A RADIAL ANALOGUE OF POISSON'S SUMMATION FORMULA WITH APPLICATIONS TO POWDER DIFFRACTION AND PINWHEEL PATTERNS

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Abstract. Diffraction images with continuous rotation symmetry arise from amorphous systems, but also from regular crystals when investigated by powder diffraction. On the theoretical side, pinwheel patterns and their higher dimensional generalisations display such symmetries as well, in spite of being perfectly ordered. We present first steps and results towards a general frame to investigate such systems, with emphasis on statistical properties that are helpful to understand and compare the diffraction images. An alternative substitution rule for the pinwheel tiling, with two different prototiles, permits the derivation of several combinatorial and spectral properties of this still somewhat enigmatic example. These results are compared with properties of the square lattice and its powder diffraction.

1. Introduction

Since the discovery of quasicrystals some 20 years ago, mathematicians and physicists have gained a reasonable understanding of aperiodically ordered systems, in particular of those obtained from the projection method. Such sets are called cut and project sets, or model sets [17]. These are Delone sets of finite local complexity with respect to translations, which also means that any finite patch occurs in finitely many orientations only.

Much less is known about aperiodically ordered systems with local patches occurring in infinitely many orientations, such as the pinwheel tiling of the plane or its three-dimensional counterpart, see [19] and references therein. Arguably, these are closer to amorphous systems, but still perfectly ordered. To our knowledge, no mathematically satisfactory frame for the analysis of radially symmetric systems and the comparison of their spectral properties has been developed so far. It is the aim of this contribution to show first steps in this direction, by combining results and methods from discrete geometry with the more recent approach of mathematical diffraction theory.

Our guiding examples are the square lattice and the pinwheel tiling of the plane. The diffraction of the square lattice is well understood, and it is not difficult to get some insight into its powder diffraction. The latter emerges from the presence of many grains in random mutual orientations, and thus requires a setting with circular symmetry.

Circular symmetry is also a fundamental property of the pinwheel tiling, resp. its compact hull. This tiling has recently been reinvestigated from the autocorrelation and diffraction point of view [18]. However, hardly any explicit calculation exists in the literature, the reason being the enigmatic nature of the substitution generated pinwheel tiling. New insight is gained by means of an alternative construction on the basis of a substitution rule with two distinct prototiles. This gives access to quantities such as frequencies (hence also to the frequency module), distance sets and the ring structure of the diffraction measure.

In Section 2, we derive a radial analogue of Poisson's summation formula for tempered distributions, which is needed in the following analysis. In the last section, we outline the general structure by presenting a number of results. They are clearly distinguished according to their present status into theorems (with proofs or references), claims (with a sketch of the idea and a reference to future work) and observations (based on numerical or preliminary evidence). Since our alternative substitution will no doubt enable other developments as well, we hope that further progress is stimulated by the results presented in this paper.

1.1. **Notation and preliminaries.** A rotation through α about the origin is denoted by R_α, and $B_r(x)$ is the closed ball of radius r centred in x. Whenever we speak of an *absolute frequency* (e.g., of a point set), we mean the average number per unit volume, whereas *relative frequency* of a subset of objects is used with respect to the entire number of objects. The absolute frequency of the points in a point set X (if it exists) is also called the *density* of X, denoted by $\mathrm{dens}(X)$. The set of non-negative integers is called $\mathbb{N}_0$, and the unit circle is $\mathbb{S}^1 = \{z \in \mathbb{C} : |z| = 1\}$. If M is a locally finite point set, the corresponding *Dirac comb* $\delta_M := \sum_{x\in M} \delta_x$, where δ_x is the normalised point (or Dirac) measure in x, is a well-defined measure. The Fourier transform of g is denoted by $\widehat{g}$. Whenever we use Fourier transform for measures below, we are working in the framework of tempered distributions [20].

2. A radial analogue of Poisson's summation formula

The diffraction pattern of an ideal crystal, supported on a point lattice $\varGamma \subset \mathbb{R}^d$, can be obtained by the Poisson summation formula (PSF) for lattice measures or Dirac combs [20, 7, 8]

$$\widehat{\delta_\varGamma} = \mathrm{dens}(\varGamma) \cdot \delta_{\varGamma^*}, \tag{1}$$

where $\varGamma^* := \{x \in \mathbb{R}^d : x \cdot y \in \mathbb{Z} \text{ for all } y \in \varGamma\}$ is the dual lattice. The distribution-valued (or measure-valued) version follows from the classical PSF, compare [7, 13], via applying it to a (compactly supported) Schwartz function. It is often used to derive the diffraction measure $\widehat{\gamma_\omega}$ of a lattice periodic measure $\omega = \varrho * \delta_\varGamma$ (with ϱ a finite measure). One obtains the autocorrelation measure

$$\gamma_\omega = \mathrm{dens}(\varGamma) \cdot (\varrho * \widetilde{\varrho}\,) * \delta_\varGamma, \tag{2}$$

where $\widetilde{\varrho}(g) := \overline{\varrho(\widetilde{g})}$ with complex conjugation $\bar{\cdot}$ and $\widetilde{g}(x) = \overline{g(-x)}$, and the diffraction measure

$$\widehat{\gamma_\omega} = (\mathrm{dens}(\varGamma))^2 \cdot |\widehat{\varrho}\,|^2 \cdot \delta_{\varGamma^*},$$

see [12, 1] for details. Our interest is to extend this approach to situations with circular (or spherical) symmetry.

Let us first consider the square lattice $\mathbb{Z}^2$, and recall that its circular shells have radii precisely in the set

$$\mathcal{D}_\square := \{r \geq 0 : r^2 = m^2 + n^2 \text{ with } m, n \in \mathbb{Z}\} = \{0, 1, \sqrt{2}, 2, \sqrt{5}, 2\sqrt{2}, 3, \ldots\}. \tag{3}$$

This is the set of non-negative numbers whose squares are integers that contain primes $p \equiv 3 \bmod 4$ only to even powers. Moreover, on a shell of radius $r \in \mathcal{D}_\square$, one finds finitely many lattice points, their number being given by

$$\eta_{\square}(r) = \begin{cases} 1, & r = 0, \\ 4a(r^2), & r \in \mathcal{D}_{\square} \setminus \{0\}. \end{cases} \tag{4}$$

Here, $a(n)$ is the number of ideals of norm n in $\mathbb{Z}[i]$, the ring of Gaussian integers. This is a multiplicative arithmetic function, thus specified completely by its values at prime powers (see [3, 11]). They are given by

$$a(p^{\ell}) = \begin{cases} 1, & \text{if } p = 2, \\ \ell + 1, & \text{if } p \equiv 1 \bmod 4, \\ 0, & \text{if } p \equiv 3 \bmod 4 \text{ and } \ell \text{ odd}, \\ 1, & \text{if } p \equiv 3 \bmod 4 \text{ and } \ell \text{ even}. \end{cases}$$

As $\mathbb{Z}^2$ is self-dual as a lattice, with $\mathrm{dens}(\mathbb{Z}^2) = 1$, the PSF (1) simplifies to $\widehat{\delta_{\mathbb{Z}^2}} = \delta_{\mathbb{Z}^2}$.

