B = m$. There are an uncountably infinite number of Fibonacci sequences, but all have the same local properties and the same diffraction pattern. It is easy to see that every Fibonacci sequence has

$$\lim_{m\to\infty} \frac{p_m^A}{p_m^B} = \tau, \quad \text{where} \quad \tau = \frac{1+\sqrt{5}}{2}. \tag{2}$$

For definiteness, we will work with the sequence ([22])

$$\vec{p}_m = (\left\|\frac{m}{\tau}\right\|, m - \left\|\frac{m}{\tau}\right\|). \tag{3}$$

Here $\|\cdot\|$ is the nearest integer function: If $m \in \mathbb{Z}$ and $m \le x < m+1$ then:

$$\|x\| = \begin{cases} m & \text{if} \quad x \in [m, m+1/2), \\ m+1 & \text{if} \quad x \in [m+1/2, m+1). \end{cases} \tag{4}$$

Now pick two positive numbers (also called A and B) that determine the space between each "A" or "B" atom and its predecessor. That is, the atomic positions are given by

$$x_m = \vec{p}_m \cdot (A, B). \tag{5}$$

We call the sequence $\{x_m\}$ a *modified Fibonacci chain.* If $A = B$, then the atoms are equally spaced, and this is simply a periodic array. If $A/B = \tau$, then the atomic positions are those obtained from the canonical "cut and project" method. By varying the ratio A/B, we interpolate between these two cases. Note that the average atomic spacing is $\frac{\tau A + B}{1+\tau}$. We will keep this average spacing fixed and consider the one-parameter family

$$A = \tau - \frac{\epsilon}{\tau}, \qquad B = 1 + \epsilon, \tag{6}$$

depending on the control parameter ϵ.

3 2D Analysis of the Modified Fibonacci Chain

The modified Fibonacci chain can be obtained by a "cut and project" method with a nonstandard projection. From this construction we can compute the diffraction pattern.

Let $\mathcal{L}_2^\nu$ be the 2 dimensional square lattice with spacing ν. The Voronoï cell of each lattice point is a square. Let l_0 be the line $y = x/\tau$ through the origin, making an angle $\beta_0 = \cot^{-1}(\tau)$ with the x-axis. Let X be the subset of $\mathcal{L}_2^\nu$ whose Voronoï cells are cut by l_0. It is well known (see e.g., [22]) that $X = \{\vec{x} \mid \vec{x} = \nu\vec{p}_m, m \in \mathbb{Z}\}$ where $\vec{p}_m$ are population vectors given by (3).

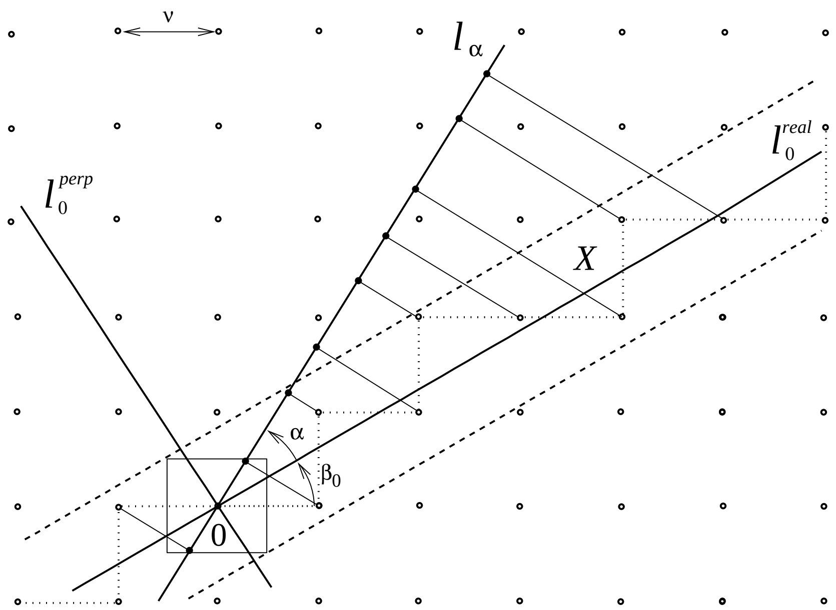

Figure 1: The 2D construction of the modified Fibonacci chain. Details in text.

