



Diffraction from visible lattice points and k th power free integers

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Abstract

We prove that the set of visible points of any lattice of dimension $n \geq 2$ has pure point diffraction spectrum, and we determine the diffraction spectrum explicitly. This settles previous speculation on the exact nature of the diffraction in this situation. Using similar methods we show the same result for the one-dimensional set of k th-power-free integers with $k \geq 2$. Of special interest is the fact that neither of these sets is a Delone set — each has holes of unbounded inradius. We provide a careful formulation of the mathematical ideas underlying the study of diffraction from infinite point sets. © 2000 Elsevier Science B.V. All rights reserved.

1. Introduction

It has long been known that the diffraction spectrum of a crystal consists of pure Bragg peaks only, being a pure point measure supported on the lattice dual to the lattice of periods. Until about 15 years ago it was tacitly believed that crystals were the only discrete point sets with this property. Now, however, we know that many quasicrystals have pure point diffraction spectra (though in a significantly different sense, since the locations of the peaks are no longer discrete). These quasicrystals are all Meyer sets, that is, sets S that are both uniformly discrete and relatively dense and whose difference sets $\Delta = S - S$ also have these properties. (For a discussion of Meyer sets, see [20]). There has consequently been a feeling that a perfectly diffracting discrete point set, if not precisely a Meyer set, must be closely related to a Meyer set. Indeed, the Meyer condition cannot possibly be strictly necessary since, as we shall see later, adding or removing a set of density zero does not alter the diffraction spectrum of a discrete

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point set, and one can clearly destroy the relative denseness of any uniformly discrete point set by removing a set of density zero.

In this paper we give some simple examples of perfectly diffractive discrete point sets that deviate much further from the Meyer properties than this; in fact we consider sets which, for arbitrarily large D , have a lattice of holes of inner diameter at least D . Such a set cannot differ from a Meyer set (or from a model set, which is a particular case of a Meyer set) only by a set of density zero. The sets comprising our examples are well known in number theory: they are the sets of visible (or primitive) points of a lattice in any dimension $n \geq 2$, see [1,14] and the front cover of [1] for a picture of the case $n = 2$, and the one-dimensional sets consisting of the k th-power-free integers for $k \geq 2$, see [14, Section 6.6].

As well as giving a rigorous derivation of the diffraction spectra that depends on explicitly calculating the autocorrelation of the point set, we precede it by a shorter derivation of the pure point parts of the spectra only, via the Fourier transform of the point set. This takes a similar line to previous attempts and uses a general result of A. Hof. It provides a quick, elegant way of calculating the discrete parts of the spectra which gives the correct results but does not have a full mathematical justification at present.

The rigorous approach is a response to the history of the problem for the visible lattice points, described in [3]. In particular, there is a clear disagreement between earlier results in [29,21] regarding the nature of the diffraction. This was partially resolved in favour of [21] by a calculation of the point part of the diffraction spectrum in terms of Dirichlet series and its comparison with a real optical experiment [3]. The older numerical calculations in [29], using the fast Fourier transform, suffer from an insufficient resolution and are misleading. In this article, we give the definitive description of the nature of the diffraction spectrum by making the previous formal calculation of the pure point part [21,3] rigorous and by proving that there is no continuous part.

The paper is organized as follows. We start by describing the results from number theory and related areas we need, then describe some basic properties of the set of visible points. Next, we discuss the background material of Fourier transforms and autocorrelations needed for diffraction spectra. This is first framed in the language of tempered distributions and then connected to measure theoretical considerations which are a basic part of the theory of diffraction. We then give the short intuitively motivated method of computing the pure point part of the diffraction spectrum, both for the visible points and the k th-power-free integers. The following two sections are devoted to an explicit calculation of the autocorrelation of the set of visible points, followed by a rigorous derivation of the diffraction spectrum. The ensuing section treats the set of k th-power-free numbers in the same way, followed by an extensive outlook and a summary.

Strictly speaking, neither the measure theoretical picture nor the intuitive approach to computing the diffraction are necessary for the logic of the paper, and they could be omitted by the reader whose primary concern is verifying the mathematical validity of

the results. But we would like to stress that the additional information provided in this article is needed to locate our results in the wider context of mathematical diffraction theory.

2. Tools from number theory

Here we set out some results we need from number theory and related areas.

2.1. Notation

We use the notation $(l, m) = \text{gcd}(l, m)$ to denote the greatest common divisor of two integers l and m . For integers d and x , $d|x$ means that d is a divisor of x . Summation conditions like ' $d|x$ ' are to be interpreted as meaning that d runs through positive divisors of x only (even when x is negative). The divisor function $\sigma(m)$ (defined for $m \in \mathbb{Z}^+$) counts the number of positive divisors of m , so $\sigma(m) = \sum_{d|m} 1$.

Also, we will frequently use the O-notation for error estimates. For example, we say that a function $f(r)$ is $O(1/r)$ if there is a constant c such that $|f(r)|$ is bounded by c/r for $r \geq 0$, see [1, Section 3.2] for details.

2.2. Lattices

A lattice in \mathbb{R}^n is a set Γ of the form

$$\Gamma = \mathbb{Z}\mathbf{b}_1 \oplus \cdots \oplus \mathbb{Z}\mathbf{b}_n, \quad (1)$$

where $\{\mathbf{b}_1, \dots, \mathbf{b}_n\}$ is a set of n linearly independent vectors called a *basis* of Γ . We define $\text{vol}(\Gamma)$ to be the volume of a fundamental region of the lattice, e.g. of $\{t_1\mathbf{b}_1 + \cdots + t_n\mathbf{b}_n \mid 0 \leq t_1, \dots, t_n < 1\}$. Consequently, $\text{vol}(\Gamma)$ can be calculated as $\text{vol}(\Gamma) = |\det(\mathbf{b}_1, \dots, \mathbf{b}_n)|$ which turns out to be independent of the basis chosen. Every lattice is uniformly discrete and relatively dense in \mathbb{R}^n and is a subgroup of \mathbb{R}^n under vector addition.

Proposition 1. *Let Γ be a lattice and \mathbf{a} an arbitrary vector (not necessarily in Γ). Let $N(R)$ be the number of points \mathbf{x} in $\Gamma + \mathbf{a}$ with $|\mathbf{x}| < R$. Then there are constants c_1 and c_2 , depending only on Γ , such that, for all $R > 0$,*

$$|N(R)\text{vol}(\Gamma) - v_n R^n| \leq c_1 R^{n-1} + c_2, \quad (2)$$

where v_n is the volume of the unit ball in \mathbb{R}^n , i.e. $v_n = \pi^{n/2}/\Gamma(1 + n/2)$.

Proof. The translates of the fundamental region of Γ by vectors in $\Gamma + \mathbf{a}$ tile \mathbb{R}^n . Let \mathcal{U} be the total volume of those translates that meet the open ball $B_R(\mathbf{0})$ and v the total volume of those translates that lie entirely inside this ball. Then the volume $v_n R^n$ of the ball and the number $N(R)\text{vol}(\Gamma)$ are both bounded above by \mathcal{U} and below by v .

So their difference is at most $\mathcal{V} - v$, which is the total volume of the translates of the fundamental region that meet the boundary of the ball. If D is the diameter¹ of the fundamental region, then this volume is at most $v_n(R + D)^n - v_n(R - D)^n \leq 2^n v_n D R^{n-1}$, when $R \geq D$, and at most $v_n(R + D)^n < 2^n v_n D^n$, when $R < D$. The second of these estimates is obvious, while the first (when $R \geq D$) follows from

$$\begin{aligned} (R + D)^n - (R - D)^n &= \sum_{m=0}^n \binom{n}{m} R^{n-m} (D^m - (-D)^m) \\ &\leq 2 \sum_{m \text{ odd}} \binom{n}{m} R^{n-1} D \\ &= 2DR^{n-1} \sum_{m \text{ odd}} \binom{n}{m} = 2^n DR^{n-1}. \end{aligned} \tag{3}$$

This gives the result with $c_1 = 2^n v_n D$ and $c_2 = 2^n v_n D^n$. \square

If Γ is a lattice and r is a nonzero real number then $r\Gamma$ is also a lattice (a basis of $r\Gamma$ is $\{r\mathbf{b}_1, \dots, r\mathbf{b}_n\}$). When r is an integer $r\Gamma \subseteq \Gamma$ and $r\Gamma$ is a sublattice (and a subgroup) of Γ , of index r^n . For a nonzero integer m and two points \mathbf{a} and \mathbf{b} in Γ we write $\mathbf{a} \equiv \mathbf{b} \pmod{m\Gamma}$ to mean that $\mathbf{a} - \mathbf{b} \in m\Gamma$. With this notation we have the following Chinese Remainder Theorem for a lattice Γ .

Proposition 2. *Let Γ be a lattice and $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_r \in \Gamma$. If $m_1, m_2, \dots, m_r \in \mathbb{Z}^+$ are chosen so that $(m_j, m_k) = 1$, for $1 \leq j < k \leq r$, then there is a point $\mathbf{a} \in \Gamma$ such that the solutions of the simultaneous congruences*

$$\mathbf{x} \equiv \mathbf{a}_1 \pmod{m_1\Gamma}, \dots, \mathbf{x} \equiv \mathbf{a}_r \pmod{m_r\Gamma} \tag{4}$$

are precisely the points $\mathbf{x} \in \Gamma$ with

$$\mathbf{x} \equiv \mathbf{a} \pmod{(m_1 \cdot m_2 \cdot \dots \cdot m_r)\Gamma}. \tag{5}$$

Proof. This follows by applying the Chinese Remainder Theorem for integers [14, Theorem 2.7.1] to each coordinate with respect to a basis of Γ . \square

We define the *content* of a nonzero lattice point \mathbf{x} in a lattice Γ by

$$\text{cont}(\mathbf{x}) := \max\{l \mid \mathbf{x} \in l\Gamma\}. \tag{6}$$

If \mathbf{x} is expressed in terms of a basis of Γ , $\mathbf{x} = \sum x_j \mathbf{b}_j$, then $\text{cont}(\mathbf{x}) = \text{gcd}(x_1, \dots, x_n)$ (which is therefore independent of the particular basis chosen). For consistency and convenience, we define $\text{cont}(\mathbf{0}) = \infty$. For $m \in \mathbb{Z}^+$ and $\mathbf{x} \in \Gamma$, we have

$$\text{cont}(m\mathbf{x}) = m \cdot \text{cont}(\mathbf{x}). \tag{7}$$

¹The diameter of a bounded set $S \subset \mathbb{R}^n$ is the supremum of all distances between points of S .

It is clear from (6) that for $\mathbf{x} \in \Gamma \setminus \{\mathbf{0}\}$

$$\text{cont}(\mathbf{x}) \leq \frac{|\mathbf{x}|}{L(\Gamma)}, \tag{8}$$

where $|\mathbf{x}|$ is the Euclidean length of \mathbf{x} and $L(\Gamma)$ is the length of the shortest nonzero vector in Γ .

The set $V = V(\Gamma)$ of *visible points* of a lattice Γ (also known as the *primitive points* of Γ) is

$$V := \{\mathbf{x} \in \Gamma \mid \text{cont}(\mathbf{x}) = 1\}. \tag{9}$$

In terms of a lattice basis, V consists of all points whose coordinates have no common divisor. These are precisely the lattice points that are visible from the origin, in the sense that the line segment joining them to the origin contains no other lattice point. When $n = 1$, V consists of two points, equidistant from 0, but otherwise V is infinite and, indeed, contains more than half the lattice points, as we shall see. For $m \in \mathbb{Z}^+$ we have

$$mV = \{\mathbf{x} \in \Gamma \mid \text{cont}(\mathbf{x}) = m\}. \tag{10}$$

2.3. Density

Let S be a uniformly discrete set of points in \mathbb{R}^n (i.e. there is a $c > 0$ so that $\mathbf{x}, \mathbf{y} \in S$ with $\mathbf{x} \neq \mathbf{y}$ implies $|\mathbf{x} - \mathbf{y}| \geq c$). We say S has *natural density* $\mathcal{D} = \text{dens}(S)$ if

$$\mathcal{D}_R = \mathcal{D}_R(S) := \frac{|\{\mathbf{x} \in S \mid |\mathbf{x}| < R\}|}{v_n R^n} \rightarrow \mathcal{D} \tag{11}$$

as $R \rightarrow \infty$. The expression $|\mathcal{D} - \mathcal{D}_R|$ (a function of R) is called the *error term* for the natural density. For example, by Proposition 1, $\mathcal{D} = \text{dens}(\Gamma)$ exists for every lattice Γ and is equal to $1/\text{vol}(\Gamma)$ (with error term $O(1/R)$).

If $\text{dens}(S)$ exists and if T is an orthogonal transformation then $\text{dens}(T(S)) = \text{dens}(S)$, but it is a failing of the natural density that it is not always true that $\text{dens}(T(S)) = \text{dens}(S)/|\det(T)|$ when T is a general affine transformation, see Appendix A.

When we use the word ‘density’ from now on we shall mean natural density.

2.4. Power-free numbers

For an integer exponent $k \geq 1$ the set $F = F_k$ of *kth-power-free integers* is

$$F := \{n \in \mathbb{Z} \mid n \text{ is not divisible by } d^k \text{ for any integer } d > 1\}. \tag{12}$$

An equivalent characterization of the numbers $n \in F$ is that in their prime power factorization $n = \pm p_1^{a_1} p_2^{a_2} \cdots p_r^{a_r}$ every exponent a_j is less than k . In close analogy with V , the case $k = 1$ is trivial, F_1 consisting of just the two numbers ± 1 , but for $k \geq 2$, F_k is infinite and contains more than half the integers. These numbers have been studied for a long time, see [22,19] for two sources relevant in our context.

2.5. Inclusion–exclusion

The Möbius function $\mu(m)$ is defined for $m \in \mathbb{Z}^+$ by

$$\mu(m) := \begin{cases} 1 & \text{when } m = 1, \\ (-1)^r & \text{when } m \text{ is a product of } r \text{ distinct primes,} \\ 0 & \text{when } m \text{ is divisible by the square of a prime.} \end{cases} \quad (13)$$

It is multiplicative in the sense that $\mu(lm) = \mu(l)\mu(m)$ when $(l, m) = 1$ (and clearly $\mu(lm) = 0$ when $(l, m) \neq 1$).

A number of inversion formulæ and variants of the inclusion–exclusion principle can be expressed in terms of this function. The result we need in this paper is

$$\sum_{d|m} \mu(d) = \begin{cases} 1 & \text{if } m = 1, \\ 0 & \text{if } m > 1, \end{cases} \quad (14)$$

see [14, Theorem 6.3.1]. For a point \mathbf{x} in a lattice Γ this shows that

$$\chi_V(\mathbf{x}) := \sum_{d|\text{cont}(\mathbf{x})} \mu(d) \quad (15)$$

is the characteristic function of the visible points V of Γ (except that it is undefined when $\mathbf{x} = \mathbf{0}$).

