Canad. Math. Bull. 2026, pp. 1–14
http://dx.doi.org/10.4153/S0008439526101854
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Circles in diffraction

Emily R. Korfanty and Nicolae Strungaru

Abstract. Given a Fourier transformable measure in two dimensions, we find a formula for the intensity of its Fourier transform along circles. In particular, we obtain a formula for the diffraction measure along a circle in terms of the autocorrelation measure. We then look at some applications of this formula.

1 Introduction

Since the early 1900s, crystallographers have used diffraction experiments to determine the structure of crystals. Until the discovery of quasicrystals in 1984 by Dan Shechtman [SBGC84], pure-point diffraction was taken as evidence of an underlying periodic structure in the material. Quasicrystals, however, exhibit sharp diffraction patterns, and typically show symmetries that are impossible in materials with a periodic structure. Shechtman's discovery, for which he was awarded the 2011 Nobel Prize in Chemistry, inspired a new interest in aperiodic structures and mathematical diffraction theory. For an overview of this area, we recommend the monographs [BG13, BG17].

A rigorous mathematical treatment of diffraction was introduced by Hof in [Hof95]. He defined the diffraction measure as the Fourier transform of the so-called autocorrelation measure. Diffraction is now well understood for systems with pure-point spectrum [LSS24], and systems with finite local complexity (FLC) coming from cut-and-project schemes [BHS17, BM04, KR18, RS17, Sch00, Str05, Str17, Str20a].

On the other hand, diffraction is generally much less understood for systems without FLC with respect to translations. One such example is the pinwheel tiling [Rad94]. Its diffraction is rotationally invariant and has a Bragg peak of unit intensity at the origin [MPS06], but nothing else is known. In particular, it is not known if the diffraction is absolutely continuous, singular continuous, or mixed.

There are many examples of rotationally invariant diffraction patterns. The diffraction of any rotationally invariant measure, or of any substitution tiling with statistical circular symmetry, is rotationally invariant [DSV00, FHG25, Fre08, Sad98]. Rotational invariance also appears in X-ray powder diffraction experiments, where the sample is ground into many smaller samples prior to the usual diffraction process

Received by the editors July 4, 2025; revised January 5, 2026; accepted January 5, 2026.
Published online on Cambridge Core March 2, 2026.
E.R.K. was supported by NSERC via a CGS D scholarship. N.S. was supported by the NSERC via grants 2020-00038 and 2024-04853.
AMS subject classification: **78A45**, 42B10, 33C10.
Keywords: Diffraction, Bessel functions, Fourier transform.

https://doi.org/10.4153/S0008439526101854 Published online by Cambridge University Press

[Cow81, War69]. During the grinding process, the samples tend to rotate in random directions. This random distribution of rotations on the unit circle is typically statistically circular, and hence the powder diffraction is rotationally invariant. Similarly, diffraction patterns from glass are also rotationally invariant, due to the randomness in the liquid frozen to obtain the glass [War34, War37].

Another interesting class of highly ordered structures are Vogel spirals, which seem to have circularly symmetric diffraction patterns supported on rings (see, e.g., [NLT12, TCD11]). As far as we know, the nature of their spectrum is not known.

In [BFG07a, BFG07b, GD11], numerical approximations of the pinwheel diffraction were compared to a powder diffraction from $\mathbb{Z}^2$. These numerical approximations suggest that the pinwheel diffraction may include bright circles with the same radii as the circles in the powder diffraction, which would imply the existence of a singular continuous component of the spectrum. Despite this observed similarity to the powder diffraction from $\mathbb{Z}^2$, it is still unknown whether or not there exists any circle in the pinwheel diffraction. Besides numerical simulations, we are not aware of any progress made toward understanding the diffraction of the pinwheel tiling in the last 20 years.

There are two steps which are necessary in order to prove the existence (or nonexistence) of circles in the diffraction of a point set. First, one must understand the relationship between the autocorrelation measure and circles appearing in the diffraction. Then, one must better understand the autocorrelation measure. It is our goal in this article to address the first step only. More precisely, we derive a formula for computing the intensity of a circle in the diffraction in terms of the autocorrelation. We show that the diffraction intensity $\widehat{\gamma}(C_r)$ along the circle $C_r = \{x \in \mathbb{R}^2 : \|x\| = r\}$ is given by

$$\widehat{\gamma}(C_r) = \lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, \mathrm{d}\gamma(y)\,, \tag{1.1}$$

where γ is the autocorrelation measure and J_0 is the Bessel function of the first kind of order 0 (see Corollary 3.3). The formula is similar, in some sense, to the classical formula for calculating the intensity of Bragg peaks via the average integral of a character with respect to the autocorrelation measure [BG17, Theorem 4.10.14].