Let l_α be the line through the origin making an angle

$$\beta = \beta_0 + \alpha \tag{7}$$

with the x-axis, and define Π_α to be the orthogonal projection onto l_α. Finally, let Λ be the projection of X onto l_α:

$$\Lambda = \Pi_\alpha(X). \tag{8}$$

The set Λ is then a modified Fibonacci chain. The two distances are

$$A = \nu \cos\beta, \qquad B = \nu \sin\beta. \tag{9}$$

Their sequence is fully determined by X and does not depend on α. The average distance between nearest neighbors in Λ is

$$\lim_{m\to\infty} \frac{\vec{p}_m \cdot (A, B)}{\vec{p}_m \cdot (1,1)} = \nu \frac{\sqrt{\tau+2}}{\tau+1} \cos\alpha. \tag{10}$$

To keep this average spacing constant we take

$$\nu = \frac{\sqrt{\tau+2}}{\cos\alpha}. \tag{11}$$

The angle α, the displacement parameter ϵ of (6) and the ratio $\kappa = A/B$ are related by

$$\epsilon = \frac{\tau - \kappa}{\kappa + \tau - 1} = \tau \tan(\alpha), \tag{12}$$

$$\kappa = \cot(\beta) = \frac{\tau - \tan(\alpha)}{1 + \tau \tan(\alpha)} = \frac{\tau + \epsilon(1-\tau)}{1+\epsilon}, \tag{13}$$

$$\tan(\alpha) = \frac{\epsilon}{\tau} = \frac{\tau - \kappa}{\kappa\tau + 1}. \tag{14}$$

We assume that every point of the set Λ is an atom with scattering power equal to unity. Our aim is to calculate the diffraction pattern of such a structure. We begin by calculating the 2-dimensional diffraction pattern of X. The diffraction pattern of Λ is then a section of the diffraction pattern of X along the direction l_α.

To get the diffraction pattern of X we note that X is $\mathfrak{L}_2^\nu$ times the characteristic function of a strip of width

$$h_\alpha = \nu \frac{\tau + 1}{\sqrt{\tau + 2}} = \frac{\tau + 1}{\cos\alpha} \tag{15}$$

around l_0. The Fourier transform of a product is the convolution of the Fourier transforms, and the Fourier transform of a lattice is the reciprocal lattice. The diffraction pattern of X in 2D has normalized intensity

$$I(\vec{k}) = \sum_{m_x}\sum_{m_y} \Big(\frac{\sin((h_\alpha|\vec{k} - \vec{k}_{m_x m_y}|)/2)}{(h_\alpha|\vec{k} - \vec{k}_{m_x m_y}|)/2)}\Big)^2 \delta\big((\vec{k} - \vec{k}_{m_x m_y}) \cdot (\tau, 1)\big), \tag{16}$$

where $\vec{k}_{m_x m_y} = \frac{2\pi}{\nu}(m_x, m_y)$ and $m_x,\ m_y \in \mathbb{Z}$ label points of the reciprocal lattice to $\mathfrak{L}_2^\nu$. Along the direction l_α, the peaks can be observed at positions

$$k^{phys} = \frac{\vec{k}_{m_x m_y} \cdot (\tau, 1)}{\cos\alpha\sqrt{\tau + 2}} = 2\pi \frac{\tau m_x + m_y}{\tau + 2}. \tag{17}$$

Note that these positions are independent of α (or ϵ or κ). Their intensities are

$$I_{m_x m_y} = \Big(\frac{\sin w}{w}\Big)^2, \qquad w = \frac{h_\alpha \vec{k}_{m_x m_y} \cdot (-1 - \tau\tan\alpha, \tau - \tan\alpha)}{2\sqrt{\tau + 2}}. \tag{18}$$

After simplifying and rewriting in terms of ϵ we obtain

$$w = \frac{\pi(\tau + 1)}{\tau + 2}(-m_x(1 + \epsilon) + m_y(\tau - \epsilon/\tau)). \tag{19}$$