Similarly, since $d^k|x$ if and only if d divides the largest integer whose k th-power divides x ,

$$\chi_F(x) := \sum_{d^k|x} \mu(d) \quad (16)$$

is the characteristic function of the k th-power-free integers (except for being undefined when $x = 0$).

2.6. Dirichlet series

The well-known Riemann zeta-function (see, for example, [1, Chapter 12] or [14, Section 9.2]) is defined for complex numbers s with $\text{Re}(s) > 1$ by

$$\zeta(s) := \sum_{m=1}^{\infty} \frac{1}{m^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}, \quad (17)$$

where the sum is called a *Dirichlet series* and the product (in which p runs through all positive prime numbers) is called an *Euler product*. The sum and product are absolutely convergent for s in the half-plane $\text{Re}(s) > 1$, but $\zeta(s)$ can be meromorphically continued to the whole of \mathbb{C} , for example $\zeta(0) = -\frac{1}{2}$. The only singularity of $\zeta(s)$ is a simple pole at $s = 1$ with residue 1. Using the Euler product, we see that the Dirichlet series of $1/\zeta(s)$ is given by

$$\frac{1}{\zeta(s)} = \prod_p \left(1 - \frac{1}{p^s}\right) = \sum_{m=1}^{\infty} \frac{\mu(m)}{m^s}. \quad (18)$$

This function has infinitely many poles (all in the half-plane $\text{Re}(s) < 1$). Its value at 1 is 0 and its value at 0 is -2 .

Another Dirichlet series we shall encounter is

$$\zeta(s) := \sum_{m=1}^{\infty} \frac{\mu(m)\sigma(m)}{m^s} = \prod_p \left(1 - \frac{2}{p^s}\right). \tag{19}$$

Again, both the Dirichlet series and Euler product are absolutely convergent in the half-plane $\text{Re}(s) > 1$. It can also be seen from the Euler product that $\zeta(1) = 0$.

3. Visible points of a lattice

Here we summarize some elementary and well-known properties of the set of visible points V of a lattice Γ , together with complete proofs.

Since Γ is a free Abelian group of rank n , its automorphism group, $\text{Aut}(\Gamma)$, is isomorphic to the matrix group $\text{GL}(n, \mathbb{Z})$. Explicit isomorphisms can be found by taking coordinates with respect to any lattice basis.

Proposition 3. *The orbits of the action of $\text{GL}(n, \mathbb{Z})$ on Γ are the sets mV , $m \in \mathbb{N}_0$. In particular, $\text{GL}(n, \mathbb{Z})$ acts transitively on V .*

Proof. Since the elements of $\text{GL}(n, \mathbb{Z})$ cannot decrease content and are invertible, they preserve content. Hence each set mV is invariant under $\text{GL}(n, \mathbb{Z})$. The transitivity of $\text{GL}(n, \mathbb{Z})$ on V can be seen from the facts that every visible point belongs to some basis of Γ [10, Section 3, Theorem 5] and that any two bases of Γ are related by a transformation in $\text{GL}(n, \mathbb{Z})$. For $m \in \mathbb{Z}^+$ the transitivity of $\text{GL}(n, \mathbb{Z})$ on mV follows from its transitivity on V . Transitivity on the singleton orbit $0 \cdot V = \{\mathbf{0}\}$ is trivial. \square

Proposition 4. *V is uniformly discrete, but has arbitrarily large holes. Moreover, for any $r > 0$, there is a set of holes in V of inradius at least r whose centres have positive density.*

Proof. The uniform discreteness is trivial, as V is a subset of a lattice. Now, let $C = \{\mathbf{a}_1, \dots, \mathbf{a}_s\}$ be any finite configuration of points in Γ (e.g. all points in a ball or a cube). Choose s integer moduli m_1, \dots, m_s that are > 1 and coprime in pairs (for example, they could be the first s primes). By Proposition 2 there is a point $\mathbf{a} \in \Gamma$ with

$$\mathbf{a} \equiv -\mathbf{a}_1 \pmod{m_1\Gamma}, \dots, \mathbf{a} \equiv -\mathbf{a}_s \pmod{m_s\Gamma}. \tag{20}$$

Now for any $\mathbf{x} \equiv \mathbf{a} \pmod{m_1m_2 \dots m_s\Gamma}$ the configuration $C + \mathbf{x} = \{\mathbf{a}_1 + \mathbf{x}, \dots, \mathbf{a}_s + \mathbf{x}\}$ is congruent, in the geometric sense, to C but no point in $C + \mathbf{x}$ is visible, since $\mathbf{a}_j + \mathbf{x} \in m_j\Gamma$. The points \mathbf{x} have density $\text{dens}(\Gamma)/(m_1m_2 \dots m_s) > 0$. \square

For $n = 2$, and with the density of holes not mentioned, this is Theorem 5.29 of [1]. We note that the hole nearest the origin provided by this argument can be expected to be at a distance of the order s^s and that the density guaranteed for holes of inradius r is of the order $r^{-n^2 r^n}$, so large holes, while having positive density, are probably extremely sparse.

This proposition shows that V , though uniformly discrete, is not relatively dense, and hence not a Delone set. Consequently it is not a Meyer set either. (Recall that A is a Meyer set if and only if both A and $A - A := \{x - y \mid x, y \in A\}$ are Delone sets [17].) Also, V cannot be transformed into a Delone set by adding a set of zero density. However, we do have:

Proposition 5. *If $n \geq 2$ then $V - V = \Gamma$.*

Proof. Clearly, $V - V \subseteq \Gamma$. Now let $\mathbf{x} = \sum_{j=1}^n x_j \mathbf{b}_j \in \Gamma$, where $n \geq 2$. Then, $(x_1, x_2, \dots, x_n) = (x_1 + 1, 1, x_3, \dots, x_n) - (1, 1 - x_2, 0, \dots, 0)$, and \mathbf{x} is the difference of two visible points. \square

The existence of arbitrarily large holes also implies that the set of visible points cannot have a uniform density (not, at least, when its density is positive in some sense, as is the case for $n \geq 2$). It does have a natural density, however:

Proposition 6. *The visible points V of a lattice $\Gamma \in \mathbb{R}^n$ have a natural density given by*

$$\text{dens}(V) = \frac{\text{dens}(\Gamma)}{\zeta(n)}, \tag{21}$$

with error term $O(1/R)$ when $n \neq 2$ and $O(\log R/R)$ when $n = 2$.

This is a standard example of the use of Möbius inversion given (at least for the case $\Gamma = \mathbb{Z}^2$) in most introductory number theory books (for example, [14, Theorem 6.6.3; 1, Theorem 3.9]). In these particular references the averages are taken over triangles and squares, respectively, instead of balls. Indeed the density is independent of the shape of the region averaged over. We say more about this in Appendix A.

Proof. The proposition is trivially true for $n = 1$, when the pole of $\zeta(s)$ at 1 gives a density of 0, so we assume from now on that $n \geq 2$.

The density of V , if it exists, is the limit as $R \rightarrow \infty$ of

$$\frac{1}{v_n R^n} \sum_{\substack{|\mathbf{x}| < R \\ \mathbf{x} \in V}} 1, \tag{22}$$

which by (15) is

$$\frac{1}{v_n R^n} \sum_{\substack{\mathbf{x} \in \Gamma \setminus \{\mathbf{0}\} \\ |\mathbf{x}| < R}} \sum_{m|\text{cont}(\mathbf{x})} \mu(m) = \frac{1}{v_n R^n} \sum_{1 \leq m < cR} \mu(m) \sum_{\substack{\mathbf{x} \in m\Gamma \setminus \{\mathbf{0}\} \\ |\mathbf{x}| < R}} 1, \tag{23}$$

where $c = 1/L(\Gamma)$ (using (8)). The inner sum is equal to the number of nonzero points $\mathbf{y} \in \Gamma$ with $|\mathbf{y}| < R/m$, which by Proposition 1 is

$$\frac{v_n}{\text{vol}(\Gamma)} \left(\frac{R}{m}\right)^n + O\left(\left(\frac{R}{m}\right)^{n-1}\right) + O(1). \tag{24}$$

Substituting this into the right-hand side of (23) gives

$$\text{dens}(\Gamma) \sum_{1 \leq m < cR} \frac{\mu(m)}{m^n} + O\left(\frac{1}{R} \sum_{1 \leq m < cR} \frac{1}{m^{n-1}}\right) + O\left(\frac{1}{R^{n-1}}\right) \tag{25}$$

which tends to $\text{dens}(\Gamma)/\zeta(n)$ as $R \rightarrow \infty$ when $n \geq 2$ by (18). The total error is $O(1/R^{n-1})$, from the last term and the tail of the sum in the main term, and $O(1/R)$ (or $O(\log R/R)$ when $n = 2$ and the series diverges logarithmically), from the middle term. \square

Calculations of densities by Möbius inversion form the core of this paper. This is the first of many.

4. Diffraction spectra

In this section we assemble the facts we need about distributions, Fourier transforms and diffraction spectra. The mathematics underlying diffraction is quite subtle and needs to be spelt out carefully. Although the discussion in this section does not contain much that is new, it is nonetheless difficult to extract it all from any convenient source. We shall use a formulation based upon tempered distributions. For an essentially parallel approach which starts with measures, we refer to [12]. We shall link the two approaches later in this section.

4.1. Autocorrelations

In dealing with diffraction, and therefore Fourier transforms, it is appropriate to use tempered distributions, whose test space \mathcal{S} consists of the Schwartz functions (also known as ‘rapidly decreasing functions’). We refer to [30,25] for this and the details on the standard topology which is used to describe convergence in \mathcal{S} . A *tempered distribution* T is a continuous (in the sense of this topology) linear functional on \mathcal{S} . The space of tempered distributions is denoted by \mathcal{S}' and is equipped with the weak*-topology. A simple example is δ_x , *Dirac’s delta-distribution*² at the point x ,

²Nowadays, it is usually called Dirac’s point measure for reasons that will become clear shortly.

defined by $(\delta_x, \psi) := \psi(\mathbf{x})$ for all $\psi \in \mathcal{S}$. We prefer this notation to $\delta_x(\psi)$ because it emphasizes the duality between \mathcal{S}' and \mathcal{S} .

If S is a uniformly discrete subset of \mathbb{R}^n , we call

$$\omega_S := \sum_{\mathbf{x} \in S} \delta_{\mathbf{x}} \quad (26)$$

its *Dirac comb*. It is also a tempered distribution, and in fact the sum (26) is convergent (with any ordering) in the weak*-topology.

To describe the diffraction from a Dirac comb $\omega = \omega_S$ we need its *natural autocorrelation distribution* (also called its generalized Patterson function) defined by

$$\gamma_\omega := \lim_{R \rightarrow \infty} \frac{1}{v_n R^n} \sum_{\mathbf{x}, \mathbf{y} \in S_R} \delta_{\mathbf{x} - \mathbf{y}}, \quad (27)$$

where $S_R = S \cap B_R(\mathbf{0})$ and $B_R(\mathbf{0})$ is the ball of radius R centre $\mathbf{0}$. We shall simply call γ_ω the ‘autocorrelation’ of S from now on. The existence of this limit in the weak*-topology is a prerequisite for the diffraction spectrum to be well defined. (The word ‘natural’ refers to the use of the expanding ball $B_R(\mathbf{0})$ in the averaging process. Replacing it by an expanding region of some other shape might lead to a different limit.) It is clear from the definition that enlarging or diminishing S by a set of density 0 does not change its autocorrelation γ_ω . In particular, adding or removing any finite number of points does not change γ_ω , as for natural density.

We say that S has *finite local complexity* if $\Delta = S - S$ is discrete and closed in \mathbb{R}^n (as is clearly the case for all sets whose diffraction spectra we seek in this paper). Such an S is uniformly discrete because $\mathbf{0} \in \Delta$ is isolated. The existence of limit (27) in the weak*-topology is now controlled by the following result.

Lemma 1. *Let S be a set of finite local complexity and $\omega = \omega_S$ its Dirac comb. Then S has a natural autocorrelation γ_ω if and only if the coefficients $w(\mathbf{a})$*

$$w(\mathbf{a}) := \lim_{R \rightarrow \infty} \frac{1}{v_n R^n} \sum_{\substack{|\mathbf{x}|, |\mathbf{x} - \mathbf{a}| < R \\ \mathbf{x}, \mathbf{x} - \mathbf{a} \in S}} 1 \quad (28)$$

exist, i.e. the right-hand side is convergent for all $\mathbf{a} \in \Delta$. In this case, $w(\mathbf{a}) \geq 0$ for all $\mathbf{a} \in \Delta$ and γ_ω is the tempered distribution of positive type³ given by the weak*-convergent sum

$$\gamma_\omega = \sum_{\mathbf{a} \in \Delta} w(\mathbf{a}) \delta_{\mathbf{a}}. \quad (29)$$

Proof. The existence of γ_ω clearly implies the existence of $w(\mathbf{a})$ for all $\mathbf{a} \in \Delta$ because Δ is discrete by assumption and the Schwartz space \mathcal{S} contains all C^∞ -functions of compact support, whence we can focus on any individual \mathbf{a} .

³ See the next section for a definition.

Conversely, assume that the $w(\mathbf{a})$ exist (they are then clearly ≥ 0). Since Δ is closed and discrete, its intersection with any compact subset of \mathbb{R}^n contains only finitely many points. Consequently, the $w(\mathbf{a})$ are locally summable and the right-hand side of (29) defines a distribution over the space \mathcal{D} of all C^∞ -functions of compact support. We have to show that it is actually also a tempered distribution. This follows from the translation boundedness⁴ of ω which is then inherited by γ_ω , see [12, Proposition 2.2]. Finally, γ_ω can also be written as a certain volume-normalized convolution (see below) which implies that it is a distribution of positive type. \square

4.2. Fourier transforms

The Fourier transform \hat{T} of a tempered distribution $T \in \mathcal{S}'$ is defined by $(\hat{T}, \psi) := (T, \hat{\psi})$, where we use the definition

$$\hat{\psi}(\mathbf{y}) := \int_{\mathbb{R}^n} e^{-2\pi i \mathbf{y} \cdot \mathbf{x}} \psi(\mathbf{x}) \, d\mathbf{x} \tag{30}$$

for the Fourier transform of functions $\psi \in \mathcal{S}$. The Fourier transform maps the space \mathcal{S} onto itself and is continuous on \mathcal{S} in the standard topology for Schwartz functions [25, Theorem 7.7], hence it maps \mathcal{S}' onto itself and is continuous on \mathcal{S}' in the weak*-topology [25, Theorem 7.15].