This formula shows potential for many applications to the study of the diffraction for substitution tilings with statistical circular symmetry, once the autocorrelation measures are better understood.

Our approach to obtain (1.1) is as follows. Heuristically, we should have the equalities $\widehat{\gamma}(C_r) = \widehat{\gamma}(1_{C_r})$ " = " $\gamma(\widehat{1_{C_r}})$. Of course, the last equality above cannot hold since $\widehat{1_{C_r}} = 0$. Moreover, the equality $\widehat{\gamma}(f) = \gamma(\widehat{f})$ holds for Schwartz functions, but 1_{C_r} is not even continuous. To get around this issue, we instead approximate 1_{C_r} by a sequence of Schwartz functions of the form $f_n = g_n * \theta_r$, where θ_r is the uniform probability measure on C_r (defined in (2.1)), and g_n is an approximate identity sequence of Gaussian functions, renormalized such that f_n converges to 1 on C_r. We obtain Theorem 3.2 by applying the formula $\widehat{\gamma}(f_n) = \gamma(\widehat{f_n})$ and letting $n \to \infty$.

Our article is organized as follows. We review basic definitions and our framework in Section 2. We introduce the Fourier transform of strongly tempered measures (see

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Definition 2.1), which extends the classical theory of Fourier transformable measures in $\mathbb{R}^d$. We then briefly review the Bessel functions J_0 and I_0. Section 2.4 provides the fundamental tool for proving Theorem 3.2 (stated above). Specifically, we show via a straightforward application of the dominated convergence theorem that the intensity $\widehat{\gamma}(C_r)$ can be calculated as the limit of integrals $\int_{\mathbb{R}^2} f_n(x)\,\mathrm{d}\widehat{\gamma}(x)$, provided that the sequence f_n of Schwartz functions satisfies certain conditions (we call such sequences approximate r-circles). In Section 3, our main result (Theorem 3.2) is obtained by constructing an explicit approximate r-circle with easily computable Fourier transforms. In Section 4, we look at several examples and applications of Theorem 3.2. In particular, the Poisson summation formula for $\mathbb{Z}^2$ yields the following result.

Proposition 4.5 *For all $k > 0$, the sum of two squares function r_2 satisfies*

$$\lim_{n\to\infty} \frac{2\pi\sqrt{\pi k}}{n} \sum_{m=0}^{\infty} r_2(m) e^{-\frac{\pi^2 m}{n^2}} J_0(2\pi\sqrt{km}) = \begin{cases} r_2(k) & k \in \mathbb{N} \\ 0 & k \notin \mathbb{N}. \end{cases}$$

We discuss a connection between this result and Hardy–Landau summation formula in Remark 4.6.

2 Preliminaries

2.1 Definitions and notation

Throughout the article, $\mathbb{R}^d$ denotes the Euclidean d-space. We will denote the standard Euclidean norm on $\mathbb{R}^d$ by $\|\cdot\|$. We use λ or $\mathrm{d}x$ to denote the Lebesgue measure on $\mathbb{R}^d$. As usual, $C_c(\mathbb{R}^d)$ denotes the space of continuous functions with compact support, and $C_c^\infty(\mathbb{R}^d)$ denotes the subspace of $C_c(\mathbb{R}^d)$ consisting of smooth functions. The space of Schwartz functions is denoted by $\mathcal{S}(\mathbb{R}^d)$ and the space of tempered distributions by $\mathcal{S}'(\mathbb{R}^d)$. We write $\|f\|_\infty := \sup_{x\in\mathbb{R}^d} |f(x)|$ for the supremum norm of any bounded function f.

Recall that the Fourier transform $\widehat{f}$ of a function $f \in L^1(\mathbb{R}^d)$ at $y \in \mathbb{R}^d$ is defined by $\widehat{f}(y) := \int_{\mathbb{R}^d} f(x) e^{-2\pi i x\cdot y}\,\mathrm{d}x$. This induces a bijection $T \to \widehat{T}$ on $\mathcal{S}'(\mathbb{R}^d)$ (see [GS16] for background on tempered distributions and their Fourier theory).