4 Structure Factors and Average Unit Cells

The concept of a reference lattice has previously been proposed in [27]. Suppose we have a 1 dimensional Delone set $\{r_n\}$. Its points represent atoms, whose scattering instensities are equal to unity. We get the following expression for the structure factor:

$$F(k) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \exp(ikr_n) = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \exp(iku_n) = \int_{-\lambda/2}^{\lambda/2} P(u)\exp(iku)\mathrm{d}u, \tag{20}$$

where $P(u)$ is the probability distribution of distances u_n from the atoms to reference lattice positions $m\lambda$, $\lambda = 2\pi/k$. That is,

$$u_n = r_n - \left\|\frac{r_n}{\lambda}\right\|\lambda. \tag{21}$$

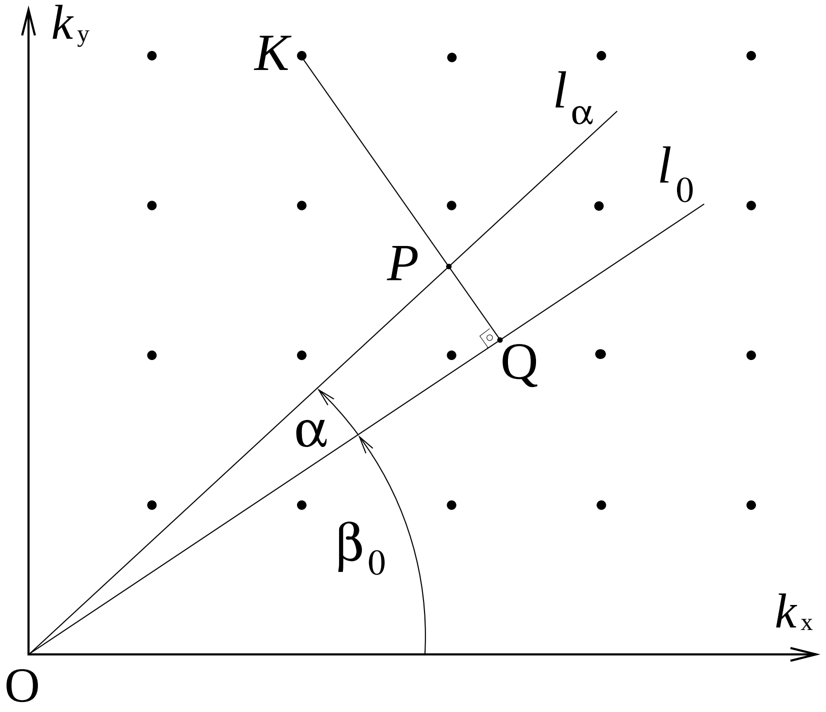

Figure 2: Diffraction pattern of the modified Fibonacci structure is a section of the diffraction pattern of X through direction l_α. $k^{phys} = \overline{OP}$ is the position of the peak, $\overline{KP}$ determines the intensity.

We call the series u_n the *displacements sequence* of r_n (induced by the reference lattice with period λ). Any series u'_n such that

$$u_n = u'_n - \left\| \frac{u'_n}{\lambda} \right\| \lambda, \tag{22}$$

will be called an *unreduced displacements sequence* (of r_n).

Theorem 1. *Let $r_n = \alpha_n + \beta_n$ be a sum of two real series. If d_n is a displacements sequence of α_n induced by a reference lattice, then*

$$u'_n = d_n + \beta_n \tag{23}$$

is an unreduced displacements sequence of r_n induced by the same lattice.

Proof. Let λ be the period of the reference lattice. We have to show that

$$u_n = r_n - \left\| \frac{r_n}{\lambda} \right\| \lambda = u'_n - \left\| \frac{u'_n}{\lambda} \right\| \lambda. \tag{24}$$

Note that for any real number x, y, $\|x - \|y\|\| = \|x\| - \|y\|$, since $\|y\|$ is an integer. We can write the right hand side of (24) as

$$\beta_n + \alpha_n - \left\| \frac{\alpha_n}{\lambda} \right\| \lambda - \left\| \frac{\beta_n + \alpha_n - \|\alpha_n/\lambda\| \lambda}{\lambda} \right\| \lambda = r_n - \left\| \frac{r_n}{\lambda} \right\| \lambda, \tag{25}$$

which is the left hand side. $\square$

The quantity $P(u)$ may be viewed as a probability distribution for an *average unit cell.* The structure factor for the scattering vector k is just the first Fourier mode of this distribution.