Choose an irrational number $\alpha \in (0, 1)$. By Weyl's lemma [15], the sequence $(n\alpha \bmod 1)_{n\geq 1}$ is uniformly distributed in $(0, 1)$. Consider the sequence $(\omega_N)_{N\geq 1}$ of measures defined by

$$\omega_N = \frac{1}{N} \sum_{n=1}^{N} \delta_{R^n \mathbb{Z}^2}, \tag{5}$$

where $R = R_{2\pi\alpha}$ is the rotation through $2\pi\alpha$. If $|x| = r > 0$, the sequence $(R^n x)_{n\geq 1}$ is uniformly distributed on $\partial B_r(0)$, again by Weyl's lemma. Observe that all lattices $R^n\mathbb{Z}^2$ share the same set of possible shell radii, namely $\mathcal{D}_{\square}$ of (3). This implies that, given an arbitrary compactly supported continuous function φ, one has

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \delta_{R^n\mathbb{Z}^2}(\varphi) = \sum_{r \in \mathcal{D}_{\square}} \eta_{\square}(r) \mu_r(\varphi),$$

where the measure μ_r is the normalised uniform distribution on $\partial B_r(0) = \{x \in \mathbb{R}^2 : |x| = r\}$, with $\mu_0 = \delta_0$. This establishes the following result.

Proposition 1. *The sequence $(\omega_N)_{N\geq 1}$ of (5) converges in the vague topology, and*

$$\omega := \lim_{N\to\infty} \omega_N = \sum_{r\in\mathcal{D}_{\square}} \eta_{\square}(r)\, \mu_r,$$

with shelling numbers $\eta_{\square}(r)$ and probability measures μ_r as introduced above. $\square$

It is obvious that the limit is, at the same time, also a limit of tempered distributions, i.e., a limit in $\mathcal{S}'(\mathbb{R}^2)$. As the Fourier transform is continuous on $\mathcal{S}'(\mathbb{R}^2)$, one has

$$\widehat{\omega} = \Bigl(\lim_{N\to\infty} \omega_N\Bigr)^{\widehat{}} = \lim_{N\to\infty} \widehat{\omega}_N.$$

Employing the ordinary PSF (1), one finds

$$\widehat{\omega}_N = \frac{1}{N} \sum_{n=1}^{N} \widehat{\delta}_{R^n\mathbb{Z}^2} = \frac{1}{N} \sum_{n=1}^{N} \delta_{(R^n\mathbb{Z}^2)^*} = \frac{1}{N} \sum_{n=1}^{N} \delta_{R^n\mathbb{Z}^2} = \omega_N$$

where we used that $(R\varGamma)^* = R\varGamma^*$ for an isometry R, and $\operatorname{dens}(R^n\mathbb{Z}^2) = \operatorname{dens}(\mathbb{Z}^2) = 1$. Combining the last two equations, one sees that

$$\widehat{\omega} = \lim_{N\to\infty} \widehat{\omega}_N = \lim_{N\to\infty} \omega_N = \omega.$$

Using polar coordinates, the Fourier transform of μ_r — which is an analytic function because μ_r has compact support — can be expressed by a Bessel function of the first kind via the following calculation,

$$\begin{aligned} \widehat{\mu}_r(k) &= \int_{\mathbb{R}^2} e^{-2\pi i k\cdot x}\, \mathrm{d}\mu_r(x) = \int_0^\infty \frac{1}{2\pi}\int_0^{2\pi} e^{-2\pi i |k| \varrho \cos\varphi}\, \mathrm{d}\varphi\, \mathrm{d}\delta_r(\varrho) \\ &= \int_0^\infty J_0(2\pi|k|\varrho)\, \mathrm{d}\delta_r(\varrho) = J_0(2\pi|k|r), \end{aligned} \tag{6}$$

where $J_0(z) = \sum_{\ell=0}^\infty \frac{(-1)^\ell}{(\ell!)^2}(\frac{z}{2})^{2\ell}$. This yields the identity

$$\widehat{\omega} = \sum_{r\in\mathcal{D}_\square} \eta_\square(r) J_0(2\pi|k|r), \tag{7}$$

to be understood in the distribution sense. It has the following consequence.

Corollary 2. *With $\eta_\square(r)$ and μ_r as introduced above, one has*

$$\sum_{r\in\mathcal{D}_\square} \eta_\square(r)\, \mu_r = \Big(\sum_{r\in\mathcal{D}_\square} \eta_\square(r)\, \mu_r\Big)^{\widehat{}} = \sum_{r\in\mathcal{D}_\square} \eta_\square(r) J_0(2\pi|k|r),$$

where the last expression is to be understood in the distribution sense. □

Identities of this type can be viewed as measure-valued generalisations of classic Hardy-Landau-Voronoi summation formulae, see [13, Sec. 4.4] and references given there for details. However, in view of the rather delicate convergence properties, a direct verification via the PSF (1) seems a simpler approach.

Observe that one can alternatively reduce the problem to one dimension and employ a Hankel transform, compare [13, Sec. 4.4]. This requires a separate treatment of the transformed measure at the origin in k-space. As this looks slightly artificial from the point of view of diffraction, we stick to ordinary Fourier transform.

The version for a general lattice $\varGamma \subset \mathbb{R}^d$ reads as follows, where, in analogy to $\eta_\square(r)$, $\eta_\varGamma(r)$ and $\eta_{\varGamma^*}(r)$ denote the number of points of $\varGamma$ and $\varGamma^*$ on centred shells $\partial B_r(0)$ of radius r.

Theorem 3 (Radial PSF)**.** *Let $\varGamma$ be a lattice of full rank in $\mathbb{R}^d$, with dual lattice $\varGamma^*$. If the sets of radii for non-empty shells are $\mathcal{D}_\varGamma$ and $\mathcal{D}_{\varGamma^*}$, with shelling numbers $\eta_\varGamma(r)$ and $\eta_{\varGamma^*}(r)$, the classical PSF (1) has the radial analogue*

$$\Big(\sum_{r\in\mathcal{D}_\varGamma} \eta_\varGamma(r)\, \mu_r\Big)^{\widehat{}} = \sum_{r\in\mathcal{D}_\varGamma} \eta_\varGamma(r)\, \widehat{\mu}_r = \operatorname{dens}(\varGamma) \sum_{r\in\mathcal{D}_{\varGamma^*}} \eta_{\varGamma^*}(r)\, \mu_r, \tag{8}$$

where μ_r denotes the uniform probability measure on the sphere of radius r around the origin.