2.2 Strongly tempered measures

In this section, we introduce a space of measures with a certain property (see Definition 2.1 below) that is compatible with diffraction theory. We will prove our results in this general setting.

Let us recall that a (Radon) measure is a linear functional $\mu : C_c(\mathbb{R}^d) \to \mathbb{C}$ that is continuous in the inductive topology (see, e.g., [RS17]). Via the Riesz Representation Theorem [RS00, Rud87], any Radon measure is a linear combination of positive regular Borel measures. Furthermore, for each measure μ, there exists a unique smallest positive measure $|\mu|$, called the variation measure of μ, satisfying $|\mu(f)| \le |\mu|(|f|)$ for all $f \in C_c(\mathbb{R}^d)$ (see [Ped89, RS17]).

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In what follows, we use the distributional Fourier transform for measures. Let us first note that, in general, $\int_{\mathbb{R}^d} f(x)\,\mathrm{d}\mu(x)$ may not be defined for a measure μ and Schwartz function f. Since we will work with integrals of this type, we will need to restrict the class of measures we are studying. Recall from [BS23] that μ is strongly tempered[1] if there exists a polynomial $P(x) \in \mathbb{C}[x_1, x_2, \ldots, x_d]$ such that $\int_{\mathbb{R}^d} \frac{1}{1+|P(x)|}\,\mathrm{d}|\mu|(x) < \infty$.

For the rest of this article, we only consider strongly tempered measures.

The following fact about strongly tempered measures explains why this definition is important for us.

Fact 2.1 [BS23, Theorem 2.7] *A measure μ is strongly tempered if and only if for all $f \in \mathcal{S}(\mathbb{R}^d)$ we have $\int_{\mathbb{R}^d} |f(x)|d|\mu|(x) < \infty$. Moreover, in this case, the mapping $T_\mu : \mathcal{S}(\mathbb{R}^d) \to \mathbb{C}$ given by $T_\mu(f) := \int_{\mathbb{R}^d} f(t)d\mu(t)$ defines a tempered distribution, and μ and T_μ uniquely determine each other.*

Let us now discuss the Fourier transformability of strongly tempered measures. Every strongly tempered measure is Fourier transformable as a distribution. Its Fourier transform is a tempered distribution, but it may not be a measure. Even if it is a measure, it may not be strongly tempered (see, e.g., [AG74, Proposition 7.1] or [BS23, Section 3]). Since our results rely on the distributional Fourier transform being a strongly tempered measure, we introduce the following definition.

Definition 2.1 A measure μ is called *Fourier transformable in the strongly tempered sense* if μ is a strongly tempered measure and there exists a strongly tempered measure ν such that, as tempered distributions, we have $\widehat{T_\mu} = T_\nu$. In the case, we write $\widehat{\mu} := \nu$ and refer to this measure as the *Fourier transform of μ in the strongly tempered sense*.

We denote by $\mathcal{SM}(\mathbb{R}^d)$ the space of all strongly tempered measures μ which are Fourier transformable in the strongly tempered sense.

Remark 2.2

(a) A strongly tempered measure μ is Fourier transformable in the measure sense (see [AG74, MS17] for a definition of Fourier transformability for measures) if and only if $\mu \in \mathcal{SM}(\mathbb{R}^d)$ and $\widehat{\mu}$ is translation bounded [Str20b, Theorem 5.2]. Moreover, in this case, the two Fourier transforms coincide.

In particular, if μ is a strongly tempered measure that is also Fourier transformable in the measure sense, then $\mu \in \mathcal{SM}(\mathbb{R}^d)$ and the Fourier transforms coincide. This allows us to use the same notation for both Fourier transforms.

(b) Given a translation-bounded measure ω, we obtain a translation-bounded, and hence strongly tempered, autocorrelation measure γ. Since γ is positive definite, it is Fourier transformable in the measure sense [AG74, BF75]. By (a), we have $\gamma \in \mathcal{SM}(\mathbb{R}^d)$ and $\widehat{\gamma}$ is the Fourier transform of γ in the strongly tempered sense.