Unfortunately, for each scattering vector we get, in principle, a different average unit cell and a different distribution. However, the structure factor for mk, $m \in \mathbb{Z}$ can be computed from the reference lattice for k; it is the m-th Fourier mode of the distribution $P(u)$. Thus, a single average unit cell is sufficient to analyze structures whose scattering occurs at multiples of a fixed scattering vector k_0. This situation includes, but is not limited to, the case where the original point pattern was periodic with period $2\pi/k_0$.

For modulated structures (including quasicrystals), there are usually two periods, a and b, which may be incommensurate. Using two reference lattices, the first one having periodicity a and the second having periodicity b, the structure factor for the sum of two scattering vectors $k_0 \equiv 2\pi/a$ and $q_0 \equiv 2\pi/b$ can be expressed by:

$$\begin{aligned} F(k_0+q_0) &= \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \exp(i(k_0+q_0)x_n) = \lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \exp(i(k_0u_n+q_0v_n)) \\ &= \int_{-a/2}^{a/2}\int_{-b/2}^{b/2} P(u,v)\exp(i(k_0u+q_0v))\mathrm{d}u\mathrm{d}v, \end{aligned} \tag{26}$$

where u and v are the shortest distances of the atomic position from the appropriate points of two reference lattices and $P(u,v)$ is the corresponding probability distribution, which thus describes a *two dimensional* average unit cell. Likewise, the structure factor for a linear combination $nk_0 + mq_0$, n, $m \in \mathbb{Z}$ is given by the (n,m) Fourier mode of $P(u,v)$. This means that the average unit cell, calculated for the wave vectors of the main structure and its modulation, can be used to calculate the peak intensities of any of the main reflections and its satellites of arbitrary order. Using (26) and its generalization, it is possible to calculate the intensities of all peaks observed in the diffraction patterns.

5 1D Analysis of the Modified Fibonacci Chain

Let $a = \frac{\tau+2}{\tau+1}$, the average spacing between atoms in a modified Fibonacci chain, and let $b = \tau a$. The positions of atoms in our chain are:

$$\begin{aligned} x_m &= \vec{p}_m \cdot (A,B) \\ &= \left\| \frac{m}{\tau} \right\| A + mB - \left\| \frac{m}{\tau} \right\| B \\ &= (A-B)\left\| \frac{m}{\tau} \right\| + mB = (A-B)\left[\frac{m}{\tau}+\frac{1}{2}\right] + mB \\ &= (A-B)\frac{m}{\tau} + mB + (A-B)\Big(\frac{1}{2} - \Big\{\frac{m}{\tau}+\frac{1}{2}\Big\}\Big) \\ &= ma + u_0 M(ma), \end{aligned} \tag{27}$$

where $M(x) = \frac{1}{2} - \{\frac{x}{b} + \frac{1}{2}\}$ is a periodic function with period b and

$$u_0 = \tau - 1 - \epsilon\tau. \tag{28}$$

Here $[x] = \|x - \frac{1}{2}\|$ is the greatest integer function and $\{x\} = x - [x]$ is the fractional part of x.

When $u_0 \neq 0$, the modified Fibonacci chain is thus an incommensurately modulated structure. A similar derivation for $\epsilon = 0$ can be found in [22].

We are going to construct a two dimensional average unit cell based on the two natural periodicities for x_m: a and b. For the scattering vector $k_0 = 2\pi/a$, it is obvious that the series $u'_m = u_0 M(ma)$ is an unreduced displacements sequence of x_m induced by the reference lattice with period a.