As special cases, we mention $\hat{\delta}_0 = 1$ and the well-known *Poisson summation formula* for lattice Dirac combs

$$\hat{\omega}_\Gamma = \text{dens}(\Gamma) \cdot \omega_{\Gamma^*} \tag{31}$$

where Γ^* is the dual or reciprocal lattice defined by

$$\Gamma^* := \{\mathbf{y} \mid \mathbf{y} \cdot \mathbf{x} \in \mathbb{Z} \text{ for all } \mathbf{x} \in \Gamma\}. \tag{32}$$

(Eq. (31) can easily be derived from Poisson’s summation formula for Schwartz functions [30, p. 254].)

For a set S of finite local complexity with autocorrelation γ_ω , its *diffraction pattern* (also called its *diffraction distribution* or *diffraction spectrum*) is the Fourier transform $\hat{\gamma}_\omega$. In view of the remarks above, $\hat{\gamma}_\omega$ is a tempered distribution. It is also a positive measure, as we shall see.

The autocorrelation of a lattice Γ , for example, is supported on Γ itself (since $\Delta = \Gamma - \Gamma = \Gamma$) and each peak has equal amplitude $\text{dens}(\Gamma)$. So the autocorrelation is $\gamma_\omega = \text{dens}(\Gamma)\omega_\Gamma$ and the corresponding diffraction spectrum is $\hat{\gamma}_\omega = \text{dens}(\Gamma)^2\omega_{\Gamma^*}$, a constant multiple of the Fourier transform of ω_Γ itself. However, as we shall see, the Fourier transform of a general point set (even of finite local complexity) does not describe its diffraction in such a simple way.

⁴ We will explain this below in the context of measures.

4.3. Pure point distributions

Our principal concern is with showing that the visible points and k th-power-free points have a pure point spectrum. In this section we consider a special class of point measures which we will use in the sequel. We already borrow from the terminology of measures here, although we will establish the precise connection only in the next section.

Consider an arbitrary complex point measure. It can be expressed in the form

$$\nu = \sum_{\mathbf{x} \in S} w(\mathbf{x}) \delta_{\mathbf{x}}, \quad (33)$$

where the point set S is countable, but not necessarily uniformly discrete, and the coefficients or *weights* $w(\mathbf{x}) \in \mathbb{C}$ are not necessarily constant. Note that the weights may be complex numbers. Let us assume in addition that the measure is translation bounded. This can be expressed as the condition that for every compact set $K \subset \mathbb{R}^n$ the sum

$$\sum_{\mathbf{x} \in S \cap (K+\mathbf{a})} |w(\mathbf{x})| \quad (34)$$

is convergent and bounded uniformly in \mathbf{a} . We denote the space of all translation bounded point measures by \mathcal{T} . All these measures are tempered, and we identify ν with T_ν , the corresponding tempered distribution.

As a subset of \mathcal{S}' , \mathcal{T} is not closed in the weak*-topology. For example, the sequence of pure point distributions

$$\{j^{-n} \omega_{\mathbb{Z}^n|j}\} \quad (35)$$

tends to the constant function 1 as $j \rightarrow \infty$. (For a test function ψ the numbers $j^{-n} \omega_{\mathbb{Z}^n|j}(\psi)$ are approximating sums to the integral⁵ of ψ .) A similar argument shows that every bounded continuous function is a limit of pure point distributions, compare the more detailed discussion in [24, Section IV.5]. Unfortunately, as this example shows, the weak*-limit of such a sequence is not, in general, the same as its pointwise limit.

However, taking pointwise limits in \mathcal{T} is justifiable under certain circumstances, and fortunately these apply in the cases of interest to us here. We introduce a ‘locally defined’ norm on \mathcal{T} by

$$\| \nu \|_{\text{loc}} := \sup_K \int_K d|\nu| = \sup_K \sum_{\mathbf{x} \in S \cap K} |w(\mathbf{x})|, \quad (36)$$

where the supremum is taken over all compact sets K of diameter < 1 . This norm defines a topology on \mathcal{T} stronger than the weak*-topology and it provides a simultaneous “ M -test” for pointwise and weak*-convergence of infinite sums of translation bounded point measures:

⁵ Seen as a sequence of measures, (35) weak*-converges to Lebesgue measure.

Lemma 2. *If $v_j \in \mathcal{T}$ for $j \in \mathbb{Z}^+$ and $\sum_{j=1}^\infty \|v_j\|_{\text{loc}}$ is convergent then $\sum_{j=1}^\infty v_j$ is pointwise and weak*-convergent to the same sum $v \in \mathcal{T}$.*

Proof. Let $v_j = \sum_{x \in S_j} w_j(\mathbf{x})\delta_x$ and choose a fixed covering of $\{K_m\}_{m \in \mathbb{Z}^+}$ of \mathbb{R}^n by compact sets of diameter < 1 . For any $\psi \in \mathcal{S}$ we have

$$\begin{aligned} |(v_j, \psi)| &= \left| \sum_{x \in S_j} w_j(\mathbf{x})\psi(\mathbf{x}) \right| \leq \sum_{m=1}^\infty \sum_{x \in S_j \cap K_m} |w_j(\mathbf{x})\psi(\mathbf{x})| \\ &\leq \|v_j\|_{\text{loc}} \sum_{m=1}^\infty \|\psi_{K_m}\| = C_\psi \cdot \|v_j\|_{\text{loc}}, \end{aligned} \tag{37}$$

where ψ_{K_m} is the restriction of ψ to K_m and $C_\psi < \infty$ is a constant that depends only on ψ and the covering chosen. Hence $\sum_{j=1}^\infty (v_j, \psi)$ is absolutely convergent (by comparison with $\sum \|v_j\|_{\text{loc}}$) and so $\sum v_j$ is weak*-convergent to a distribution v .

Also,

$$(v, \psi) = \sum_{j=1}^\infty (v_j, \psi) = \sum_{j=1}^\infty \sum_{x \in S_j} w_j(\mathbf{x})\psi(\mathbf{x}) = \sum_{x \in \bigcup S_j} \sum_{j=1}^\infty w_j(\mathbf{x})\psi(\mathbf{x}), \tag{38}$$

the reversal of the order of summation (with $w_j(\mathbf{x}) := 0$ whenever $\mathbf{x} \notin S_j$) being justified by the fact that the double sum is absolutely convergent, in view of (37).

Hence,

$$v = \sum_{x \in \bigcup S_j} \sum_{j=1}^\infty w_j(\mathbf{x})\delta_x \tag{39}$$

is the pointwise sum of the v_j 's.

Finally, if $K \subseteq \mathbb{R}^n$ is any compact set with diameter < 1 and we write $S := \bigcup S_j$ and $w(\mathbf{x}) := \sum_{j=1}^\infty w_j(\mathbf{x})$ then

$$\sum_{x \in S \cap (K+a)} |w(\mathbf{x})| \leq \sum_{j=1}^\infty \sum_{x \in S_j \cap (K+a)} |w_j(\mathbf{x})| \leq \sum_{j=1}^\infty \|v_j\|_{\text{loc}}. \tag{40}$$

Hence v is translation bounded, and therefore tempered. \square

Note that if μ_j is the distribution in (35) then $\mu_{j+1} - \mu_j$ is translation bounded but

$$\|\mu_{j+1} - \mu_j\|_{\text{loc}} \geq \frac{v_n}{2^{n-1}} - \frac{1}{j(j+1)}, \tag{41}$$

where v_n is the volume of the n -dimensional unit ball. (The supports of μ_j and μ_{j+1} intersect in the integer points only and there is almost no cancellation in calculating the norm.) So the norms of the differences are bounded below by a positive constant for large j and their sum diverges to infinity, thus failing to satisfy the hypothesis of the lemma. (An easier calculation along the same lines is $\|\mu_{2^{k+1}} - \mu_{2^k}\| \geq v_n/2^n$.)

4.4. Distributions and measures

The diffraction pattern $\hat{\gamma}_\omega$ is a tempered distribution. However, it is also a positive measure. This remarkable fact is indispensable for the general theory of diffraction, making available to it a vast array of concepts and tools. For example, it makes it immediately evident that the diffraction pattern may be viewed as having a pure point part and a continuous part, a fact of considerable physical significance.

The next two subsections sketch out this distribution theory — measure theory connection in the context of diffraction. The proofs of the main theorems of this paper in no way depend on this background material, which can therefore be ignored as far as verifying the results is concerned. Nevertheless, it is desirable to realize the natural connection to measure theory, both to see our results in their proper setting and because it is this picture that has a generalization to the diffraction theory of translation bounded measures on locally compact Abelian groups which is an appropriate setting for more general questions, compare [11,2].

A distribution T is *positive* if for all positive test functions ψ , $(T, \psi) \geq 0$. A distribution T is of *positive type* or is *positive definite* if for all test functions ψ , $(T, \psi * \psi^*) \geq 0$, where $\psi^*(x) := \overline{\psi(-x)}$. These two concepts are related by the Bochner–Schwarz theorem (see [30, Theorem VII.XVIII] or [24, Theorem IX.10]) which asserts that a tempered distribution is positive if and only if it is the Fourier transform of a tempered distribution of positive type.

Let \mathcal{C} denote the space of complex-valued continuous functions of compact support on \mathbb{R}^n and let $\|\cdot\|$ denote the supremum norm on \mathcal{C} . A (complex) *measure* ν on \mathbb{R}^n is defined as a linear functional on \mathcal{C} such that for every compact set $K \subset \mathbb{R}^n$ there is a constant a_K such that

$$|\nu(\phi)| \leq a_K \|\phi\| \quad (42)$$

for all $\phi \in \mathcal{C}$ with support in K . Such measures are in one-to-one correspondence with regular Borel measures through the Riesz–Markov representation theorem, see [8, Chapter XIII; 4, Chapter 8, Section 69] for background material, and we thus identify these two pictures. We deal only with regular Borel measures in this paper. If for each $\phi \in \mathcal{C}$ inequality (42) holds uniformly for all translates of ϕ , we say that ν is *translation bounded*. This turns out to be a very useful concept because the Fourier transform of a tempered measure, though a tempered distribution, need not be a measure, but the Fourier transform of the autocorrelation of a translation bounded tempered distribution, if it exists, is always a measure. Let us explain how to control this subtle point in the context of diffraction theory.

Distributions and measures act on different spaces of functions and are equipped with different topologies. Nonetheless, there is an important connection between them which comes through the fact that the space \mathcal{D} of C^∞ -functions of compact support is dense both in \mathcal{C} and in \mathcal{S} .

If a measure ν defines a tempered distribution T_ν by

$$(T_\nu, \psi) = \nu(\psi) = \int \psi \, d\nu \quad (43)$$

for all $\psi \in \mathcal{S}$, the measure ν is called *tempered*. A sufficient condition for a measure to be tempered is that it is slowly increasing in the sense that $\int (1+|\mathbf{x}|)^{-k} |\nu|(\mathrm{d}\mathbf{x}) < \infty$ for some $k \in \mathbb{Z}^+$, see [30, Theorem VII.VII] or [25, Example 7.12b]. Here, $|\nu|$ is the unique absolute value of ν , i.e. the smallest positive measure ρ such that $|\nu(\phi)| \leq \rho(|\phi|)$ for all $\phi \in \mathcal{C}$. It is also called the *variational* measure of ν . As a partial converse, any positive tempered distribution is a positive tempered measure. Thus, under the assumption of positiveness, tempered measures and tempered distributions can be viewed as the same thing, and the Bochner–Schwartz theorem can be restated as follows: ν is a positive tempered measure if and only if it is the Fourier transform of a tempered distribution of positive type.

Now, let ν be a translation bounded measure. Clearly ν is tempered. Our previous definition of the autocorrelation of a Dirac comb has a natural extension to the autocorrelation γ_ν of ν by means of a volume-normalized convolution of ν with ν^* , where ν^* is defined by $\nu^*(\phi) := \overline{\nu(\overline{\phi^*})}$, see [12] for details.⁶ This construction of γ_ν guarantees that, when it exists, it is a positive-definite tempered measure (and distribution), so combining the previous arguments we see that the corresponding diffraction pattern $\hat{\gamma}_\nu$ is a tempered positive measure.

This is important because it is this object that describes what one actually sees on the screen in a diffraction experiment: each (measurable) volume is assigned a nonnegative number, namely the total intensity of radiation scattered into this volume. In this article, we will only meet the simple case that ν is a Dirac comb ω_S . However, already the convolution with a function of compact support (a “profile” of the scatterer) shows why the more general setting is useful. Let us summarize this by the following result, which is a combination of [12, Propositions 2.2, 3.3].

Proposition 7. *Let ν be a translation bounded measure. If its natural autocorrelation γ_ν exists, it is a translation bounded (hence tempered) positive-definite measure. Furthermore, $\hat{\gamma}_\nu$ is then a positive measure and also translation bounded.*

4.5. Decomposition of measures

A *pure point* of a measure ν is a point $\mathbf{x} \in \mathbb{R}^n$ with $\nu(\{\mathbf{x}\}) \neq 0$. Since ν is a regular Borel measure, it has at most countably many pure points and the sum of $|\nu(\{\mathbf{x}\})|$ over the pure points in any compact set K is convergent, and the pure points alone serve to define a measure ν_{pp} called the *pure point part* of ν . Thus ν has a unique decomposition as

$$\nu = \nu_{\text{pp}} + \nu_{\text{c}}, \tag{44}$$

⁶Note, however, that the definition of the analogous operation to $*$ in [12] is slightly incorrect in that it omits the extra complex conjugation.

where $v_c := v - v_{pp}$ is the so-called *continuous part*⁷ of v , and is characterized by having no pure points. A *pure point measure* is a measure whose continuous part is 0.

When a tempered measure v is decomposed in this way the components v_{pp} and v_c are, of course, measures, but not necessarily tempered. For a translation bounded measure v , however, the components are both translation bounded and hence tempered. If v is a *positive* tempered measure, the decomposition is automatically into tempered components.

Returning now to diffraction patterns, we meet the special situation that $\hat{\gamma}_\omega$ is a *positive* measure. Consequently, it decomposes into a pure point part and a continuous part, both of which are positive measures. The pure point part is called the *Bragg spectrum* (of the point set S that created it). We say that the diffraction pattern is *pure point* or that S has a *pure point diffraction spectrum* if its diffraction pattern is a pure point measure, i.e. if it is equal to its Bragg spectrum.

Let us finally mention that, relative to Lebesgue measure, the continuous part v_c can be further decomposed into an *absolutely continuous* and a *singular continuous* part, $v_c = v_{ac} + v_{sc}$, see [4,24] for details. In our examples, we show that v_c vanishes, which means that there is neither an absolutely continuous nor a singular continuous component present.

5. An intuitive derivation of the point spectra

This section describes a short, intuitive way of calculating the pure point part of the diffraction spectrum of the visible points V of a lattice Γ and also of the k th-power-free numbers $F = F_k$. Its purpose is to give a taste of our later number theoretic methods in a simpler setting and also to contrast this intuitively clear calculation with the more circuitous route via autocorrelations we take later in rigorously establishing the complete diffraction spectra. It seems almost miraculous when the longer method eventually reduces to the same simple result. The intuitive method depends on the fact that since the autocorrelation γ_ω is a volume-normalized convolution of $\omega = \omega_V$ with itself, its Fourier transform, the diffraction pattern $\hat{\gamma}_\omega$, should be a normalized square of $\hat{\omega}$.