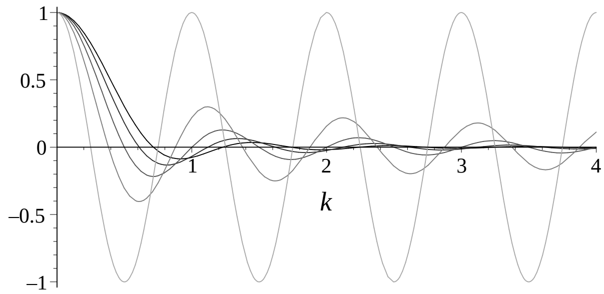


FIGURE 1. A plot of the radial structure of the function $\widehat{\mu}_1(k)$ of (9) for dimensions $d = 1$ (light grey), 2, 3, 4, and 5 (black).

Proof. Select a sequence of isometries $(R_n)_{n\geq 0}$, $R_n \in \mathrm{SO}(d)$, such that $(R_n x)_{n\geq 0}$, for a fixed x of length 1, is uniformly distributed on the unit sphere $\mathbb{S}^d$. Consider then the sequence of measures defined by

$$\omega_N = \frac{1}{N}\sum_{n=1}^{N} \delta_{R_n \varGamma}.$$

The claim now follows from Weyl's lemma and the classical PSF (1) in complete analogy to our previous planar example. □

The formula for general d can also be expressed in terms of Bessel functions of the first kind. Here, by standard calculations with spherical coordinates and integral representations of Bessel functions, one obtains

$$\widehat{\mu}_r(k) = \int_{\mathbb{R}^d} e^{-2\pi i k x}\, \mathrm{d}\mu_r(x) = \Gamma\big(\frac{d}{2}\big)\, \frac{J_{\frac{d}{2}-1}(2\pi|k|r)}{(\pi|k|r)^{\frac{d}{2}-1}}, \tag{9}$$

where $\Gamma(x)$ is the gamma function and $J_\nu(z) = (\frac{z}{2})^\nu \sum\limits_{\ell=0}^{\infty} \frac{(-1)^\ell}{\ell!\Gamma(\nu+\ell+1)} (\frac{z}{2})^{2\ell}$. In particular,

$$\widehat{\mu}_r(k) = \begin{cases} \cos(2\pi k r), & \text{if } d = 1, \\ J_0(2\pi|k|r), & \text{if } d = 2, \\ \frac{\sin(2\pi|k|r)}{2\pi|k|r}, & \text{if } d = 3. \end{cases}$$

The analogue of Corollary 2 for $d = 1$ and $\varGamma = \mathbb{Z}$ thus reads

$$\sum_{m\in\mathbb{Z}} \cos(2\pi k m) = \widehat{\delta_{\mathbb{Z}}} = \delta_{\mathbb{Z}},$$

which is just another form of the ordinary PSF in this case (as radial averaging is trivial here). Figure 1 shows (9) for $r = 1$ and various values of d.

3. A SIMPLISTIC APPROACH TO POWDER DIFFRACTION

The intensity distribution in powder diffraction emerges from a collection of grains in random and mutually uncorrelated orientations. Its precise theoretical description is difficult, compare [21] and references therein.

Here, we look into a rather simplistic approach that nevertheless captures the essence of the diffraction image. For simplicity, and for comparison with related pinwheel patterns, we explain this for the square lattice $\mathbb{Z}^2$. Instead of working with grains of finite size, we consider the superposition of entire lattices, with appropriate weights. Moreover, we make the restriction that there is a common rotation centre for all lattices, which we choose to be the origin. As a first step, let us take a look at $\mathbb{Z}^2 \cup R\mathbb{Z}^2$, where $R \in \mathrm{SO}(2)$ is a generic rotation (by which we mean that it is *not* an element of the group of coincidence rotations $\mathrm{SOC}(\mathbb{Z}^2) = \mathrm{SO}(2,\mathbb{Q})$, see [3] for more on this concept).

Lemma 4. *Let $R \in \mathrm{SO}(2)$ be a generic rotation, so that $\mathbb{Z}^2 \cap R\mathbb{Z}^2 = \{0\}$. Then, the autocorrelation of $\omega = \frac{1}{2}(\delta_{\mathbb{Z}^2} + \delta_{R\mathbb{Z}^2})$ is*

$$\gamma_\omega = \frac{1}{4}\delta_{\mathbb{Z}^2} + \frac{1}{4}\delta_{R\mathbb{Z}^2} + \frac{1}{2}\lambda, \tag{10}$$

where λ is the Lebesgue measure in $\mathbb{R}^2$. The diffraction measure of ω is

$$\widehat{\gamma}_\omega = \sum_{x\in\mathbb{Z}^2\cup R\mathbb{Z}^2} I(x)\delta_x \tag{11}$$

with $I(0) = 1$ and $I(x) = \frac{1}{4}$ for all $0 \neq x \in \mathbb{Z}^2 \cup R\mathbb{Z}^2$.

Proof. The first two terms in (10) are the autocorrelations of $\frac{1}{2}\mathbb{Z}^2$ and of $\frac{1}{2}R\mathbb{Z}^2$. The third term originates from the cross-correlation between them, where we used the identity

$$\lambda = \lim_{r\to\infty} \frac{1}{\pi r^2} \sum_{\substack{x\in\mathbb{Z}^2\cap B_r(0)\\ y\in R\mathbb{Z}^2\cap B_r(0)}} \delta_{x-y},$$

with the limit being taken in the vague topology. This identity can be derived as follows. It is easy to see that each square in the square lattice is hit by $x-y$ exactly once, if x is arbitrary but fixed and y runs through $R\mathbb{Z}^2$. (The exception is $y = 0$, but we can neglect it since it plays no role in the limit.) Thus each square in $\mathbb{Z}^2$ is hit with the same frequency in the limit. Since R is a generic rotation, the sequence $(x - y \bmod (1,1))$ is uniformly distributed in the fundamental domain $[0,1)^2$ of $\mathbb{Z}^2$, if x is arbitrary but fixed and y runs through $R\mathbb{Z}^2$. This is a consequence of the uniform distribution of $(n\alpha \bmod 1)_{n\geq 1}$ in $(0,1)$ if α is irrational. Thus, the points in the sum above are uniformly distributed in $\mathbb{R}^2$ in the limit, and the series converges in the vague topology to the Lebesgue measure.