Next we consider the (one dimensional) average unit cell for the scattering vector $q_0 = 2\pi/b$. The series

$$\mu_m = ma - \left\| \frac{ma}{b} \right\| b = -bM(ma) = -u'_m \frac{b}{u_0} \tag{29}$$

is an (unreduced) displacement sequence of ma induced by a reference lattice with period b. Using Theorem 1 we immediately get that the series

$$v'_m = \mu_m + u'_m = (u_0 - b)M(ma) = v_0 M(ma) = \xi u'_m \tag{30}$$

is an unreduced displacements sequence of x_m induced by a lattice with period b, where

$$v_0 = u_0 - b. \qquad \xi = v_0/u_0 = \frac{-\tau^2(1+\epsilon)}{1-\epsilon\tau^2}. \tag{31}$$

By Kronecker's theorem (see [11]), the series u'_m is uniformly distributed in the interval $[-|u_0|/2, |u_0|/2]$. As pointed out by Elser ([9], for a more precise discussion see also [22]) the uniformity of this distribution is crucial for our deliberations. Likewise, the series v'_m is uniformly distributed in the interval $[-|v_0|/2, |v_0|/2]$.

The structure factor (see (26)) is

$$F(n_1k_0 + n_2q_0) = \int_{-a/2}^{a/2} \int_{-b/2}^{b/2} P(u,v) \exp(i(n_1k_0u + n_2q_0v))\mathrm{d}u\mathrm{d}v. \tag{32}$$

The unreduced displacements sequences u'_m and v'_m can be used to calculate $P(u,v)$. However, this cannot be done directly because their terms may lie outside the average unit cell (i.e.: $|u_0| > a$ or $|v_0| > b$). Such a situation is shown in figure 3. We have to reduce the series to the interior of the cell. The probability function $P(u,v)$ is nonzero only along segments with slope ξ (as a result of the strong correlation between u'_m and v'_m given by (30)) and has constant value. This last fact follows from the uniformity of the marginal distributions.

The formula (32) is invariant under the changes

$$u \to u + \gamma_1 a, \qquad v \to v + \gamma_2 b, \tag{33}$$

where $\gamma_{1,2}$ are arbitrary integers. Likewise, the formula does not change if we use $P'(u,v) = C\delta(v - \xi u)$ instead of $P(u,v)$ and if we change the region of integration from $[-a/2, a/2]$,$[-b/2, b/2]$ to $[-|u_0|/2, |u_0|/2]$, $[-|v_0|/2, |v_0|/2]$. That is, we are free to integrate a part of distribution in the neighboring unit cells.

For integers n_1, n_2 we compute the location K_{n_1,n_2}, the structure factor $F(K_{n_1,n_2})$ and the normalized intensity I of the corresponding peak:

$$K_{n_1n_2} = (n_1k_0 + n_2q_0) = \frac{2\pi(\tau n_1 + n_2)}{\tau a} \qquad F(K_{n_1,n_2}) = \frac{\sin(w)}{w}, \qquad I = |F|^2, \tag{34}$$

where

$$w = (n_1k_0 + n_2q_0\xi)u_0/2 = (K_{n_1,n_2} - n_2q_1)u_0/2, \qquad q_1 = q_0(1-\xi) = \frac{2\pi\tau}{1-\epsilon\tau^2}. \tag{35}$$

The integers n_1 and n_2 label the main reflection and its satellites, respectively. Equations (34, 35) can be used to calculate the positions and intensities of all peaks.

The correspondence with the previous 2 dimensional calculation is given by

$$n_1 = m_y, \qquad n_2 = m_x - m_y. \tag{36}$$

By equations (17) and (34), the peaks are located at

$$K_{n_1,n_2} = K_{m_y, m_x - m_y} = 2\pi \frac{m_y\tau + m_x - m_y}{\tau} \frac{\tau+1}{\tau+2} = 2\pi \frac{m_x\tau + m_y}{\tau+2} = k^{phys}. \tag{37}$$

Likewise, substituting (36) into (35) and simplifying yields (19).