In this context, the coefficients of $\hat{\omega}$ are usually called *amplitudes*, even if they only exist formally, while those of $\hat{\gamma}_\omega$ are called *intensities* which relates to the fact that they are real and nonnegative. The appropriate operation now is to determine the intensities as the absolute squares of the corresponding amplitudes of peaks, as indicated in the commutative Wiener diagram in Fig. 1 where the vertical arrows represent the Fourier transform, the upper horizontal arrow the volume-normalized convolution, and the lower horizontal arrow taking the absolute squares of amplitudes.

⁷ The word ‘continuous’ here does not refer to being continuous as a function, since a line measure in the plane, for example, is continuous. It refers to the intermediate value property that if there are sets $A \subset C$ with $v_c(A) < b < v_c(C)$ then there is a set B with $A \subset B \subset C$ and $v_c(B) = b$. Some authors use the word diffuse instead of continuous and the words atomic or purely discrete instead of pure point.

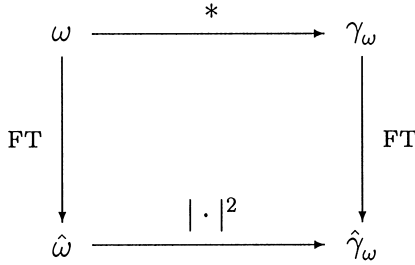


Fig. 1. Wiener diagram.

This observation dates back at least 100 years in optics and is the standard procedure in diffraction theory [7]. In the context of diffraction from infinite arrangements, it has been made rigorous (at least for the pure point part of the spectrum) by Hof [12,13]. The intuitive approach to the visible points runs through the Wiener diagram along the ‘low road’, via the difficult to interpret $\hat{\omega}$.

5.1. Visible points

We start from

$$\omega_V = \sum_{m=1}^{\infty} \mu(m) \omega_{m\Gamma \setminus \{0\}}, \tag{45}$$

which follows from (15) since the sum on the right-hand side is supported on $\Gamma \setminus \{0\}$ and the amplitude of the peak at $x \in \Gamma \setminus \{0\}$ is

$$\chi_V(x) = \sum_{m|\text{cont}(x)} \mu(m). \tag{46}$$

Although the sum on the right-hand side of (46) is finite for each x , these pointwise sums are not uniformly convergent, so the sum on the right-hand side of (45) does not pass the M -test of Proposition 2 as a sum of pure point distributions. Nevertheless, it is clear that the sum does converge to ω_V in the weak*-topology (though not in the local norm topology). Taking the Fourier transform of (45) term-by-term we obtain

$$\hat{\omega}_V = \sum_{m=1}^{\infty} \mu(m) \left(\frac{1}{m^n} \omega_{\Gamma^*/m} - 1 \right), \tag{47}$$

where here and in the remainder of this subsection we assume Γ to have unit density, i.e. $\text{vol}(\Gamma) = 1$. Since ω_V is a tempered distribution it has a Fourier transform $\hat{\omega}_V$ which is also a tempered distribution, and since the Fourier transform is a continuous operator on the space of tempered distributions with the weak*-topology [24] the sum on the right-hand side of (47) converges to $\hat{\omega}_V$ in the weak*-topology (though again it does not pass the M -test). This time the sums of the amplitudes at individual points of $\mathbb{Q}\Gamma^*$ are infinite sums but uniformly convergent, when $n \geq 2$.

It is difficult to interpret (47) as a distribution and we suspect that it is not a measure. Nevertheless, we can identify the pure points and their amplitudes formally (even though they may not be real peaks).

Define the *denominator* of a nonzero point $x \in \mathbb{Q}\Gamma^*$ by

$$\text{den}(x) := \text{gcd}\{m \in \mathbb{Z} \mid mx \in \Gamma^*\} \tag{48}$$

(it is the smallest positive integer such that $mx \in \Gamma^*$). Then the sum of the amplitudes in (47) at a point $x \in \mathbb{Q}\Gamma^* \setminus \{0\}$ with denominator d is

$$\begin{aligned} \sum_{l=1}^{\infty} \frac{\mu(ld)}{(ld)^n} &= \frac{\mu(d)}{d^n} \sum_{\substack{l=1 \\ (l,d)=1}}^{\infty} \frac{\mu(l)}{l^n} = \frac{\mu(d)}{d^n} \prod_{p \nmid d} \left(1 - \frac{1}{p^n}\right) \\ &= \frac{\mu(d)}{\zeta(n)d^n} \prod_{p \mid d} \left(1 - \frac{1}{p^n}\right)^{-1} = \frac{\mu(d)}{\zeta(n)} \prod_{p \mid d} \frac{1}{p^n - 1}. \end{aligned} \tag{49}$$

When $n \geq 2$, the pointwise sum of the pure point parts is thus nonzero at all points of $\mathbb{Q}\Gamma^*$ with squarefree denominator but is not absolutely locally summable. It is, however, locally square summable. The squaring operation gives, for the diffraction spectrum $\hat{\gamma}_\omega$ of V , the distribution with a pure point at each point of $\mathbb{Q}\Gamma^*$ with squarefree denominator, the peak at such a point with denominator d having intensity

$$\frac{1}{\zeta^2(n)} \prod_{p \mid d} \frac{1}{(p^n - 1)^2}. \tag{50}$$

These coefficients are uniformly absolutely locally summable and in fact are the correct intensities of the diffraction pattern. This will be proved below in Theorem 3. They were first derived, based on similar arguments, in [3]. However, one may well ask why this works. How can we justify the squaring operation as the appropriate mechanism for obtaining the intensities? The intuition is supported as follows.

5.2. Hof's results

Two results of Hof [12,13] are:

Proposition 8. *Let ν be a translation bounded measure on \mathbb{R}^n such that $\hat{\nu}$ is also a translation bounded measure. Then*

$$\hat{\nu}(\{x\}) = \lim_{R \rightarrow \infty} \frac{1}{v_n R^n} \int_{B_R(a)} e^{-2\pi i x \cdot y} \nu(dy) \tag{51}$$

for every $x \in \mathbb{R}^n$ and the limit exists uniformly in a .

Proposition 9. *Let ν be a translation bounded measure with natural autocorrelation γ and suppose that for all $x \in \mathbb{R}^n$,*

$$m_x := \lim_{R \rightarrow \infty} \frac{1}{v_n R^n} \int_{B_R(a)} e^{-2\pi i x \cdot y} \nu(dy) \tag{52}$$

exists uniformly in \mathbf{a} . Then, for all \mathbf{x} , we have

$$\hat{\gamma}(\{\mathbf{x}\}) = |m_{\mathbf{x}}|^2. \tag{53}$$

Taken together, these show that if the Fourier transform $\hat{\nu}$ of a translation bounded tempered distribution ν is also translation bounded (and hence can be decomposed as a pure point part and a continuous part) then the pure points of the diffraction spectrum $\hat{\gamma}_{\nu}$ are the same as the pure points of the Fourier transform $\hat{\nu}$, but their intensities are the absolute squares of the amplitudes of $\hat{\nu}$. Proposition 9 alone says that this continues to be true even when $\hat{\nu}$ is not translation bounded, at least as long as the formal expressions for the pure point amplitudes, also called Fourier–Bohr coefficients, of $\hat{\nu}$ (which may now not represent peaks of $\hat{\nu}$ in the accepted sense) converge uniformly with respect to translation of physical space. We shall say more about the status of the method after giving the analogous intuitive derivation for the k th-power-free integers.

5.3. k th-power-free integers

The parallel intuitive calculation for the pure point part of the diffraction spectrum of the set $F = F_k$ of k th-power-free integers in \mathbb{R} goes like this. We have

$$\omega_F = \sum_{m=1}^{\infty} \mu(m) \omega_{m^k \mathbb{Z} \setminus \{0\}}, \tag{54}$$

hence

$$\hat{\omega}_F = \sum_{m=1}^{\infty} \mu(m) \left(\frac{1}{m^k} \omega_{\mathbb{Z}/m^k} - 1 \right). \tag{55}$$

Let d_k be the smallest positive integer such that d_k^k is divisible by d . We note that d_k is a divisor of d but is divisible by every prime factor of d and that $d \mid m^k$ if and only if $d_k \mid m$. Then the formal sum of the amplitudes of the peaks of (55) at a point $x \in \mathbb{Q}$ with denominator d is

$$\begin{aligned} \sum_{l=1}^{\infty} \frac{\mu(ld_k)}{(ld_k)^k} &= \frac{\mu(d_k)}{d_k^k} \sum_{\substack{l=1 \\ (l,d)=1}}^{\infty} \frac{\mu(l)}{l^k} \\ &= \frac{\mu(d_k)}{\zeta(k) d_k^k} \prod_{p \mid d} \left(1 - \frac{1}{p^k} \right)^{-1} = \frac{\mu(d^*)}{\zeta(k)} \prod_{p \mid d} \frac{1}{p^k - 1}, \end{aligned} \tag{56}$$

since, when d_k is squarefree, we have $d_k = d^* = \prod_{p \mid d} p$ (the squarefree kernel of d) and $d_k^k = \prod_{p \mid d} p^k$. Consequently, the pure point part of the diffraction spectrum of F has peaks at the points of \mathbb{Q} with $(k + 1)$ th-power-free denominator, and its intensity at a such a point, with denominator d , is

$$\frac{1}{\zeta^2(k)} \prod_{p \mid d} \frac{1}{(p^k - 1)^2}. \tag{57}$$

This is a pure point distribution and also agrees with the result of Theorem 5 below.

5.4. Status of the method

In the remaining sections of this paper, which contain the heart of the proofs, we completely avoid Hof’s formula (52) (which in any case could only determine the pure point part of the spectrum without any assurance that there is no continuous part). What prevents us from making our derivation of the pure point part of the spectrum rigorous by citing Proposition 9 is that for our examples the limit in (52) is not uniform in \mathbf{a} . This is most easily seen by noting that our point sets have arbitrarily large holes, so that no matter how large R is there will be an \mathbf{a} such that $B_R(\mathbf{0}) + \mathbf{a}$ lies entirely within a hole. However, large holes are very sparse, so the limit is, in a sense, “nearly uniform”. For $\mathbf{x} \notin \mathbb{Q}\Gamma^*$ the limit (52) can be shown to be 0 (as it should be) but again is almost certainly not uniform in \mathbf{a} .

The fact that our examples are outside the domain where Hof’s result applies underscores the fact that we are in new territory not only for calculating the continuous part of the diffraction spectrum but even for calculating the diffraction peaks. In other words: the answer to the question which distributions of matter diffract is still largely unknown.

6. Autocorrelation of the visible points

The remainder of this paper consists of a rigorous derivation of the results of the previous section via the ‘high road’ of the autocorrelation. So we begin by using an elaboration of the kind of Möbius inversion argument used in proving Proposition 6 to calculate the autocorrelation of the visible points V of a lattice Γ .

Theorem 1. *For $n \geq 3$, the natural autocorrelation γ of the set V of visible points of a lattice Γ exists and is supported on Γ , the weight of a point $\mathbf{a} \in \Gamma$ in the autocorrelation of V being given by*

$$w(\mathbf{a}) = \text{dens}(\Gamma)\zeta(n) \prod_{p|\text{cont}(\mathbf{a})} \left(1 + \frac{1}{p^n - 2}\right) \tag{58}$$

with error term (as defined just after (11)) equal to $O(1/R)$, where the implied constant depends on \mathbf{a} as well as on Γ .

Proof. By Proposition 5, $V - V = \Gamma$, so the autocorrelation of V (if it exists) is supported on Γ . The weight of a point $\mathbf{a} \in \Gamma$ in the autocorrelation of V is the limit as $R \rightarrow \infty$ of

$$\frac{1}{v_n R^n} \sum_{\substack{|\mathbf{x}|, |\mathbf{x}-\mathbf{a}| < R \\ \mathbf{x}, \mathbf{x}-\mathbf{a} \in V}} 1 \tag{59}$$

and by Lemma 1 the existence of this limit for each $\mathbf{a} \in \Gamma$ is sufficient to ensure the existence of the autocorrelation.

It is convenient to drop the condition $|\mathbf{x} - \mathbf{a}| < R$ in (59), which then becomes

$$\frac{1}{v_n R^n} \sum_{\substack{|\mathbf{x}| < R \\ \mathbf{x}, \mathbf{x} - \mathbf{a} \in V}} 1. \tag{60}$$

The difference between these sums is $O(1/R)$, due to the extra lattice points \mathbf{x} within a constant distance $|\mathbf{a}|$ of the boundary of $B_R(\mathbf{0})$ that are included in the latter. We note that the latter sum has a natural geometric interpretation as the proportion of integer points in a large ball that are visible both from the origin and from the viewpoint \mathbf{a} . By (15) and (8), (60) can be expressed as

$$\begin{aligned} & \frac{1}{v_n R^n} \sum_{\substack{\mathbf{x} \in \Gamma \setminus \{\mathbf{0}, \mathbf{a}\} \\ |\mathbf{x}| < R}} \sum_{l | \text{cont}(\mathbf{x})} \mu(l) \sum_{m | \text{cont}(\mathbf{x} - \mathbf{a})} \mu(m) \\ &= \frac{1}{v_n R^n} \sum_{1 \leq l < S} \sum_{1 \leq m < S} \mu(l) \mu(m) \sum_{\substack{\mathbf{x} \in \Gamma \setminus \{\mathbf{0}, \mathbf{a}\} \\ \mathbf{x} \equiv \mathbf{0} \pmod{l\Gamma} \\ \mathbf{x} \equiv \mathbf{a} \pmod{m\Gamma} \\ |\mathbf{x}| < R}} 1, \end{aligned} \tag{61}$$

where $S = (R + |\mathbf{a}|)/L(\Gamma)$. Collecting together terms with the same value of $d = (l, m)$, noting that all solutions \mathbf{x} of the congruences belong to $d\Gamma$ and that the congruences have no solution at all unless $\mathbf{a} \in d\Gamma$, and putting $l' = l/d$, $m' = m/d$, $\mathbf{x}' = \mathbf{x}/d$, $\mathbf{a}' = \mathbf{a}/d$, we obtain

$$\frac{1}{v_n R^n} \sum_{d | \text{cont}(\mathbf{a})} \sum_{1 \leq l' < S/d} \sum_{\substack{1 \leq m' < S/d \\ (l', m') = 1}} \mu(l'd) \mu(m'd) \sum_{\substack{\mathbf{x}' \in \Gamma \setminus \{\mathbf{0}, \mathbf{a}'\} \\ \mathbf{x}' \equiv \mathbf{0} \pmod{l'\Gamma} \\ \mathbf{x}' \equiv \mathbf{a}' \pmod{m'\Gamma} \\ |\mathbf{x}'| < R/d}} 1. \tag{62}$$

Since l' and m' are bound variables of summation and \mathbf{x}' and \mathbf{a}' will not be referred to again, we can drop the dashes: from now on l and m are the new l' and m' but \mathbf{a} is the original \mathbf{a} .