Now, Equation (11) follows immediately from $\widehat{\lambda} = \delta_0$ and the PSF (1). □

For completeness, let us briefly comment on the situation that $R \in \mathrm{SOC}(\mathbb{Z}^2)$. In this case, $\varTheta := \mathbb{Z}^2 \cap R\mathbb{Z}^2$ is a sublattice of $\mathbb{Z}^2$ of finite index, which is $1/\operatorname{dens}(\varTheta)$. It is possible to show that $\omega = \frac{1}{2}(\delta_{\mathbb{Z}^2} + \delta_{R\mathbb{Z}^2})$ has diffraction

$$\widehat{\gamma}_\omega = \delta_\varTheta + \frac{1}{4}\delta_{\mathbb{Z}^2\setminus\varTheta} + \frac{1}{4}\delta_{R\mathbb{Z}^2\setminus\varTheta}.$$

The difference to the diffraction formula in Lemma 4 is concentrated on $\varTheta \setminus \{0\}$, and hence plays no role in our further discussion when $\operatorname{dens}(\varTheta) \to 0$, which happens under multiple coincidence intersections [3]. We may thus disregard coincidence rotations for our present purposes.

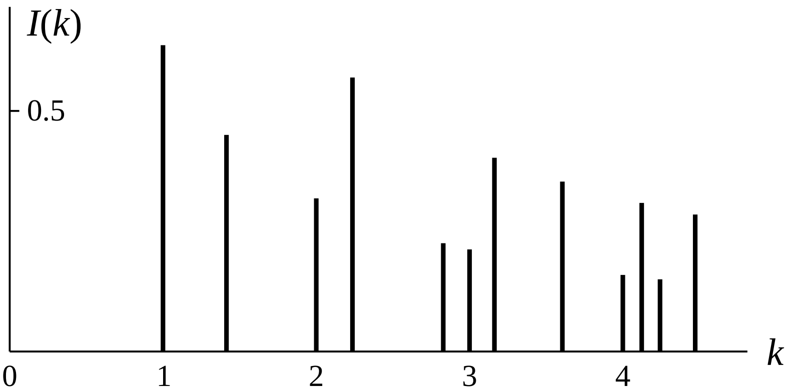


FIGURE 2. Radial dependence of ring intensities of square lattice powder diffraction. The central intensity is not shown, see text for details.

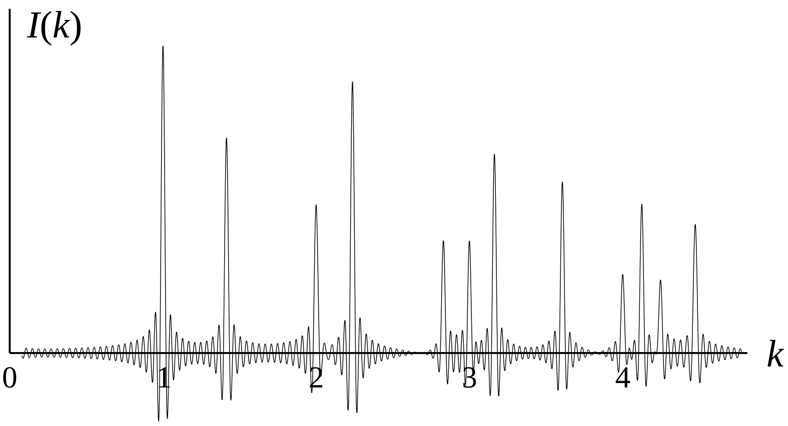


FIGURE 3. Numerical approximation of Figure 2, based on summing Bessel functions, for radii $r \leq 25$. The required radial autocorrelation coefficients $\eta_{\square}(r)$ are taken from Equation (4).

Let us continue by considering multiple intersections. If all rotations are generic (in the sense that the lattices $R_i\mathbb{Z}^2$ and $R_j\mathbb{Z}^2$ are distinct apart from the origin) and satisfy a uniform distribution property, we obtain the following result.

Proposition 5. *Let $\varGamma = \mathbb{Z}^2$, $\varGamma_j = R_j\mathbb{Z}^2$ with generic R_j, i.e., $\varGamma_j \cap \varGamma_k = \{0\}$ for $j \neq k$, and define $\omega = \frac{1}{N}\sum_{j=1}^{N} \delta_{\varGamma_j}$. Then, one has the identities*

$$\gamma_\omega = \frac{N-1}{N}\lambda \, + \sum_{j=1}^{N} \frac{1}{N^2}\delta_{\varGamma_j} \quad \text{and} \quad \widehat{\gamma}_\omega = \frac{N-1}{N}\delta_0 + \frac{1}{N}\Big(\frac{1}{N}\sum_{j=1}^{N}\widehat{\delta}_{\varGamma_j}\Big).$$

If $(R_j x)_{j\geq 0}$ is uniformly distributed on $\mathbb{S}^1$ for some fixed $x \in \mathbb{S}^1$, we obtain

$$\lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N}\widehat{\delta}_{\varGamma_j} = \sum_{r\geq 0} \eta_{\square}(r)\mu_r,$$

with $\eta_{\square}(r)$ *as in* (4).

Proof. The first statement — about γ_ω — follows as in Lemma 4. Observing $(\varGamma_j)^* = R_j \varGamma^*$, this implies

$$\widehat{\gamma}_\omega = \sum_{x \in \bigcup_j R_j \varGamma^*} I(x) \delta_x,$$

where $I(0) = 1$ and $I(x) = \frac{1}{N^2}$ otherwise. Consequently, one finds

$$\widehat{\gamma}_\omega = \frac{N-1}{N} \delta_0 + \frac{1}{N} \Big(\frac{1}{N} \sum_{j=1}^{N} \widehat{\delta}_{\varGamma_j} \Big).$$

By Theorem 3 in connection with Weyl's lemma and the self-duality of $\mathbb{Z}^2$, the term in the brackets converges to $\sum_{r \geq 0} \eta_{\square}(r) \mu_r$ as $N \to \infty$. $\square$

This simple argument shows that, after discarding the central intensity and multiplying the remainder by N, one is left with a circular diffraction pattern in the spirit of the radial PSF in Theorem 3. Disregarding the central intensity, the shelling numbers $\eta_{\square}(r)$ reflect the total intensity, integrated over the rings of radius r, in this idealized approach to powder diffraction. Consequently, in a measurement that displays the intensity along a given direction, the resulting radial dependence is given by $\frac{\eta_{\square}(r)}{2\pi r}$, compare Figure 2. The numerical approximation in Figure 3, included for later comparison, shows a strong oscillatory behaviour, as a result of summing Bessel functions. Note that this approximation disregards positivity in favour of including circular symmetry. The comparison gives a good impression on the overshooting that originates from this approach.