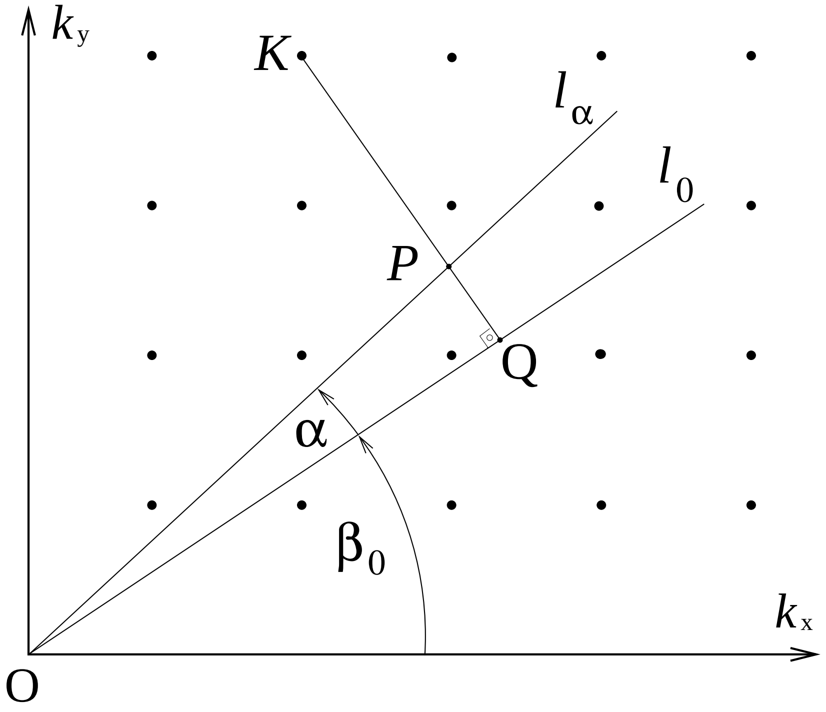

Figure 3: (a) shows two parameter average unit cell. The distribution $P(u, v)$ is non zero only along the thick lines and has constant value. Projections of it onto directions u and v determine the probability distributions for scattering vectors k_0 and q_0 ((b) and (c) respectively). (d) presents set of vectors $\{(u'_m, v'_m) \mid m \in \mathbb{Z}\}$. It may happen its elements lie outside the average unit cell and have to be reduced to its interior (like for the presented example with $\epsilon = -0.7$). Invariance under the substitution (33) assures that integration of functions on (a) and (d) gives the same results. Our parameter space has discrete translational symmetry like a periodic crystal.

6 Discussion of the Results

It has been shown that the deformation rule in physical space changes only the amplitude of modulation (equation (27)). Positions of peaks do not depend on the parameter ϵ; only their intensities vary. Using equations (34) and (35) we can easily build envelope functions, which go through the satellite reflections of the same order (indexed by n_2). The shift of the envelope functions is q_1, as given by (35).

The set of positions of Bragg peaks is always periodic, since the spectrum of a one-dimensional dynamical system is an Abelian group. By a *commensurate* diffraction pattern we mean a pattern in which the amplitudes are periodic as well. However, aside from the special case $A = B$, the Bragg peaks are described by two incommensurate periods, and should not be confused with the diffraction of a periodic crystal. For our diffraction patterns, one period (of length q_1) is connected with envelope functions, while the second, with period k_0, is associated with peaks ascribed to each envelope function. This behavior is characteristic of modulated crystals and was discussed in [26]. Only the first periodicity could assure equality of intensities.

It is convenient to describe our results in terms of the ratio $\kappa = A/B$. When κ is rational, say equal to p/q, then every atomic location x_m is a multiple of $A/p = B/q$. Plane waves whose frequencies are multiples of $2\pi p/A$ have value 1 at each atomic position, and the entire diffraction pattern is periodic with period $2\pi p/A$.

Conversely, if the diffraction pattern is periodic, then the underlying periods k_0 and q_1 must be commensurate. A simple algebraic calculation then shows that κ must be rational. Thus, the pattern is commensurate if and only if κ is rational, which corresponds to projecting the set X onto a rational direction ($\kappa = \cot\beta$; see (9)).