By Propositions 2 and 1 (with $lm\Gamma$ in place of Γ) the inmost sum is

$$\text{dens}(\Gamma) v_n \left(\frac{R}{d l m} \right)^n + O\left(\frac{R}{d l m} \right)^{n-1} + O(1). \tag{63}$$

These three terms give a main term and two error terms in (62).

The first error term is majorized by

$$O\left(\frac{1}{R} \sum_{1 \leq l < S} \frac{1}{l^{(n-1)}} \sum_{1 \leq m < S} \frac{1}{m^{(n-1)}} \right) = \begin{cases} O(1/R) & \text{if } n \geq 3, \\ O((\log S)^2/R) & \text{if } n = 2, \end{cases} \tag{64}$$

since the sums are convergent when $n - 1 \geq 2$ and increase logarithmically when $n - 1 = 1$.

The second error term is majorized by $O(S^2/R^n) = O(1/R^{n-2})$. So when $n \geq 3$ both error terms are $O(1/R)$ (since $S = O(R)$) and tend to 0 as $R \rightarrow \infty$.

The main term is (with $\mathcal{D} = \text{dens}(\Gamma)$)

$$\begin{aligned} & \mathcal{D} \sum_{d|\text{cont}(\mathbf{a})} \sum_{1 \leq l < S/d} \sum_{\substack{1 \leq m < S/d \\ (l,m)=1}} \frac{\mu(ld)\mu(md)}{(dlm)^n} \\ &= \mathcal{D} \sum_{d|\text{cont}(\mathbf{a})} \sum_{\substack{1 \leq l < S/d \\ (l,d)=1}} \sum_{\substack{1 \leq m < S/d \\ (m,d)=1 \\ (l,m)=1}} \frac{\mu^2(d)\mu(l)\mu(m)}{(dlm)^n}, \end{aligned} \tag{65}$$

since $\mu(ld)$ is $\mu(l)\mu(d)$ when $(l, d) = 1$ and 0 otherwise, and similarly for $\mu(md)$,

$$= \mathcal{D} \sum_{d|\text{cont}(\mathbf{a})} \frac{\mu^2(d)}{d^n} \sum_{\substack{1 \leq l < S/d \\ (l,d)=1}} \sum_{\substack{1 \leq m < S/d \\ (m,d)=1}} \frac{\mu(lm)}{(lm)^n}, \tag{66}$$

since $\mu(l)\mu(m)$ is $\mu(lm)$ when $(l, m) = 1$ and 0 otherwise

$$\rightarrow \mathcal{D} \sum_{d|\text{cont}(\mathbf{a})} \frac{\mu^2(d)}{d^n} \sum_{\substack{r=1 \\ (r,d)=1}}^{\infty} \frac{\mu(r)\sigma(r)}{r^n} \text{ as } R \rightarrow \infty, \tag{67}$$

since the double sum is absolutely convergent. The difference between this limit and the partial sum (66) is $O(1/R^{n-1})$, so falls within the error term estimate $O(1/R)$.

Using (19), the expression for limit (67) can be rearranged as

$$\begin{aligned} & \mathcal{D} \sum_{\substack{d|\text{cont}(\mathbf{a}) \\ d \text{ square-free}}} \frac{1}{d^n} \prod_{p|d} \left(1 - \frac{2}{p^n}\right) = \mathcal{D} \zeta(n) \sum_{\substack{d|\text{cont}(\mathbf{a}) \\ d \text{ square-free}}} \frac{1}{d^n} \prod_{p|d} \left(1 - \frac{2}{p^n}\right)^{-1} \\ &= \mathcal{D} \zeta(n) \prod_{p|\text{cont}(\mathbf{a})} \left(1 + \frac{1}{p^n} \left(1 - \frac{2}{p^n}\right)^{-1}\right) = \mathcal{D} \zeta(n) \prod_{p|\text{cont}(\mathbf{a})} \left(1 + \frac{1}{p^n - 2}\right). \end{aligned} \tag{68}$$

This completes the proof. \square

To establish the existence of the autocorrelation function for the visible points when $n = 2$, we need to reduce the second error term in the above proof. This we do by modifying the argument slightly, first using the characteristic function (15) to replace the constraint on $\mathbf{x} - \mathbf{a}$ only, then discarding large values of m from the sum before using (15) again to replace the constraint on \mathbf{x} .

Theorem 2. *Theorem 1 holds for $n = 2$ with the error term increased to $O(1/\sqrt{R})$.*

Proof. Using (15) to replace the constraint on $\mathbf{x} - \mathbf{a}$, (60) becomes

$$\frac{1}{\pi R^2} \sum_{\substack{\mathbf{x} \in V \\ \mathbf{x} \neq \mathbf{a} \\ |\mathbf{x}| < R}} \sum_{\substack{m | \text{cont}(\mathbf{x} - \mathbf{a}) \\ 1 \leq m < S}} \mu(m) = \frac{1}{\pi R^2} \sum_{1 \leq m < S} \mu(m) \sum_{\substack{\mathbf{x} \in V \\ \mathbf{x} \neq \mathbf{a} \\ \mathbf{x} \equiv \mathbf{a} \pmod{m\Gamma} \\ |\mathbf{x}| < R}} 1, \tag{69}$$

where S is as before. The inner sum is trivially $O(R^2/m^2)$ (since $m < S = O(R)$) so the contribution to (60) from the terms with $m \geq \sqrt{R}$ is

$$O\left(\sum_{m \geq \sqrt{R}} \frac{1}{m^2}\right) = O(1/\sqrt{R}). \tag{70}$$

For the terms in (69) with $m < \sqrt{R}$ we use the characteristic function (15) to replace the constraint on \mathbf{x} , obtaining

$$\begin{aligned} &\frac{1}{\pi R^2} \sum_{1 \leq m < \sqrt{R}} \mu(m) \sum_{\substack{\mathbf{x} \in \Gamma \setminus \{\mathbf{0}, \mathbf{a}\} \\ \mathbf{x} \equiv \mathbf{a} \pmod{m\Gamma} \\ |\mathbf{x}| < R}} \sum_{l | \text{cont}(\mathbf{x})} \mu(l) \\ &= \frac{1}{\pi R^2} \sum_{1 \leq l < S} \sum_{1 \leq m < \sqrt{R}} \mu(l)\mu(m) \sum_{\substack{\mathbf{x} \in \Gamma \setminus \{\mathbf{0}, \mathbf{a}\} \\ \mathbf{x} \equiv \mathbf{0} \pmod{l\Gamma} \\ \mathbf{x} \equiv \mathbf{a} \pmod{m\Gamma} \\ |\mathbf{x}| < R}} 1. \end{aligned} \tag{71}$$

This is now identical to (61), except that the second S is replaced by \sqrt{R} , and as before contributes to (60) a main term that tends to

$$\mathcal{D} \xi(2) \prod_{p | \text{cont}(\mathbf{a})} \left(1 + \frac{1}{p^2 - 2}\right) \tag{72}$$

as $R \rightarrow \infty$ and two error terms $O((\log R)^2/R)$ and $O(1/\sqrt{R})$. The difference between the main term and its limit is also $O(1/\sqrt{R})$. So the total error term is majorized by $O(1/\sqrt{R})$. \square

Note that this modified argument does not reduce the error term when $n \geq 3$, which contains a term $O(1/R)$ arising from the boundary of the ball when $l=m=1$. For $n=2$, a similar but more complicated argument gives an improved error term $O(R^{-3/4}(\log R)^c)$ for some constant c , but we do not need this here.

Remark. Theorems 1 and 2 show that the weight $w(\mathbf{a})$ in the autocorrelation of V (also called the autocorrelation coefficient⁸) depends only on the content of \mathbf{a} and

⁸Note that $w(\mathbf{a})$ can also be interpreted as the density of lattice points that are simultaneously visible both from the origin and from the lattice point \mathbf{a} . Extending this to the condition of simultaneous visibility from an arbitrary (but finite) set of points of Γ results in higher-order correlation coefficients, see [5] for some recent results.

the density of Γ . This enables us to calculate how the application of a nonsingular linear transformation T to V affects the autocorrelation of V . Clearly T preserves content, in the sense that, for any lattice Γ and $\mathbf{x} \in \Gamma$, the content of $T\mathbf{x}$ as a vector of $T\Gamma$ is equal to the content of \mathbf{x} as a vector of Γ . In particular, TV is the set of visible points of $T\Gamma$. The autocorrelation of TV is supported on $T\Gamma$ and (58) shows that

$$w_{TV}(T\mathbf{a}) = \frac{\text{dens}(T\Gamma)}{\text{dens}(\Gamma)} w_V(\mathbf{a}) = \frac{1}{|\det T|} w_V(\mathbf{a}), \tag{73}$$

where the suffix on w indicates which autocorrelation it is associated with. Thus, the autocorrelation of TV is $|\det T|^{-1}$ times the T -image of the autocorrelation of V .

The direct way of calculating $w_{TV}(T\mathbf{a})$ from (59) is

$$w_{TV}(T\mathbf{a}) = \lim_{R \rightarrow \infty} \frac{1}{v_n R^n} \sum_{\mathbf{x}, \mathbf{x}-T\mathbf{a} \in RB \cap TV} 1, \tag{74}$$

where $B = B_1(\mathbf{0})$ is the unit ball in \mathbb{R}^n , and substituting this in (73) gives

$$w_V(\mathbf{a}) = \lim_{R \rightarrow \infty} \frac{|\det T|}{v_n R^n} \sum_{\mathbf{y}, \mathbf{y}-\mathbf{a} \in RT^{-1}B \cap V} 1 = \lim_{R \rightarrow \infty} \frac{1}{\text{vol}(E)R^n} \sum_{\mathbf{y}, \mathbf{y}-\mathbf{a} \in RE \cap V} 1, \tag{75}$$

where $E = T^{-1}B$ is an ellipsoid. Hence, averaging over the expanding ellipsoid RE gives the same value for the autocorrelation of V as using the natural density and averaging over an expanding ball. The choice of ellipsoid here is completely arbitrary, since for any E there is a linear transformation T with $TE = B$. In Appendix A this is generalized further and we show how to replace E by any bounded measurable region (not necessarily centred at $\mathbf{0}$) with finite $(n - 1)$ -dimensional surface area.

7. Diffraction spectrum of the visible points

The final step in obtaining the diffraction spectrum of the visible points V is to take the Fourier transform of the autocorrelation of V .

Theorem 3. *The diffraction spectrum of the set of visible points of an n -dimensional lattice Γ (with $n \geq 2$) exists and is a pure point measure which is concentrated on the set of points in $\mathbb{Q}\Gamma^*$ with squarefree denominator and whose intensity at a point with such a denominator q is given by*

$$\frac{\text{dens}(\Gamma)^2}{\zeta^2(n)} \prod_{p|q} \frac{1}{(p^n - 1)^2}. \tag{76}$$

This measure can also be represented as

$$\text{dens}(\Gamma)^2 \zeta(n) = \sum_{\substack{d=1 \\ d \text{ square-free}}}^{\infty} \left(\prod_{p|d} \frac{1}{p^{2n} - 2p^n} \right) \omega_{\Gamma^*/d}, \tag{77}$$

a weak*-convergent sum of Dirac combs.

Proof. Let γ be the autocorrelation of V . The right-hand side of (68) can be expressed in the form (again, with $\mathcal{D} = \text{dens}(\Gamma)$)

$$w(\mathbf{a}) = \mathcal{D} \zeta(n) \sum_{\substack{d=1 \\ d \text{ square-free} \\ \mathbf{a} \in d\Gamma}}^{\infty} \frac{1}{d^n} \prod_{p|d} \left(1 - \frac{2}{p^n} \right)^{-1}. \tag{78}$$

So by Theorems 1 and 2 and Lemma 1

$$\gamma = \mathcal{D} \zeta(n) \sum_{\substack{d=1 \\ d \text{ square-free}}}^{\infty} \frac{1}{d^n} \prod_{p|d} \left(1 - \frac{2}{p^n} \right)^{-1} \omega_{d\Gamma}. \tag{79}$$

Since $\|\omega_{d\Gamma}\|_{\text{loc}} = O(1)$ and the coefficient of $\omega_{d\Gamma}$ is $O(1/d^n)$ when $n \geq 2$, this sum of tempered distributions is convergent in the weak*-topology by Lemma 2 (and this is easy to see by other means in this case, where the resulting sum is uniformly discrete). Its term-by-term Fourier transform is

$$\mathcal{D}^2 \zeta(n) \sum_{\substack{d=1 \\ d \text{ square-free}}}^{\infty} \frac{1}{d^{2n}} \prod_{p|d} \left(1 - \frac{2}{p^n} \right)^{-1} \omega_{\Gamma^*/d}, \tag{80}$$

which weak*-converges to the diffraction spectrum of V , since the Fourier transform operator is weak*-continuous. Since $\|\omega_{\Gamma^*/d}\|_{\text{loc}} = O(d^n)$ and the coefficient of $\omega_{\Gamma^*/d}$ is $O(1/d^{2n})$, Lemma 2 tells us that the weak*-sum is a translation bounded pure point measure equal to the pointwise sum of its terms.

This establishes the series form (77) for the diffraction spectrum. The explicit values of the intensities can now be evaluated quite simply. Let \mathbf{p} be a point in $\mathbb{Q}\Gamma^*$ with denominator q . We can suppose that q is square-free, since otherwise there is no contribution to (77) at all. The terms in (77) that contribute to the intensity at \mathbf{p} are those with $d = mq$ (m square-free in \mathbb{Z}^+ and prime to q), so the intensity at \mathbf{p} is

$$\mathcal{D}^2 \zeta(n) \prod_{p|q} \frac{1}{p^{2n} - 2p^n} \sum_{\substack{m=1 \\ m \text{ square-free} \\ (m,q)=1}}^{\infty} \prod_{p|m} \frac{1}{p^{2n} - 2p^n}. \tag{81}$$

This simplifies to

$$\begin{aligned}
 & \mathcal{D}^2 \zeta(n) \prod_{p|q} \frac{1}{p^{2n} - 2p^n} \prod_{p \nmid q} \left(1 + \frac{1}{p^{2n} - 2p^n} \right) \\
 &= \mathcal{D}^2 \zeta(n) \prod_{p|q} \frac{1}{p^{2n}} \left(1 - \frac{2}{p^n} \right)^{-1} \prod_{p \nmid q} \left(1 - \frac{1}{p^n} \right)^2 \left(1 - \frac{2}{p^n} \right)^{-1} \\
 &= \frac{\mathcal{D}^2}{\zeta^2(n)} \prod_{p|q} \frac{1}{p^{2n}} \left(1 - \frac{1}{p^n} \right)^{-2} \tag{82}
 \end{aligned}$$

(using the Euler products in (18) and (19)) which agrees with (76). \square

An explicit example of the diffraction (for $\Gamma = \mathbb{Z}^2$) is shown in [3], and compared with an optical experiment. The diffraction image in this case is both D_4 -symmetric and $GL(2, \mathbb{Z})$ invariant which results in a beautiful image with a rather unusual symmetry structure, reminiscent of self-similar patterns common in fractals.