4. Application to tilings with statistical circular symmetry

4.1. **The pinwheel tiling.** The prototile of the pinwheel tiling is a rectangular triangle with side length 1, 2 and $\sqrt{5}$. The smallest angle in T is $\arctan(\frac{1}{2})$. Here, we choose the prototile T with vertices $(-\frac{1}{2}, -\frac{1}{2})$, $(\frac{1}{2}, -\frac{1}{2})$, $(-\frac{1}{2}, \frac{3}{2})$, and equip T with a control point at $(0,0)$. Every tile in a pinwheel tiling is either of the form $R_\alpha T + x$, or of the form $R_\alpha S T + x$ for some $x \in \mathbb{R}^2$, where S denotes the reflection in the horizontal axis and R_α rotation through α. The substitution σ for the pinwheel tiling is shown in Figure 4 (left). By the action of σ, T is expanded, rotated by $-\arctan(\frac{1}{2})$ and dissected into five triangles that are congruent to T. Formally, we define $\sigma(T) := \{Q_1(T) + x_1, Q_2(T) + x_2, Q_3(T) + x_3, Q_4(T) + x_4, Q_5(T) + x_5\}$, with $Q_i \in \mathrm{O}(2)$ and $x_i \in \mathbb{R}^2$. The appropriate choices of Q_i and x_i can be derived from the figure. In particular, $\sigma(T)$ contains a triangle *equal* to T, thus we may choose $Q_1 =$ and $x_1 = 0$. The substitution σ extends in a natural way to all isometric copies $QT + x$ (where $Q \in \mathrm{O}(2)$ and $x \in \mathbb{R}^2$) by $\sigma(QT + x) := Q\sigma(T) + \sqrt{5}x$. Since one of the triangles in $\sigma(T)$ equals T, the tiling PW can be defined as a fixed point of the substitution σ. This results in $\sigma(PW) = PW = \bigcup_{n \geq 0} \sigma^n(T)$. This convention follows [18] but deviates from [19], because it is advantageous for us to include the rotation in the definition of σ.

4.2. **The kite domino tiling.** It is advantageous to consider a second substitution which yields a closely related tiling. Consider the two prototiles K and D (for 'kite' and 'domino'),

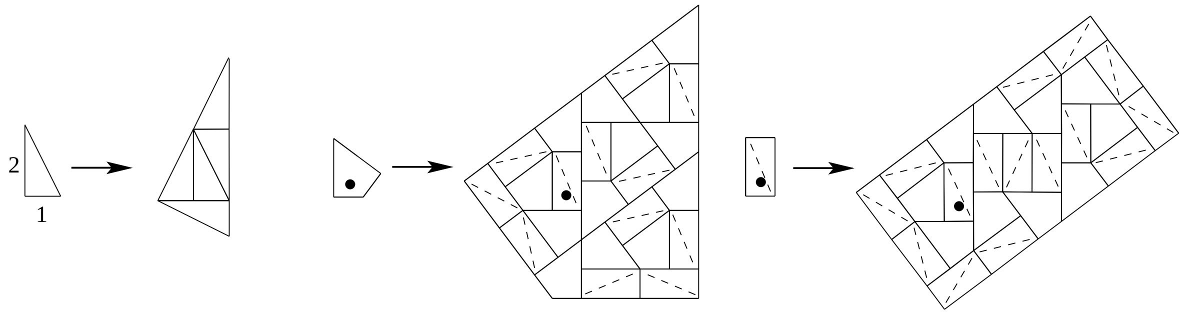


FIGURE 4. The substitution for the pinwheel tiling (left) and for the kite domino tiling (right). The dashed lines indicate how the dominos have to be dissected to obtain a pinwheel tiling. They are also needed to turn the global substitution rule for KD into a local one for its hull.

where D is the rectangle with vertices $(-\frac{1}{2}, -\frac{1}{2})$, $(\frac{1}{2}, -\frac{1}{2})$, $(\frac{1}{2}, \frac{3}{2})$, $(-\frac{1}{2}, \frac{3}{2})$, and K is the quadrangle with vertices $(-\frac{1}{2}, -\frac{1}{2})$, $(\frac{1}{2}, -\frac{1}{2})$, $(\frac{11}{10}, \frac{3}{10})$, $(-\frac{1}{2}, \frac{3}{2})$. Both tiles consist of two copies of the pinwheel triangle T, glued together along their long edges. Every pinwheel tiling gives rise to a kite domino tiling by deleting all edges of length $\sqrt{5}$. The substitution for the kite domino tiling is shown in Figure 4 (right). Essentially, it is σ^2 applied to the new prototiles, where σ is the substitution for the pinwheel tiling. If ϱ denotes this new substitution, a fixed point is given by $KD = \bigcup_{n\geq 0} \varrho^n(D)$. This is a *global* substitution that works on the specific D defined above, compare [9] for a discussion of the general substitution concept. The two tilings, PW and KD, are mutually locally derivable (MLD) in the sense of [6]. Essentially, this means that one is obtained from the other by local replacement rules and vice versa. These rules are evident from Figure 4.

As PW and KD are MLD, the global substitution ϱ also induces a *local* substitution in the sense of [5], where two (oriented) copies of the domino have to be distinguished. Loosely speaking, this follows from the observation that the local surrounding of any domino in KD or one of the other elements in the hull defined by KD determines the type of the domino, and hence how to apply the substitution to it.

We equip K with control points at $(0,0), (\frac{2}{5}, \frac{1}{5})$, and D with control points at $(0,0), (0,1)$. Then, the set of all control points in KD is equal to the set of control points in PW. This specific discrete point set is a Delone set, denoted by $\varLambda$ in the sequel. It is not hard to see that $\varLambda$ is MLD with both PW and KD, even though one direction of the replacement rule is less obvious than the one linking PW and KD.

Observe that the relative and absolute frequencies of triangles T in the pinwheel tiling are both equal to 1. For the relative frequencies, this is clear since there is only one prototile. The absolute frequency then follows from the fact that this prototile has area 1. Every triangle of PW carries exactly one control point, so $\mathrm{dens}(\varLambda) = 1$, too. For the kite domino tiling, standard Perron-Frobenius theory yields the relative frequencies of kite (resp. domino) as $\frac{5}{11}$ (resp. $\frac{6}{11}$). Thus, the absolute frequency of a kite (resp. domino) is $\frac{5}{22}$ (resp. $\frac{6}{22}$). The substitution matrix can be extracted from Figure 4.