(c) Instead of the Fourier theory of strongly tempered measures, one could instead use the theory of mild distributions [Fei80, Fei89].

We now list some easy observations about $\mathcal{SM}(\mathbb{R}^d)$.

[1] In [AG74], the authors call such a measure slowly increasing. The term strongly tempered is used in [BS23].

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Fact 2.3 *Let $\mu \in \mathcal{SM}(\mathbb{R}^d)$. Then the following statements hold:*

(a) *The measures μ and $\widehat{\mu}$ uniquely determine each other.*

(b) *For all $f \in \mathcal{S}(\mathbb{R}^d)$, we have $\widehat{f} \in L^1(|\mu|)$, $f \in L^1(|\widehat{\mu}|)$, and*

$$\int_{\mathbb{R}^d} \widehat{f}(y)\, d\mu(y) = \int_{\mathbb{R}^d} f(x)\, d\widehat{\mu}(x)\,.$$

(c) *$\widehat{\mu} \in \mathcal{SM}(\mathbb{R}^d)$ and $\widehat{\widehat{\mu}} = \mu^\dagger$, where $\mu^\dagger(f) := \int_{\mathbb{R}^d} f(-x)\, d\mu(x)$. In particular, the Fourier transform is a bijection from $\mathcal{SM}(\mathbb{R}^d)$ onto $\mathcal{SM}(\mathbb{R}^d)$.*

We conclude this section by recalling a classical result about convolutions that we will need in Section 3.

Theorem 2.4 [Gra08, Theorem 2.3.20] *Let $T \in \mathcal{S}'(\mathbb{R}^d)$ be a tempered distribution, and let $f \in \mathcal{S}(\mathbb{R}^d)$ be a Schwartz function. Then $f * T$ is a C^∞ function, where*

$$f * T(\varphi) := T(f^\dagger * \varphi) \qquad \forall \varphi \in \mathcal{S}(\mathbb{R}^d)\,,$$

and $f^\dagger(x) := f(-x)$. Furthermore, if T has compact support, then $f * T \in \mathcal{S}(\mathbb{R}^d)$.

2.3 Bessel functions

In Section 3, we encounter certain integrals that turn out to be exactly the integrals defining the Bessel function J_0 of the first kind of order 0 and the modified Bessel function I_0 of the first kind of order 0. In this section, we collect the facts about these functions that will be important for our computations. Since these results are well known, we skip them, and refer the reader to [Wat44] for the general theory of Bessel functions. The reader may also refer to the extended arXiv version of this article [KS24] for short proofs of the specific results needed in Section 3.

For $r > 0$, we denote by $\theta_r : C_c(\mathbb{R}^2) \to \mathbb{C}$ the uniform probability measure on the circle $C_r := \{x \in \mathbb{R}^2 : \|x\| = r\}$. More precisely,

$$\theta_r(f) := \frac{1}{2\pi} \int_{-\pi}^{\pi} f(r\cos\theta, r\sin\theta)\, \mathrm{d}\theta \qquad \forall f \in C_c(\mathbb{R}^2)\,. \tag{2.1}$$

Now, recall that the Bessel function J_0 satisfies

$$J_0(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-iz\cos\theta}\, \mathrm{d}\theta \qquad \forall z \in \mathbb{C}\,.$$

Using this integral representation, it is easy to see that J_0 appears in the Fourier transform of θ_r. More specifically, a short, trivial computation shows that for all $r > 0$, the Fourier transform of θ_r is an absolutely continuous measure with density function

$$\widehat{\theta_r}(y) = J_0(2\pi r\|y\|) \qquad \forall y \in \mathbb{R}^2\,. \tag{2.2}$$

Next, we recall that the modified Bessel function I_0 satisfies

$$I_0(t) = J_0(it) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{t\cos\theta}\, \mathrm{d}\theta \qquad \forall t \geq 0\,.$$

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This function will appear naturally in Section 3 as a convolution of a Gaussian function and θ_r. Lastly, we will need the following well-known asymptotic property of I_0 (compare [AS72, Equation 9.7.1] and [Wat44, Section 7.23, Equations (2)–(3)]):

$$I_0(t) \sim \frac{e^t}{\sqrt{2\pi t}} \qquad \text{as } t \to \infty\,. \tag{2.3}$$

2.4 The measure of circles

We restrict our attention to $\mathbb{R}^2$. In this section, we show that the measure of a circle can be computed as a limit via a sequence of Schwartz functions. For a Fourier transformable measure μ, this will allow us to express the measure $\widehat{\mu}(C_r)$ as a limit in terms of integrals with respect to the original measure μ.