Figure 4a shows the diffraction pattern of an unmodified Fibonacci chain. The pattern is clearly non-periodic, as A/B equals to τ. For $\epsilon = 0$ our approach is identical with that presented in [28]. Figure 4b shows the pattern for $\epsilon = -0.7$ (corresponding to the average unit cell presented in figure 3). As we can see, analytical calculations of envelope functions are in full agreement with numerical calculations of the diffraction pattern.

Figures 5 and 6 show diffractions patterns for κ equal to $2/3$ and $3/2$ respectively. The regular series of peaks are clearly visible, but the diffraction patterns are still quasicrystaline. It is significant that for any value of ϵ except $1 - 1/\tau$ (discussed below) the structure is not periodic in physical space, but may have periodic diffraction patterns.

For $\epsilon = 1 - 1/\tau$ one gets fully periodic structure with $\kappa = 1$, hence $A = B$. Our deformed Fibonacci chain is then simply a lattice, and its diffraction pattern is the reciprocal lattice, with period k_0. At this special value of κ, all the other Bragg peaks have intensity zero.

Finally, it must be noted that the amplitude of each peak is a continuous function of κ. In fact, it is infinitely differentiable. As κ is varied, there is no phase transition between commensurate and incommensurate diffraction patterns; the evolution is smooth. As such, with measurement apparatus of fixed accuracy, it is impossible to determine whether a given pattern is precisely periodic.

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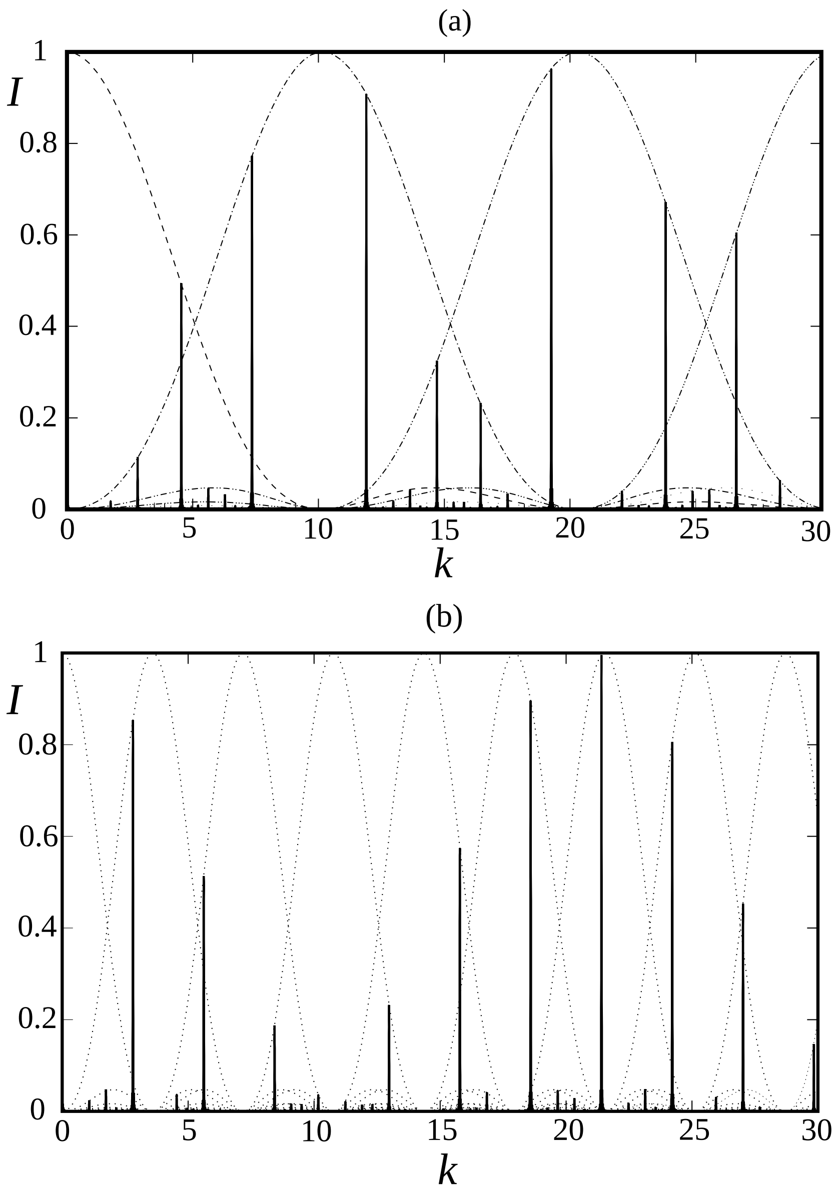