Discrete structures that are MLD lead to dynamical systems that are topologically conjugate [14]. Therefore, we formulate the hull on the basis of the Delone sets of the control

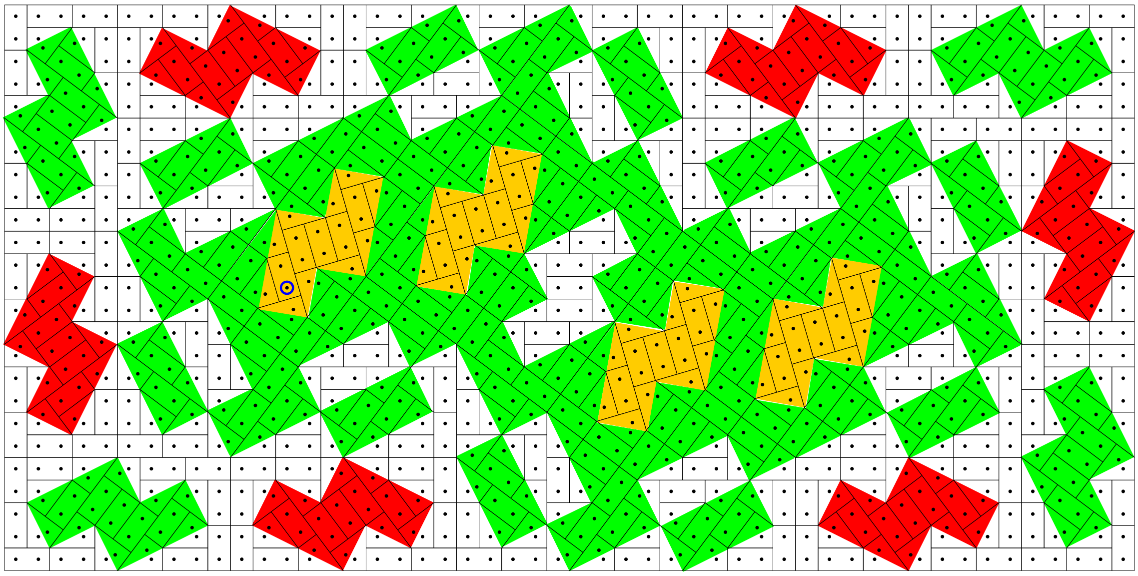


FIGURE 5. A patch from a kite domino tiling. The control points of the white tiles are contained in $\mathbb{Z}^2$. The control points in the other tiles are contained in rotated copies of $\mathbb{Z}^2$, where the common rotation centre is indicated in the figure. The possible rotations are described in Claim 1.

points. Let $\varLambda$ be one such set, e.g., the set $\varLambda$ of control points of PW as defined above. Define the orbit closure

$$\mathbb{X}(\varLambda) = \overline{\mathbb{R}^2 + \varLambda}^{\mathsf{LRT}}$$

in the local rubber topology (LRT) [4], which is compact. This topology is slightly different from the one introduced in [19]. But in the present case, both topologies yield the same hull and are equivalent on $\mathbb{X}(\varLambda)$.

The following result is well-known [19, 18].

Theorem 6. *The hull $\mathbb{X}(\varLambda)$ is $\mathbb{S}^1$-symmetric. Moreover, $(\mathbb{X}(\varLambda), \mathbb{R}^2)$ is a strictly ergodic dynamical system, i.e., it is uniquely ergodic and minimal. All elements of $\mathbb{X}(\varLambda)$ possess the same autocorrelation measure $\gamma = \gamma_{\varLambda}$ and the same diffraction measure $\widehat{\gamma}_{\varLambda}$. Both measures are $\mathbb{S}^1$-symmetric.* □

In this sense, speaking of the diffraction of the pinwheel tiling or its control points has a unique meaning. At this point, we know that

$$\widehat{\gamma} = (\mathrm{dens}(\varLambda))^2\, \delta_0 + (\widehat{\gamma})_{\mathsf{cont}} = \delta_0 + (\widehat{\gamma})_{\mathsf{cont}}$$

because a translation bounded circularly symmetric measure cannot contain Bragg peaks other than the trivial one at $k = 0$. That the intensity coefficient of δ_0 is $(\mathrm{dens}(\varLambda))^2$, hence 1 in our case, is a consequence of the equation

$$\widehat{\gamma}(\{0\}) = \lim_{r\to\infty} \frac{1}{\pi r^2}\, \gamma(B_r(0)) = \left(\lim_{r\to\infty} \frac{1}{\pi r^2}\, \delta_{\varLambda}(B_r(0)) \right)^2 = (\mathrm{dens}(\varLambda))^2 \,.$$

It can be proved by means of a Fourier concentration argument in connection with results from [16]; alternatively, see [12] for another approach and [18] for details on the case at hand.

It remains to determine the structure of $(\widehat{\gamma})_{\mathsf{cont}}$ more closely, in particular the separation into singular and absolutely continuous components.

4.3. **Results and observations.** The following claims and conjectures are stated for the particular tiling KD or for its set of control points $\varLambda$. Since mutual local derivability extends to entire hulls, we remain in the situation of Theorem 6. Proofs of the claims are either outlined here or will appear in [2]. Let us start with our main observation.

Observation 1. *The diffraction measure $\widehat{\gamma}$ of the pinwheel tiling is of the form*

$$\widehat{\gamma} = \delta_0 + (\widehat{\gamma})_{\mathsf{sc}} + (\widehat{\gamma})_{\mathsf{ac}}.$$

There is a countable set $\mathcal{D}^* \subset \mathbb{R}_{\geq 0}$ such that

$$(\widehat{\gamma})_{\mathsf{sc}} = \sum_{r \in \mathcal{D}^* \setminus \{0\}} I(r)\, \mu_r .$$

The set $\mathcal{D}^*$ seems to be locally finite, i.e., discrete and closed. Moreover, $(\widehat{\gamma})_{\mathsf{ac}}$ seems to be non-vanishing.

The set $\mathcal{D}^*$ is a subset of another set, $\mathcal{D} = \mathcal{D}_{\varLambda}$, which shows up in the determination of the autocorrelation and is described in more detail below.

Claim 1. *Let $\varLambda$ be the set of all control points of KD. Then, $\varLambda$ is a Delone subset of a countable union of rotated square lattices. More precisely, with $\theta = 2\arctan(\frac{1}{2})$,*

$$\varLambda \subset \bigcup_{k \in \mathbb{Z}} R_{k\theta}(\mathbb{Z}^2).$$

Using the geometry of the kite domino tiling, it is not difficult to establish this property. Figure 5 may serve as a visualisation on a small scale. This structure suggests that the diffraction of the pinwheel tiling might share some features with that of the powder diffraction of $\mathbb{Z}^2$, see the comment after the proof of Lemma 4. Since R_θ acts as multiplication by $\frac{1}{5}\left(\begin{smallmatrix} 3 & -4 \\ 4 & 3 \end{smallmatrix}\right)$, the next result is immediate. Note that R_θ is well known from the coincidence site lattice problem of the square lattice, compare [3], and has played a crucial rule in the explicit calculations in [18].