8. k th-power-free numbers

In this section we derive the diffraction spectrum of the one-dimensional set F consisting of the k th-power-free numbers in \mathbb{Z} . Again, this has arbitrarily long gaps but it nevertheless has a pure point diffraction spectrum. The proof of the second assertion closely parallels the corresponding proof for the visible points V in the previous two sections, with the parameter k for F playing the rôle of the dimension n of V in the formalism. There are some differences of detail, however, particularly with the error terms.

Let us note here that the results on the autocorrelation derived below also follow from [22] ($k = 2$) and from [19, Theorem 1], where also more general correlation functions have been derived. The error term given in [19] is $O(R^{-1+2/(k+1)})$, which is slightly better than the error term we derive in Theorem 4. We include our proof to make this paper self-contained and to show up the close parallel between visible lattice points and k -free numbers.

Proposition 10. *F is uniformly discrete, but has gaps of arbitrary length. Moreover, for any $L > 0$ the set of gaps of length at least L has positive density.*

Proof. The uniform discreteness is trivial since $F \subset \mathbb{Z}$. Choose L integer moduli m_1, \dots, m_L that are > 1 and coprime in pairs (for example, the first L primes). By the Chinese Remainder Theorem there is an integer N with

$$N \equiv -j + 1 \pmod{m_j^k} \quad \text{for } j = 1, \dots, L. \tag{83}$$

Now for $x \equiv N \pmod{m_1^k m_2^k \dots m_L^k}$ we have $m_1^k | x, m_2^k | (x+1), \dots, m_L^k | (x+L-1)$, so none of the numbers $x, x+1, \dots, x+L-1$ is k th-power-free. The numbers x have density $(m_1 m_2 \dots m_L)^{-k}$. \square

This argument gives a distance of the order L^{kL} between gaps of length L , so again long gaps can be expected to be extremely sparse. Nevertheless, gaps of length L have a definite frequency (its expression in terms of Dirichlet series can be extracted from [19]). It is interesting to note that the corresponding distribution is *not* Poissonian, but that these frequencies decline faster than exponentially in L [15,9].

Proposition 11. *For $k \geq 2$, the k th-power-free integers F have a natural density given by*

$$\text{dens}(F) = \frac{1}{\zeta(k)}, \tag{84}$$

with error term $O(R^{-1+(1/k)})$.

At least for the squarefree numbers, this is again a standard example of Möbius inversion, see [14, Theorem 6.6.1].

Proof. The natural density of F is the limit as $R \rightarrow \infty$ of

$$\frac{1}{2R} \sum_{\substack{|x| < R \\ x \in F}} 1, \tag{85}$$

which by (16) is

$$\begin{aligned} \frac{1}{2R} \sum_{\substack{|x| < R \\ x \neq 0}} \sum_{m^k | x} \mu(m) &= \frac{1}{2R} \sum_{1 \leq m < R^{1/k}} \mu(m) \sum_{\substack{|x| < R \\ x \equiv 0 \pmod{m^k} \\ x \neq 0}} 1 \\ &= \sum_{1 \leq m < R^{1/k}} \frac{\mu(m)}{m^k} + O\left(\frac{R^{1/k}}{R}\right), \end{aligned} \tag{86}$$

since the inner sum on the right-hand side of (86) is $2R/m^k + O(1)$. This last expression tends to $1/\zeta(k)$ as $R \rightarrow \infty$ when $n \geq 2$, with the errors due to the tail of the sum and to the explicit error term both $O(R^{-1+(1/k)})$. \square

Theorem 4. *For $k \geq 2$, the natural autocorrelation of the set F of k th-power-free integers exists and is supported on \mathbb{Z} , the weight of an integer a in the autocorrelation of V being given by*

$$w(a) = \zeta(k) \prod_{p^k | a} \left(1 + \frac{1}{p^k - 2}\right) \tag{87}$$

with error term $O(R^{-(1-(1/k))^2})$, where the implied constant depends on a .

Proof. Clearly the autocorrelation is supported on \mathbb{Z} . The weight of an integer a in the autocorrelation of F is the limit as $R \rightarrow \infty$ of

$$\frac{1}{2R} \sum_{\substack{|x|, |x-a| < R \\ x, x-a \text{ } k\text{-free}}} 1 \tag{88}$$

and, as in the proof of Theorem 1, to show the existence of the autocorrelation it is enough to show that this limit exists for every a . Again as in the proof of Theorem 1, we can drop the condition $|x - a| < R$ from the sum to obtain

$$\frac{1}{2R} \sum_{\substack{|x| < R \\ x, x-a \text{ } k\text{-free}}} 1 \tag{89}$$

with error $O(1/R)$.

This can be evaluated by an argument exactly parallel to that for the visible points, using the characteristic function (16) in place of (15). We use the argument in the modified form we used in the proof of Theorem 2 since, in the context of k th-power-free numbers, it gives an improved error term in all cases owing to the fact that, for a one-dimensional set, errors due to the boundary of a large region are trivial. (Using the unmodified form would give error term $O(R^{-1+(2/k)})$ instead of the $O(R^{-1+(2/k)-(1/k)^2})$ we obtain here. As with the visible points, this would not be small enough to establish the existence of the limit for the squarefree numbers $k = 2$ — the paradigm case.)

Using the characteristic function (16) to replace the constraint on $x - a$, (89) becomes

$$\frac{1}{2R} \sum_{\substack{|x| < R \\ x \text{ } k\text{-free} \\ x \neq a}} \sum_{m^k | (x-a)} \mu(m) = \frac{1}{2R} \sum_{1 \leq m < S^{1/k}} \mu(m) \sum_{\substack{|x| < R \\ x \text{ } k\text{-free} \\ x \neq a \\ x \equiv a \pmod{m^k}}} 1, \tag{90}$$

where $S = R + |a|$. The inner sum is trivially $O(R/m^k)$ (since $m^k < S$) so the contribution to (89) from the terms with $m \geq T$, where T is a parameter tending to infinity with R to be chosen later, is

$$O\left(\sum_{m \geq T} \frac{1}{m^k}\right) = O(T^{1-k}). \tag{91}$$

For the terms in (90) with $m < T$ we use the characteristic function (16) to replace the constraint on x , obtaining

$$\frac{1}{2R} \sum_{1 \leq m < T} \mu(m) \sum_{\substack{|x| < R \\ x \neq 0, a \\ x \equiv a \pmod{m^k}}} \sum_{l^k | x} \mu(l)$$

$$= \frac{1}{2R} \sum_{1 \leq l < R^{1/k}} \sum_{1 \leq m < T} \mu(l)\mu(m) \sum_{\substack{|x| < R \\ x \neq 0, a \\ x \equiv 0 \pmod{l^k} \\ x \equiv a \pmod{m^k}}} 1. \tag{92}$$

Collecting together terms with the same value of $d = (l, m)$, noting that all solutions x of the congruences are divisible by d^k and that the congruences have no solution unless $d^k | a$, and putting $l' = l/d$, $m' = m/d$, $x' = x/d^k$, $a' = a/d^k$, we obtain

$$\frac{1}{2R} \sum_{d^k | a} \sum_{1 \leq l' < R^{1/k}/d} \sum_{\substack{1 \leq m' < T/d \\ (l', m')=1}} \mu(l'd)\mu(m'd) \sum_{\substack{|x'| < R/d^k \\ x' \neq 0, a' \\ x' \equiv 0 \pmod{l'^k} \\ x' \equiv a' \pmod{m'^k}}} 1. \tag{93}$$

As in the proof of Theorem 1, we can drop the dashes from now on.

By the Chinese Remainder Theorem the inner sum is

$$\frac{2R}{(dlm)^k} + O(1) \tag{94}$$

giving a main term and another error term in (89).

The error term is majorized by $O(R^{-1+(1/k)T})$.

The main term is

$$\begin{aligned} & \sum_{d^k | a} \sum_{1 \leq l < R^{1/k}/d} \sum_{\substack{1 \leq m < T/d \\ (l, m)=1}} \frac{\mu(ld)\mu(md)}{(dlm)^k} \\ &= \sum_{d^k | a} \sum_{\substack{1 \leq l < R^{1/k}/d \\ (l, d)=1}} \sum_{\substack{1 \leq m < T/d \\ (m, d)=1 \\ (l, m)=1}} \frac{\mu^2(d)\mu(l)\mu(m)}{(dlm)^k}, \end{aligned} \tag{95}$$

since $\mu(ld)$ is $\mu(l)\mu(d)$ when $(l, d) = 1$ and 0 otherwise, and similarly for $\mu(md)$,

$$= \sum_{d^k | a} \frac{\mu^2(d)}{d^k} \sum_{\substack{1 \leq l < R^{1/k}/d \\ (l, d)=1}} \sum_{\substack{1 \leq m < T/d \\ (m, d)=1}} \frac{\mu(lm)}{(lm)^k}, \tag{96}$$

since $\mu(l)\mu(m)$ is $\mu(lm)$ when $(l, m) = 1$ and 0 otherwise

$$\rightarrow \sum_{d^k | a} \frac{\mu^2(d)}{d^k} \sum_{\substack{r=1 \\ (r, d)=1}}^{\infty} \frac{\mu(r)\sigma(r)}{r^k} \text{ as } R \rightarrow \infty \tag{97}$$

since the double sum is absolutely convergent. The difference between this limit and the partial sum (96) is $O(1/R^{-(k-1)/k}) + O(T^{-(k-1)})$ and each of these terms is subsumed by one of the error estimates we already have.

This last expression is

$$\begin{aligned}
 \sum_{\substack{d^k|a \\ d \text{ square-free}}} \frac{1}{d^k} \prod_{p \mid d} \left(1 - \frac{2}{p^k}\right) &= \zeta(k) \sum_{\substack{d^k|a \\ d \text{ square-free}}} \frac{1}{d^k} \prod_{p \mid d} \left(1 - \frac{2}{p^k}\right)^{-1} \\
 &= \zeta(k) \prod_{p^k|a} \left(1 + \frac{1}{p^k} \left(1 - \frac{2}{p^k}\right)^{-1}\right) \\
 &= \zeta(k) \prod_{p^k|a} \left(1 + \frac{1}{p^k - 2}\right). \tag{98}
 \end{aligned}$$

Finally, we choose $T = R^{(1/k)-(1/k)^2}$, making both error terms $O(R^{-1+(2/k)-(1/k)^2})$. \square

We can now fill a small gap in our analogy by the following result.

Corollary 1. *For $k \geq 2$, we have $F - F = \mathbb{Z}$.*

Proof. Since $F - F \subset \mathbb{Z}$, γ_ω is clearly supported on \mathbb{Z} . From Theorem 4, we get $w(a) > 0$ for all $a \in \mathbb{Z}$, hence also $\mathbb{Z} \subset F - F$. \square

Let us finally describe the diffraction of k th-power-free integers.

Theorem 5. *The diffraction spectrum of the set F of k th-power-free integers exists and is a pure point measure. It is supported on the set of numbers $a/q \in \mathbb{Q}$ with q being $(k + 1)$ -power-free. The diffraction intensity at a point with such a denominator q is*

$$\frac{1}{\zeta^2(k)} \prod_{p \mid q} \frac{1}{(p^k - 1)^2}. \tag{99}$$

This measure can also be represented as

$$\zeta(k) \sum_{\substack{d=1 \\ d \text{ square-free}}}^{\infty} \left(\prod_{p \mid d} \frac{1}{p^{2k} - 2p^k} \right) \omega_{\mathbb{Z}/d^k}, \tag{100}$$

a weak*-convergent sum of Dirac combs.

Proof. As in the proof of Theorem 3, it follows from (98) that

$$\gamma = \zeta(k) \sum_{\substack{d=1 \\ d \text{ square-free}}}^{\infty} \frac{1}{d^k} \prod_{p \mid d} \left(1 - \frac{2}{p^k}\right)^{-1} \omega_{d^k \mathbb{Z}}, \tag{101}$$

where γ is the autocorrelation of F and this sum of tempered distributions is convergent in the $\|\cdot\|_{\text{loc}}$ -topology for $k \geq 2$. Its term-by-term Fourier transform is

$$\zeta(k) \sum_{\substack{d=1 \\ d \text{ square-free}}}^{\infty} \frac{1}{d^{2k}} \prod_{p|d} \left(1 - \frac{2}{p^k}\right)^{-1} \omega_{\mathbb{Z}/d^k}, \tag{102}$$

where the sum of the local norms of the terms is convergent, so by Lemma 2 (102) weak*-converges to a translation bounded pure point measure equal to the pointwise sum of its terms. Since the Fourier transform operator is weak*-continuous this pure point distribution is the diffraction spectrum of F .

This establishes (100). To obtain (99) we note that the terms in (100) that contribute to the intensity at a/q (where q has to be $(k + 1)$ -free) are those with $d = mq^*$, where q^* is the square-free kernel of q and $m \in \mathbb{Z}^+$ is square-free and prime to q . Thus the intensity at a/q is

$$\zeta(k) \prod_{p|q} \frac{1}{p^{2k} - 2p^k} \sum_{\substack{m=1 \\ m \text{ square-free} \\ (m,q)=1}}^{\infty} \prod_{p|m} \frac{1}{p^{2k} - 2p^k}. \tag{103}$$

This is (81) without the factor \mathcal{D}^2 and with n replaced by k , so reduces to (99). \square

9. Further connections and directions

Above, we have emphasized that the sets of visible lattice points V_Γ and the set of k -th-power-free numbers F_k differ from any regular model set (see [18,20,27,28] for definitions and properties) by a set of positive density, suggesting that they cannot be obtained from the cut-and-project construction in any natural way. However, there is a way of obtaining these sets by cut-and-project using the rational adeles instead of Euclidean space as the hyperspace (or embedding space) and using windows which, although they have empty interior, are quite natural sets in this context. From this point of view, V_Γ and F_k are ‘super-singular’ model sets. This comes about because these sets are the result of sieving over primes: F_k , for example, is what remains of \mathbb{Z} after removing the zero residue class mod p^k for each p .