Figure 4: Examples of diffraction patterns: (a) unmodified Fibonacci chain ($\kappa = \tau$ and $\epsilon = 0$); (b) $\kappa \approx 6.836$ ($\epsilon = -0.7$). Broken lines present envelope functions. Given envelope function goes through satellite peaks of the same order. All envelopes have the same shape; their shift is q_1. As we can see analytical results are in full compatibility with numerical calculations.

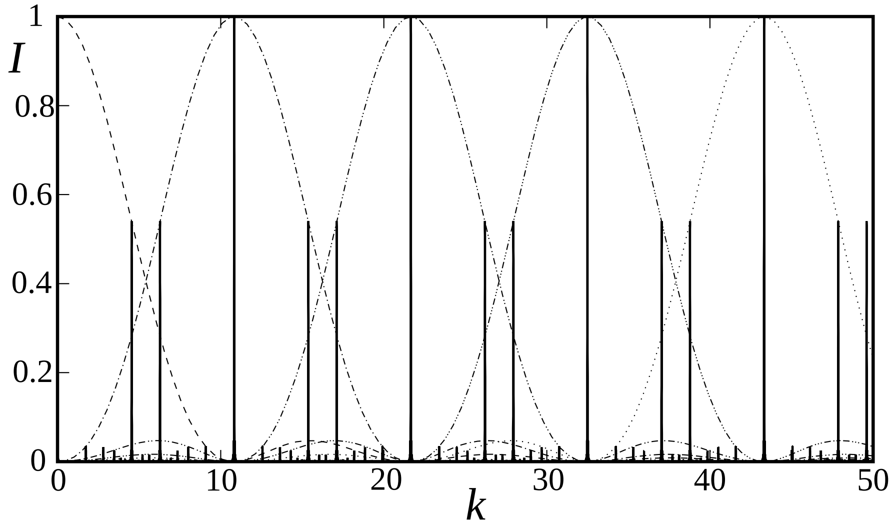

Figure 5: Modified Fibonacci chain for $\kappa = 2/3$ ($\epsilon \approx 0.741$, $q_1 \approx 10.816$).

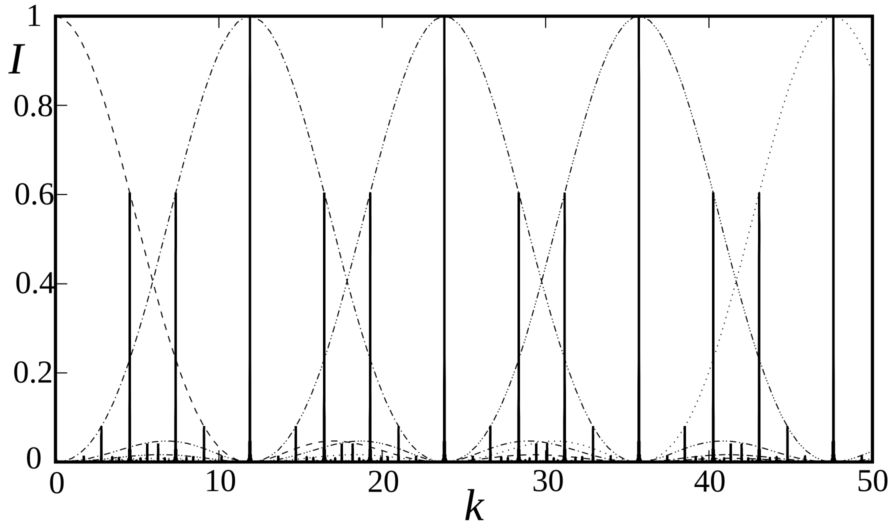

Figure 6: Modified Fibonacci chain for $\kappa = 3/2$ ($\epsilon \approx 0.056$, $q_1 \approx 11.913$).