Claim 2. *Let $\varLambda$ be the set of all control points of KD. It satisfies*

$$\varLambda \subset \big\{ \big(\tfrac{n}{5^k}, \tfrac{m}{5^k}\big) : m, n \in \mathbb{Z},\ k \in \mathbb{N}_0 \big\},$$

and the distance set $\mathcal{D} = \mathcal{D}_{\varLambda} := \{|x-y| : x, y \in \varLambda\}$ is a subset of $\{\sqrt{\frac{p^2+q^2}{5^\ell}} : p, q, \ell \in \mathbb{N}_0\}$. It is the same set for all elements of $\mathbb{X}(\varLambda)$. $\square$

We believe that this subset relation is quite sharp, i.e., that the difference between the two sets is not too large, in the following sense.

Claim 3. *All values $r = \sqrt{p^2+q^2}$ with $p, q \in \mathbb{N}_0$ occur in $\mathcal{D}$. Moreover, for each $\ell \in \mathbb{N}_0$, there are infinitely many $p, q \in \mathbb{N}_0$ such that $\sqrt{\frac{p^2+q^2}{5^\ell}}$ is contained in $\mathcal{D}$.*

In fact, numerical computations suggest the following, stronger property.

Observation 2. *For each $\ell \in \mathbb{N}_0$, $\mathcal{D}$ contains all but finitely many values of the form $\sqrt{\frac{p^2+q^2}{5^\ell}}$.*

In the sequel, the absolute frequencies of distances are of interest, wherefore we define the *radial autocorrelation function*

$$\eta(r) = \lim_{R\to\infty} \frac{1}{\mathrm{vol}(B_R)} \sum_{\substack{x,y\in\varLambda\cap B_R(0)\\ |x-y|=r}} 1. \tag{12}$$

The limit exists due to unique ergodicity, see Theorem 6. This permits us to write the autocorrelation of $\varLambda$ — and hence of $\mathbb{X}(\varLambda)$ — as

$$\gamma = \sum_{r\in\mathcal{D}} \eta(r)\, \mu_r, \tag{13}$$

with μ_r as in Section 2. This follows from Theorem 6 together with Claim 3. Note that $\varLambda$ is repetitive [18] (defined up to congruence), so that all $\eta(r)$ in (13) are strictly positive, by the definition of $\mathcal{D}$ in Claim 2. Clearly, γ is both a positive and positive definite measure, and a tempered distribution on $\mathbb{R}^2$.

The following theorem holds in more generality than the context of this paper. In fact, it holds for all substitution tilings which are of *finite local complexity* (FLC) and *self-similar.* The latter means that $\lambda T_i = \bigcup_{T\in\sigma(T_i)} T$. Roughly speaking, this means that the support of the substitution of each prototile T_i is similar to T_i. Finite local complexity means that, for some $R > 0$, the tiling contains only finitely many local patches of diameter less than R, up to congruence. Note that FLC is frequently defined with respect to translations, whereas we define FLC here with respect to congruence, because of the nature of the pinwheel tiling. Both properties, FLC and self-similarity, hold for the majority of substitution tilings in the literature [10].

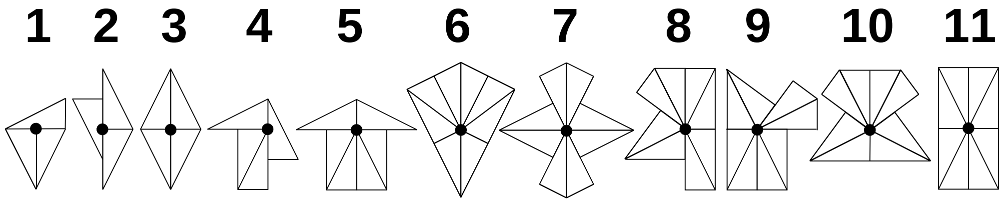
Theorem 7. *In any self-similar substitution tiling of finite local complexity (w.r.t. congruence) with substitution factor λ, all relative frequencies are contained in $\mathbb{Q}(\lambda^d)$. Moreover, the tiling can be scaled such that all absolute frequencies are contained in $\mathbb{Q}(\lambda^d)$ as well. In particular, if λ^d is an integer, and if the tiling is appropriately scaled, all relative and absolute frequencies are rational.*

For a proof, we refer to [2]. This theorem, applied to the pinwheel tiling or the kite domino tiling, yields that all frequencies are rational.

Claim 4. *All values of $r^2 \leq 5$ together with $\eta(r)$ are given in the following table. Values marked with an asterisk are numerically based conjectures, all other values are exact.*

r^2	0	$\frac{1}{5}$	1	$\frac{8}{5}$	$\frac{9}{5}$	$\frac{49}{25}$	2	$\frac{13}{5}$	$\frac{81}{25}$	$\frac{17}{5}$	4	$\frac{113}{25}$	5
$\eta(r)$	1	$\frac{5}{11}$	$\frac{439}{165}$	$\frac{1}{2}$	$\frac{67}{165}$	$\frac{4}{165}$	$\frac{7}{2}^*$	$\frac{142}{165}$	$\frac{4}{165}$	$\frac{10}{11}^*$	3^*	$\frac{8}{165}^*$	$\frac{73}{15}^*$

The value $\eta(0)$ is the absolute frequency of the control points. Since each triangle in the pinwheel tiling has area 1, we have $\eta(0) = 1$. The distance $|x - y| = 1/\sqrt{5}$ occurs precisely once within each kite. Kites have absolute frequency $\frac{5}{22}$, but the distance $|x - y|$ has to be counted twice in view of formula (12), hence $\eta(1/\sqrt{5}) = \frac{5}{11}$. The other exact values contained in the table can be established similarly, but require more sophistication. With some further effort, one can determine the *frequency module* of $\varLambda$, which is the $\mathbb{Z}$-span of the absolute



$\frac{1}{5}$ $\frac{6}{55}$ $\frac{1}{22}$ $\frac{6}{55}$ $\frac{1}{22}$ $\frac{2}{33}$ $\frac{5}{264}$ $\frac{17}{220}$ $\frac{3}{110}$ $\frac{2}{165}$ $\frac{1}{264}$

FIGURE 6. The 11 vertex stars of the pinwheel tiling (up to congruence) and their absolute frequencies (i.e., frequencies per unit area).

frequencies of all finite subsets of $\varLambda$, the latter standardised to having density 1 (which is our natural setting here).

Claim 5. *The frequency module of $\varLambda$, and hence of $\mathbb{X}(\varLambda)$, is $\mathcal{F} = \{\frac{m}{264 \cdot 5^{\ell}} \,|\, m \in \mathbb{Z},\ \ell \in \mathbb{N}_0\}$. In particular, it is countably, though not finitely generated.*

This result is derived from the absolute frequencies of the vertex stars in the pinwheel tiling, see Figure 6. These, in turn, can be derived from the frequencies of kites and darts in the kite domino tiling. Details will be given in [2].