The *cut-and-project construction* can be pictured like

$$\begin{array}{ccc} B \xleftarrow{\pi} A & \xrightarrow{\pi_{\text{int}}} & C \\ \cup & & \\ L & & \end{array} \tag{104}$$

Usually the *hyperspace* A is \mathbb{R}^{n+m} , with the *physical space* $B = \mathbb{R}^n$ and the *internal space* $C = \mathbb{R}^m$ being complementary subspaces having π and π_{int} as the associated projections with kernels C and B , respectively, and L being a lattice in A whose images in B and

C are dense. A bounded acceptance domain or *window* $\Omega \subset C$ is chosen and the *model set* in B is

$$A = A(\Omega) := \{\pi(\mathbf{x}) \mid \mathbf{x} \in L, \pi_{\text{int}}(\mathbf{x}) \in \Omega\}. \tag{105}$$

Then A is a uniformly discrete set and it is also relatively dense if Ω has non-empty interior. When B and C are orthogonal and Ω is a simple region we have

$$\text{dens}(A) = \text{vol}(\Omega)\text{dens}(L) = \text{vol}(\Omega)/\text{vol}(\mathcal{F}_L), \tag{106}$$

where \mathcal{F}_L is a fundamental region of L . This construction admits the generalization where A is allowed to be an arbitrary locally compact Abelian group and L a discrete subgroup with A/L compact (so that L plays the rôle of a lattice), see [20] and references therein. It is well known [18,20,27] that, even in this more general situation, $A(\Omega)$ is relatively dense if Ω has nonempty interior and possesses a uniform density if, in addition, $\partial\Omega$ has Haar measure 0, see [13,27] for details.

To obtain the k th-power-free numbers, we take A to be the ring of rational adèles $\mathbb{A}_{\mathbb{Q}}$. Let us explain what this is. (For the technical details and background to p -adic numbers and adèles see [6], which deals with the case of a general algebraic number field in place of \mathbb{Q} .) Given a prime $p \in \mathbb{Z}^+$ the p -adic valuation on \mathbb{Q} is defined, for $q \neq 0$, by $|q|_p = p^{-r}$, where $q = p^r a/b$ with $r \in \mathbb{Z}$ and a, b not divisible by p . This satisfies not only the triangle inequality but the stronger inequality $|q_1 + q_2|_p \leq \max\{|q_1|_p, |q_2|_p\}$. (Such valuations are called *non-Archimedean*.) The field \mathbb{Q}_p of p -adic numbers is the completion of \mathbb{Q} with respect to $|\cdot|_p$ (analogous to \mathbb{R} being the completion of \mathbb{Q} with respect to the ordinary absolute value) and is locally compact in the p -adic topology. In view of the strong triangle inequality, the p -adic numbers a with $|a|_p \leq 1$ form a ring \mathbb{Z}_p , called the *p -adic integers*. (It is the closure of \mathbb{Z} in \mathbb{Q}_p .) For any p -adic number $b \notin \mathbb{Z}_p$ the p -adic open ball $\{a \mid |a - b|_p < 1\}$ is disjoint from \mathbb{Z}_p . Hence \mathbb{Z}_p is closed in \mathbb{Q}_p and, since it is bounded, also compact. But \mathbb{Z}_p is the disjoint union of the p open balls $\{a \mid |a - i|_p < 1\}$ with $i = 1, \dots, p$, hence is also open in \mathbb{Q}_p . As a locally compact Abelian group under addition, \mathbb{Q}_p has a Haar measure, unique up to a multiplicative constant, which can be normalized so that $\text{vol}(\mathbb{Z}_p) = 1$.

Any fixed power of a non-Archimedean valuation is also a valuation, and topologically equivalent; but up to this equivalence the p -adic valuations and the ordinary absolute value are the *only* valuations on \mathbb{Q} . The *rational adèle ring* $\mathbb{A}_{\mathbb{Q}}$ is the restricted direct product with respect to the \mathbb{Z}_p 's of the completions of \mathbb{Q} with respect to these valuations, i.e.

$$\mathbb{A}_{\mathbb{Q}} = \left\{ \alpha = (\alpha_{\infty}, (\alpha_p)) \mid \begin{array}{l} \alpha_{\infty} \in \mathbb{R}, \alpha_p \in \mathbb{Q}_p, \text{ and } \alpha_p \in \mathbb{Z}_p \\ \text{for all except finitely many } p \end{array} \right\} \tag{107}$$

and has the restricted product topology for which the sets $O_{\infty} \times \prod_p O_p$, with O_{∞} open in \mathbb{R} , O_p open in \mathbb{Q}_p and $O_p = \mathbb{Z}_p$ for all except finitely many p , form a base of open sets. As a restricted product of locally compact sets with respect to compact sets, $\mathbb{A}_{\mathbb{Q}}$ is locally compact.

Now \mathbb{Q} embeds in $\mathbb{A}_{\mathbb{Q}}$ diagonally (i.e. each $q \in \mathbb{Q}$ can be identified with the adèle all of whose components are q), and with this identification \mathbb{Q} is discrete in $\mathbb{A}_{\mathbb{Q}}$ and $\mathbb{A}_{\mathbb{Q}}/\mathbb{Q}$ is compact. A fundamental region for \mathbb{Q} in $\mathbb{A}_{\mathbb{Q}}$ is $[0, 1] \times \prod_p \mathbb{Z}_p$, which has volume 1 in the normalized Haar measure on $\mathbb{A}_{\mathbb{Q}}$. This gives rise to the interesting and natural *cut-and-project scheme*

$$\begin{array}{ccc} \mathbb{R} & \xleftarrow{\pi} & \mathbb{A}_{\mathbb{Q}} & \xrightarrow{\pi_{\text{int}}} & \prod_p (\mathbb{Z}_p) & \mathbb{Q}_p \\ & & \cup & & & \\ & & \mathbb{Q} & & & \end{array} \tag{108}$$

with componentwise projections and $\prod_{(Z_p)}$ denoting the restricted product. The image $\pi(\mathbb{Q})$ is, of course, dense in \mathbb{R} and the denseness of $\pi_{\text{int}}(\mathbb{Q})$ in $\prod \mathbb{Q}_p$ is equivalent to the Strong Approximation Theorem [6, Section 15]. If we choose for the window the closed and open set $\Omega := \prod_p \mathbb{Z}_p$ we obtain the model set $A(\Omega) = \mathbb{Z} \in \mathbb{R}$. Since $\text{vol}(\Omega) = 1$ in the normalized Haar measure on $\prod \mathbb{Q}_p$ and $\text{dens}(\mathbb{Z}) = 1$ we note that this satisfies (106). If instead we choose $\Omega := \prod_p (\mathbb{Z}_p \setminus p^k \mathbb{Z}_p)$ with $k \geq 2$ we obtain the ‘thin’ model set $A(\Omega) = F_k$. We say “thin” because, being not relatively dense, F_k is not a regular model set. The reason that Schlottmann’s result does not apply here is that Ω has empty interior: Ω contains no basic open set because it projects to a proper subset of \mathbb{Z}_p in every non-Archimedean component, whereas basic open sets project to \mathbb{Z}_p in all except finitely many components. Nevertheless, Ω has a positive volume in the normalized Haar measure on $\prod \mathbb{Q}_p$ given by

$$\text{vol}(\Omega) = \prod_p \text{vol}(\mathbb{Z}_p \setminus p^k \mathbb{Z}_p) = \prod_p \left(1 - \frac{1}{p^k} \right) = \frac{1}{\zeta(k)}, \tag{109}$$

which, in view of Proposition 11, agrees with (106). This is astonishing and we have no explanation for it at present, since merely by translating Ω we can not only reduce the density of A to 0 but can cause A to vanish altogether. Let $i: P \rightarrow \mathbb{Z}$, where P is the set of positive primes, be any one–one correspondence, and for each $p \in P$ choose $\alpha_p \in \mathbb{Z}_p$ with $\alpha_p \equiv i(p) \pmod{p^k}$. Then the window $\Omega + \alpha \subseteq \prod \mathbb{Z}_p$, where $\alpha = (\alpha_p) \in \prod \mathbb{Q}_p$, leads to the empty set under the cut-and-project construction because each $i \in \mathbb{Z}$ is excluded mod p^k for the corresponding p .

The visible points V_{Γ} of a lattice $\Gamma \subset \mathbb{R}^n$, for $n \geq 2$, can be obtained by a similar construction, using $(\mathbb{A}_{\mathbb{Q}})^n$, which is topologically isomorphic to the restricted product with respect to \mathbb{Z}_p^n

$$A := \mathbb{R}^n \times \prod_p (\mathbb{Z}_p^n) \mathbb{Q}_p^n. \tag{110}$$

Choose a basis $\{\mathbf{b}_1, \dots, \mathbf{b}_n\}$ of Γ and embed $\mathbb{Q}\Gamma$ in A by

$$\mathbf{x} = q_1 \mathbf{x}_1 + \dots + q_n \mathbf{x}_n \mapsto (\mathbf{x}, ((q_1, \dots, q_n)_p)), \tag{111}$$

where $(q_1, \dots, q_n)_p = (q_1, \dots, q_n)$ for each p . (In the terminology of commutative algebra, this establishes that A is isomorphic to $\Gamma \otimes_{\mathbb{Z}} \mathbb{A}_{\mathbb{Q}}$, the $\mathbb{A}_{\mathbb{Q}}$ -ification of the \mathbb{Z} -module Γ , see [16] under the index entry ‘ification’). Then the image of $\mathbb{Q}\Gamma$ is a discrete subgroup of A and $A/\mathbb{Q}\Gamma$ is compact with $\mathcal{F} = \mathcal{F}_{\Gamma} \times \prod \mathbb{Z}_p^n$ as a fundamental region, where \mathcal{F}_{Γ} is a fundamental region of Γ in \mathbb{R}^n . The volume of this fundamental region in the normalized Haar measure on A is $1/\text{dens}(\Gamma)$. This gives the cut-and-project scheme

$$\mathbb{R}^n \xleftarrow{\pi} (\mathbb{A}_{\mathbb{Q}})^n \xrightarrow{\pi_{\text{int}}} \prod_p (\mathbb{Z}_p^n) \mathbb{Q}_p^n \cup \mathbb{Q}\Gamma \tag{112}$$

with the images of $\mathbb{Q}\Gamma$ under π and π_{int} being dense. If we choose for the window the closed and open set $\Omega := \prod_p \mathbb{Z}_p^n$ we obtain the model set $\Lambda(\Omega) = \Gamma \subset \mathbb{R}^n$ which has $\text{vol}(\Omega) = 1$ and satisfies (106). If we choose $\Omega := \prod_p (\mathbb{Z}_p^n \setminus p\mathbb{Z}_p^n)$ we obtain $\Lambda(\Omega) = V_{\Gamma}$. Again, Ω has empty interior but positive volume, given by

$$\text{vol}(\Omega) = \prod_p \left(1 - \frac{1}{p^n}\right) = \frac{1}{\zeta(n)} \tag{113}$$

so that (106) holds by Proposition 6. Again, translating Ω can cause the model set to vanish. A translation $\alpha \in \prod \mathbb{Q}_p^n$ that does this can be constructed as follows: let $i : P \rightarrow \mathbb{Z}^n$ be any one–one correspondence and for each p choose $\alpha_p \equiv i(p) \pmod{p}$; then take $\alpha = (\alpha_p)$.

These adelic constructions are nothing more than number theoretic sieves which exclude certain residue classes modulo a power of each prime. The choice of window determines the residue classes to be retained and translating the window changes the set of residue classes without changing their number. Clearly, many other examples of the same type can be constructed.

If V_{Γ} and F_k were regular model sets, we would be able to use standard results on model sets to derive their diffractiveness [28], but the constructions just described are outside the range of current diffraction results. To the best of our knowledge, the diffraction of adelic model sets has not been studied, which is why we have had to derive our diffraction results from scratch.

Obviously, one further question is how relevant the examples are. Is the set of visible lattice points an isolated example, or more of a paradigm case of a family of examples with pure point diffraction? We believe the latter is true, and there is one immediate class of examples that springs to mind. If we view the visible points of \mathbb{Z}^2 as the orbit of $(1, 0)$ under the group $\text{SL}(2, \mathbb{Z})$, it is clear that this orbit, in general, will split into several pieces when $\text{SL}(2, \mathbb{Z})$ is replaced by one of the standard congruence subgroups. However, our methods are robust under further congruence constraints, and so it is clear that there is a large class of congruence subsets of the visible points which will have interesting diffraction spectra.

We hope to report on some examples soon.

10. Summary

We have demonstrated that the set of visible lattice points in dimensions $n \geq 2$ and the set of k th-power-free integers with $k \geq 2$ both possess well-defined autocorrelations and pure point diffraction spectra. We have shown how to replace the intuitive but incomplete derivation of the spectra by a rigorous number theoretical argument based on explicit computation of the autocorrelation followed by Fourier inversion and repeated application of the Poisson summation formula.

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Appendix A.

This paper has required several calculations of densities of discrete point sets, for which we have used natural density. The natural density is in fact nowhere near as natural as one would expect from its name. Here, we briefly examine the drawbacks of the natural density and also the uniform density, and suggest a simply stated definition of density, intermediate between natural density and uniform density, that is applicable to sets of the kind we encounter here. A fuller exposition will appear elsewhere [23].

As an aid to describing the behaviour of densities we begin by introducing some standard measurements of measurable sets in \mathbb{R}^n .

A.1. Measurements of measurable sets

For a bounded, measurable set \mathcal{R} in \mathbb{R}^n we denote by $V(\mathcal{R})$ the volume of \mathcal{R} (that is, its n -dimensional measure). Given $\varepsilon > 0$ we denote by $\partial_\varepsilon \mathcal{R}$ the set of points in \mathbb{R}^n whose distance from the boundary of \mathcal{R} is less than ε . Then $\partial_\varepsilon \mathcal{R}$ is open, hence measurable, so also has a volume. We temporarily call a set \mathcal{R} *good* if

- (a) \mathcal{R} is bounded and measurable, and
- (b) $V(\partial_\varepsilon \mathcal{R})/\varepsilon$ is bounded as $\varepsilon \rightarrow 0$.

For good sets we can define the functions

$$V = V(\mathcal{R}), \tag{A.1}$$

$$M = M(\mathcal{R}) = \sup_{\mathbf{x} \in \mathcal{R}} |\mathbf{x}|, \tag{A.2}$$

$$R = R(\mathcal{R}) = \inf_{\mathbf{c} \in \mathbb{R}^n} \sup_{\mathbf{x} \in \mathcal{R}} |\mathbf{x} - \mathbf{c}|, \tag{A.3}$$

$$S = S(\mathcal{R}) = \sup_{0 < \varepsilon \leq R} \{V(\partial_\varepsilon \mathcal{R})/2\varepsilon\}. \tag{A.4}$$

The following relations are immediate from these definitions:

$$R \leq M, \quad V \leq v_n R^n, \quad RS \geq 2^{n-1}V, \quad S \geq v_n R^{n-1}/2, \tag{A.5}$$

where v_n is the volume of the unit ball in \mathbb{R}^n .

Each of these functions is invariant under Euclidean transformations and scales homogeneously with dilation of $\mathcal{R}:M$ and R proportionally to the dilation factor λ , V proportionally to λ^n and S proportionally to λ^{n-1} . They are affected by a non-singular affine transformation $A = T + \mathbf{t}$ (where T is linear and \mathbf{t} is a translation) as follows:

$$V(A(\mathcal{R})) = |\det T| V(\mathcal{R}), \tag{A.6}$$

$$M(A(\mathcal{R})) \leq \|T\| M(\mathcal{R}) + \|\mathbf{t}\|, \tag{A.7}$$

$$R(A(\mathcal{R})) \leq \|T\| R(\mathcal{R}), \tag{A.8}$$

$$S(A(\mathcal{R})) \leq 2^n |\det T| \|T\|^{n-1} \|T^{-1}\|^n S(\mathcal{R}). \tag{A.9}$$

Of these functions, V , M and R are straightforward, representing the volume, the maximum distance from the origin and the circumradius of \mathcal{R} , respectively. The function S is a substitute for the surface area of \mathcal{R} and in fact is always greater than or equal to the $(n - 1)$ -dimensional measure of the boundary $\partial\mathcal{R}$. The condition $\varepsilon \leq R$ in its definition is arbitrary, but ensures the scaling of S under dilations mentioned above. (Using any fixed multiple of R would have the same effect.)

These functions extend to arbitrary measurable sets if we define $M = R = \infty$ when \mathcal{R} is unbounded (in which case V may or may not be infinite) and $S = \infty$ when (b) fails. We note that $V(\partial_\varepsilon \mathcal{R})$ is infinite for every ε when \mathcal{R} is an unbounded set of finite volume, so $S = \infty$ for every set of finite volume that is not good.

A.2. Densities of discrete sets

Let X be a locally finite set of points in \mathbb{R}^n , that is, every bounded region of \mathbb{R}^n contains only finitely many points of X . Here we compare ways of defining a density for such a set X .

A.2.1. Uniform density

X has *uniform density* $\mathcal{D} = \mathcal{D}(X)$ if

$$|\{\mathbf{x} \in X \mid |\mathbf{x} - \mathbf{c}| < R\}| = \mathcal{D}v_n R^n + o(R^n) \quad \text{as } R \rightarrow \infty \tag{A.10}$$

uniformly in \mathbf{c} .

It is immediate from this definition that

(i) *uniform density is invariant under Euclidean transformations.* A less immediate consequence is that if \mathcal{R} is an arbitrary measurable set in \mathbb{R}^n and $f(V)$ is any function of V (no matter how slowly increasing) that tends to infinity with V then

$$|\mathcal{R} \cap X| = \mathcal{D}V(\mathcal{R}) + o(V(\mathcal{R})) + O(f(V(\mathcal{R}))S(\mathcal{R})) \quad \text{as } V(\mathcal{R}) \rightarrow \infty. \tag{A.11}$$

A consequence of (A.11) is

(ii) *uniform density is independent of shape.* That is, if X has uniform density \mathcal{D} then (A.10) continues to hold, with the same value of \mathcal{D} , when the sphere $|\mathbf{x} - \mathbf{c}| < R$ is replaced by an expanding set of any other shape and v_n is replaced by the volume of the set in the family that has $R = 1$.

Another consequence of (A.11) (using (A.6) and (A.9) to control the error terms) is

(iii) *uniform density varies as the reciprocal of the determinant under nonsingular affine transformations.*

All crystals and most quasicrystals possess a uniform density. However, the set V of the visible points of a lattice Γ does not. In fact, Proposition 6 shows that the number of points of V in a ball of radius R with centre $\mathbf{0}$ is $(\text{dens}(\Gamma)/\zeta(n))v_nR^n + o(R^n)$, whereas Proposition 5 shows that there are arbitrarily large balls that contain no points of V . Similarly, the set F_k of k th-power-free integers in \mathbb{R} does not possess a uniform density either. Consequently, uniform density is of no use for the questions considered in this paper — in fact, none of the sets whose densities we require possesses a uniform density.

A definition of density known as *van Hove density* is implicit in Chapter 2 of [26], if the identical formulæ (3.3) and (3.8) of [26, Chapter 2] are regarded as defining the density of a general potential operator Φ . This is equivalent to uniform density. The fact that uniform density implies van Hove density follows from (A.11) and the converse implication results from choosing the van Hove sets to be balls.

A.3. Natural density

As defined in (10) for uniformly discrete sets, X has *natural density* $\mathcal{D} = \mathcal{D}(X)$ if

$$|\{\mathbf{x} \in X \mid |\mathbf{x}| < R\}| = \mathcal{D}v_nR^n + o(R^n) \quad \text{as } R \rightarrow \infty. \tag{A.12}$$

This is often called *asymptotic density* in the context of number theory.

Like uniform density, natural density is

(i) *invariant under Euclidean transformations.* (Translation invariance is easy to derive, though not quite as immediate as for uniform density.) However, natural density is not independent of shape and does not transform naturally under linear transformations. For example, let $X = \{(x, y) \mid x, y \in \mathbb{Z}, |y| < 2|x|\}$ be the set of points in \mathbb{Z}^2 that lie in the double wedge with angle $2 \tan^{-1} 2$. The natural density of X is $(2/\pi) \tan^{-1} 2 = 0.7048\dots$, but the proportion of the integer points in the square $\{(x, y) \mid |x|, |y| < R\}$ that belong to X is $\frac{3}{4}$ and the proportion of the integer points in the square $\{(x, y) \mid |x| + |y| < R\}$ that belong to X is $\frac{2}{3}$. So for this set, counting points according to the L^2 , L^∞ or L^1 norm in \mathbb{R}^2 gives three distinct answers. The linear map $T(x, y) = (2x, y)$ transforms X into the set of integer points with x -coordinate even in the double wedge $\{(x, y) \mid x, y \in \mathbb{Z}, |y| < |x|\}$ with angle $\pi/2$. This set has density $\frac{1}{4}$, which is not a half of $(2/\pi) \tan^{-1} 2$, showing that natural density does not transform naturally under linear maps.

For the sets we deal with in this paper natural density does not exhibit such pathological behaviour. For example, Proposition 6, Theorems 1 and 2, which establish the densities of certain subsets of a lattice Γ in \mathbb{R}^n , all give a factor $\text{dens}(\Gamma)$ as the only dependency of the density on the lattice, confirming that the density varies as the reciprocal of the determinant under linear transformations. However, rather than having to verify this in each individual case, as in effect we have done here, it would be preferable to have a definition of density with strength intermediate between uniform density and natural density for which nonpathological behaviour is guaranteed.

A.4. Tied density

It is possible to define an alternative form of density, intermediate between uniform density and natural density, that overcomes these difficulties. This depends on the idea of making uniform density less free of the origin by replacing R by M in the error term of (A.10). We say that X has *tied density* $\mathcal{D} = \mathcal{D}(X)$ if for all $\mathbf{c} \in \mathbb{R}^n$

$$|\{\mathbf{x} \in X \mid |\mathbf{x} - \mathbf{c}| < R\}| = \mathcal{D}v_n R^n + o(M^n) \quad \text{as } R \rightarrow \infty, \quad (\text{A.13})$$

where $M = R + |\mathbf{c}|$.

Again it is easy to see that

(i) *tied density is invariant under Euclidean transformations.* In a similar way to (A.11) it can also be shown that if X has tied density \mathcal{D} and \mathcal{R} is an arbitrary measurable set in \mathbb{R}^n then

$$|\mathcal{R} \cap X| = \mathcal{D}V(\mathcal{R}) + o(M(\mathcal{R})^n) + o(M(\mathcal{R})S(\mathcal{R})) \quad \text{as } V(\mathcal{R}) \rightarrow \infty. \quad (\text{A.14})$$

This is sufficient to establish that

- (ii) *tied density is independent of shape*; and, with the help of (A.6) and (A.7),
- (iii) *tied density varies as the reciprocal of the determinant under nonsingular affine transformations.*

The error term $o(M^n)$ in the definition of tied density has the effect that, while balls centred away from the origin are not excluded from consideration, those distant from the origin by more than a few radii have little influence. It can be regarded as a reminder to experimentalists that, as the radius of a probe is increased, the next position of the probe should not be more than a few radii from the previous position. There is, nevertheless, a great deal of arbitrariness in the definition of tied density. The core idea is to make the error term in (126) depend on \mathbf{c} as well as on R , but any kind of dependency on \mathbf{c} (provided that for every R the error term tends to infinity with \mathbf{c}) would have a similar effect. The faster the rate of increase of the error term with \mathbf{c} the more widely applicable the density definition becomes. In an effort to conceal this arbitrariness we have chosen a very simple dependency on \mathbf{c} .

It is clear from these definitions that the existence of uniform density for a set X implies the existence of tied density for X , which in turn implies the existence of natural density for X , and that each of these densities has a unique value when it is defined.

To establish the existence of tied density for the sets studied in this paper we would need to count points x with $|x - c| < R$ instead of $|x| < R$. As a result, though the x and y variables in sums still have range R (but no longer centred at the origin), the l and m variables have range $R + |c| = M$. The effect is that main terms remain the same but some R 's are replaced by M 's in error terms. The new error terms for the results of this paper when the ball of radius R is centred away from the origin are as follows:

Proposition 6 ($n \geq 3$)	$O(1/R) + O(M/R^n)$,
Proposition 6 ($n = 2$)	$O(\log M/R) + O(M/R^2)$,
Theorem 1 ($n \geq 3$)	$O(1/R) + O(M^2/R^n)$,
Theorem 2 ($n = 2$)	$O(\sqrt{M}/R) + O(M/R^2)$,
Proposition 11 ($n = 1$)	$O(M^{1/k}/R)$,
Theorem 4 ($n = 1$)	$O(R^{1/k}M^{1/k}/RM^{1/k^2}) + O(M^{1/k}/R)$.

Each of these error terms, when multiplied by R^n , is well within the error estimate $o(M^n)$ required by the definition (A.13) of tied density. Consequently, we could have worked with tied densities instead of natural densities throughout. One concrete advantage of such an approach would have been that we could then have worked with the visible points of cubic lattices only, then used property (iii) of tied density to transfer the results to other lattices.

References

- [1] T.M. Apostol, Introduction to Analytic Number Theory, Springer, New York, 1976.
- [2] L. Argabright, J. Gil de Lamadrid, Fourier Analysis of Unbounded Measures on locally Compact Abelian groups, Memoirs of the American Mathematical Society, Vol. 145, AMS, Providence, RI, 1974.
- [3] M. Baake, U. Grimm, D.H. Warrington, Some remarks on the visible points of a lattice, J. Phys. A 27 (1994) 2669–2674 and 5041 (Erratum); see also math-ph/9903046.
- [4] S.K. Berberian, Measure and Integration, Macmillan, New York, 1965, reprint: Chelsea, New York, 1970.
- [5] D. Berend, in preparation.
- [6] J.W.S. Cassels, Global Fields, in: J.W.S. Cassels, A. Fröhlich (Eds.), Algebraic Number Theory, Academic Press, London, 1967, pp. 42–84.
- [7] J.M. Cowley, Diffraction Physics, 3rd Edition, North-Holland, Amsterdam, 1995.
- [8] J. Dieudonné, Treatise on Analysis, Vol. II, Academic Press, New York, 1970.
- [9] G. Grimmett, Large deviations in the random sieve, Math. Proc. Cambridge Philos. Soc. 121 (1997) 519–530.
- [10] P.M. Gruber, C.G. Lekkerkerker, Geometry of Numbers, 2nd Edition, North-Holland, Amsterdam, 1987.
- [11] E. Hewitt, K.A. Ross, Abstract Harmonic Analysis I, 2nd Edition, Springer, New York, 1979.
- [12] A. Hof, On diffraction by aperiodic structures, Comm. Math. Phys. 169 (1995) 25–43.
- [13] A. Hof, Diffraction by aperiodic structures, in: R.V. Moody (Ed.), The Mathematics of Long-Range Aperiodic Order, NATO ASI Series C, Vol. 489, Kluwer, Dordrecht, 1997, pp. 239–268.
- [14] L.K. Hua, Introduction to Number Theory, Springer, Berlin, 1982.
- [15] M.N. Huxley, Moments of differences between square-free numbers, in: G.R.H. Greaves, G. Harman, M.N. Huxley (Eds.), Sieve Methods, Exponential Sums, and their Applications in Number Theory, Lecture Notes in Mathematics, Vol. 237, Cambridge University Press, Cambridge, 1997, pp. 187–204.
- [16] J.T. Knight, Commutative Algebra, Cambridge University Press, Cambridge, 1971.
- [17] J.C. Lagarias, Meyer's concept of quasicrystal and quasiregular sets, Comm. Math. Phys. 179 (1996) 365–376.

- [18] Y. Meyer, *Algebraic Numbers and Harmonic Analysis*, North-Holland, Amsterdam, 1972.
- [19] L. Mirsky, Arithmetical pattern problem relating to divisibility by r th powers, *Proc. London Math. Soc.* 50 (1949) 497–508.
- [20] R.V. Moody, Meyer sets and their duals, in: R.V. Moody (Eds.), *The Mathematics of Long-Range Aperiodic Order*, NATO ASI Series C, Vol. 489, Kluwer, Dordrecht, 1997, pp. 403–441.
- [21] R. Mosseri, Visible points in a lattice, *J. Phys. A* 25 (1992) L25–L29.
- [22] S.S. Pillai, On sets of square-free numbers, *J. Indian Math. Soc. (New Ser.)* 2 (1936) 116–118.
- [23] P.A.B. Pleasants, in preparation.
- [24] M. Reed, B. Simon, *Methods of Modern Mathematical Physics. I: Functional Analysis*, 2nd Edition, Academic Press, San Diego, 1980.
- [25] W. Rudin, *Functional Analysis*, 2nd Edition, McGraw-Hill, New York, 1991.
- [26] D. Ruelle, *Statistical Mechanics: Rigorous Results*, Benjamin, Reading, 1969; reprint: Addison-Wesley, Redwood City, 1989.
- [27] M. Schlottmann, Cut-and-project sets in locally compact Abelian groups, in: J. Patera (Ed.), *Quasicrystals and Discrete Geometry*, Fields Institute Monographs, Vol. 10, AMS, Providence, RI, 1998, pp. 247–264.
- [28] M. Schlottmann, Generalized model sets and dynamical systems, in: M. Baake, R.V. Moody (Eds.), *Directions in Mathematical Quasicrystals*, CRM Monograph Series, AMS, Providence, RI, 2000, in press.
- [29] M.R. Schroeder, A simple function and its Fourier transform, *Math. Intelligencer* 4 (1982) 158–161, and: *Number Theory in Science and Communication*, 3rd Edition, Springer, Berlin, 1997.
- [30] L. Schwartz, *Théorie des Distributions*, 3rd Edition, Hermann, Paris, 1998.