We proceed by considering the Fourier transform in relation to the distance set $\mathcal{D}$. Since the Fourier transform is continuous on the space $\mathcal{S}'(\mathbb{R}^2)$ of tempered distributions, (13) becomes

$$\widehat{\gamma}_{\varLambda} = \widehat{\Big(\sum_{r\in\mathcal{D}} \eta(r)\,\mu_r\Big)} = \sum_{r\in\mathcal{D}} \eta(r)\,\widehat{\mu}_r, \tag{14}$$

where the sum is to be understood in the distribution sense. By Bochner's theorem, $\widehat{\gamma}_{\varLambda}$ is again a positive and positive definite measure, and the equation can be understood as a vague limit as well.

Let us apply Theorem 3 to the pinwheel pattern $\varLambda$. According to Claim 2, the distances in $\mathcal{D}$ arise from lattices of the form $\frac{1}{5^{\ell/2}}\mathbb{Z}^2$ with $\ell \in \mathbb{N}_0$. The corresponding dual lattices, which are relevant for the diffraction analysis, are $5^{\ell/2}\mathbb{Z}^2$, which have distance sets $5^{\ell/2}\mathcal{D}_{\square}$. Since $\mathbb{Z}^2$ contains a lattice congruent to $\sqrt{5}\mathbb{Z}^2$, it follows that $5^{\ell/2}\mathcal{D}_{\square} \subset \mathcal{D}_{\square}$ for all $\ell \in \mathbb{N}_0$, and that $\mathcal{D}_{\square}$ contains all distances that seem relevant from this point of view. At this stage, we have not found a compelling argument to exclude the possibility that certain subsets of $\varLambda$ contribute relevant distances in a coherent fashion, and thus – by unique ergodicity – further rings $I(r)\mu_r$ (with $r \notin \mathcal{D}_{\square}$) to $\widehat{\gamma}$. However, on the basis of Theorem 3, it is at least plausible that the set $\mathcal{D}^*$ is closely related with $\mathcal{D}_{\square}$, or even equal to it. In this case, $\widehat{\gamma}_{\varLambda}$ would show rings $I(r)\,\mu_r$ for $r \in \mathcal{D}_{\square}$ only. According to Claim 3, all distances have positive frequencies, so that this assumption would lead to

$$(\widehat{\gamma})_{\mathsf{sing}} = \sum_{r\in\mathcal{D}_{\square}} I(r)\,\mu_r = \delta_0 + (\widehat{\gamma})_{\mathsf{sc}} = \delta_0 + \sum_{0<r\in\mathcal{D}_{\square}} I(r)\,\mu_r$$

with $I(0) = 1$ and $I(r) > 0$ for all $r \in \mathcal{D}_{\square}$.

Let us continue our discussion on the basis of this hypothesis. If Observation 2 holds, then, for each $\ell \geq 0$, only finitely many distances of type $\sqrt{\frac{p^2+q^2}{5^{\ell}}}$ are missing, each one contributing

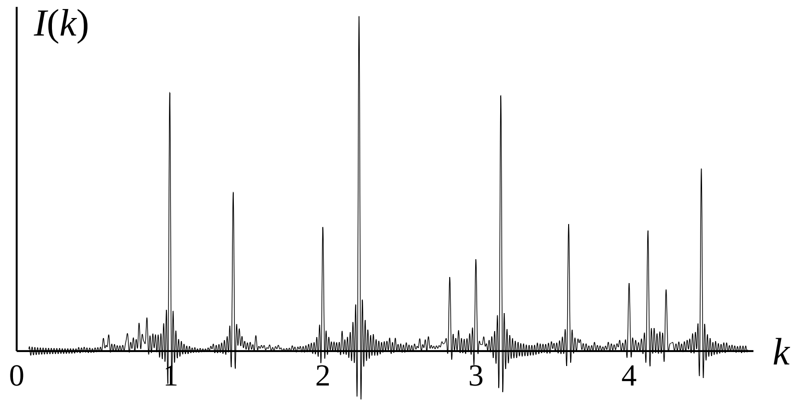


FIGURE 7. Numerical approximation of the radial intensity dependence of the pinwheel diffraction pattern. It is based on Equations (6) and (14), disregarding contributions to the central intensity. The radial autocorrelation coefficients $\eta(r)$ are estimated from a patch of radius of about 56 (thus effectively using the fifth iteration of the substitution σ). The vertical scale is arbitrary in the sense that it has no meaning without local averaging and integration.

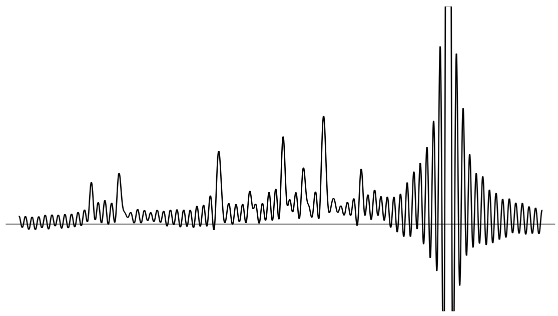


FIGURE 8. Detailed view of the shoulder to the left of the peak at $k = 1$, calculated from the sixth iteration of the substitution rule, with the large peak intensity truncated.

an absolutely continuous part to $\widehat{\gamma}$. Since $\widehat{\gamma}$ exists as a translation bounded measure, and since $\widehat{\gamma}_{\mathsf{sing}}$ is already covered by the results above, every additional contribution has to contribute to $\widehat{\gamma}_{\mathsf{ac}}$. This motivates the conjecture that $(\widehat{\gamma})_{\mathsf{ac}} \neq 0$.

Observation 1 is also supported by numerical computations of $\widehat{\gamma}$. A naive numerical analysis of a large finite portion of $\varLambda$ would yield no relevant result due to the nature of the pinwheel pattern. In particular, the number of orientations grows only logarithmically with the radius, while the number of tiles grows quadratically. The results above allow a more meaningful computation. In particular, by employing the $\mathbb{S}^1$-symmetry, the problem becomes one-dimensional, and by (7), the Fourier transform is expressed explicitly as a sum of weighted Bessel functions. As before, this approach disregards positivity of the intensity function, and the result displayed in Figure 7 shows strong oscillations with significant overshooting, similar in kind to the ones observed in Figure 3. No smoothing of any kind was used.

A comparison of the two diffraction images (Figures 3 versus 7) also supports our claim about the possible radii of pinwheel diffraction rings. One noticeable difference is the higher peak at $k = \sqrt{5}$, which is due to the pairs of points in $\varLambda$ with distance $1/\sqrt{5}$. The existence of positive shoulders in Figure 7 (such as that to the left of the first peak at $k = 1$, a blow-up of which is shown in Figure 8) is another significant difference to Figure 3, and is one of the reasons why we expect a non-vanishing radially continuous contribution, hence giving an absolutely continuous component to $\widehat{\gamma}$.

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