Definition 2.2 Let $r > 0$. We say that a sequence $\{f_n\}_{n\in\mathbb{N}}$ of functions in $\mathcal{S}(\mathbb{R}^2)$ is an *approximate r-circle* if the following conditions are satisfied:

(C1) $\lim_{n\to\infty} f_n(x) = 1_{C_r}(x)$ for all $x \in \mathbb{R}^2$;

(C2) there exists some $F \in \mathcal{S}(\mathbb{R}^2)$ such that

$$|f_n(x)| \le F(x) \qquad \forall x \in \mathbb{R}^2\,, \forall n \in \mathbb{N}\,.$$

While approximate r-circles are easy to construct, for applications, we will need sequences with nice, easily computable Fourier transforms. We will construct one such example in Section 3.

We first show that for any strongly tempered measure μ, the value of μ along C_r can be computed as a limit via an approximate r-circle.

Lemma 2.5 *Let μ be a strongly tempered measure. Then for any approximate r-circle $\{f_n\}_{n\in\mathbb{N}}$, we have*

$$\mu(C_r) = \lim_{n\to\infty} \int_{\mathbb{R}^2} f_n(x)\, d\mu(x)\,. \tag{2.4}$$

Proof By Fact 2.1, if μ is strongly tempered then $f \in L^1(|\mu|)$ for every $f \in \mathcal{S}(\mathbb{R}^2)$. In particular, if $\{f_n\}_{n\in\mathbb{N}}$ is an approximate r-circle and F is as defined in condition (C2), then $F \in L^1(|\mu|)$. Finally, by condition (C1) and the dominated convergence theorem, we have

$$\mu(C_r) = \int_{\mathbb{R}^2} 1_{C_r}(x)\, \mathrm{d}\mu(x) = \int_{\mathbb{R}^2} \lim_{n\to\infty} f_n(x)\, \mathrm{d}\mu(x) = \lim_{n\to\infty} \int_{\mathbb{R}^2} f_n(x)\, \mathrm{d}\mu(x)\,.$$

■

As an immediate consequence, we get the following.

Corollary 2.6 *If $\mu \in \mathcal{SM}(\mathbb{R}^2)$ and $\{f_n\}_{n\in\mathbb{N}}$ is an approximate r-circle, then*

$$\widehat{\mu}(C_r) = \lim_{n\to\infty} \int_{\mathbb{R}^2} f_n(x)\, d\widehat{\mu}(x) = \lim_{n\to\infty} \int_{\mathbb{R}^2} \widehat{f_n}(x)\, d\mu(x)\,.$$

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3 Circles in diffraction

We now construct an approximate r-circle via the convolution of θ_r with a family of Gaussian functions. We then use this approximate r-circle and Corollary 2.6 to derive an explicit formula for the diffraction measure of a circle in terms of the autocorrelation.

Let G_n be the following family of two-dimensional Gaussian functions:

$$G_n(x) = e^{-n^2\|x\|^2} \qquad \forall x \in \mathbb{R}^2,\ \forall n \in \mathbb{N}, \tag{3.1}$$

and let θ_r be as in (2.1). Consider the convolution $G_n * \theta_r$, defined by

$$G_n * \theta_r(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi} G_n(x_1 - r\cos\theta, x_2 - r\sin\theta)\,\mathrm{d}\theta \qquad \forall x = (x_1, x_2) \in \mathbb{R}^2.$$

Since both θ_r and G_n are rotationally invariant, so is their convolution $G_n * \theta_r$. With this observation, it is easy to show that for all $r > 0$ and $n \in \mathbb{N}$, we have

$$G_n * \theta_r(x) = I_0(2n^2 r\|x\|)e^{-n^2(\|x\|^2+r^2)} \qquad \forall x \in \mathbb{R}^2. \tag{3.2}$$

Throughout the rest of this section, we fix $r > 0$ and define the functions

$$g_n := 2nr\sqrt{\pi}G_n, \qquad f_n = g_n * \theta_r = 2nr\sqrt{\pi}G_n * \theta_r \qquad \forall n \in \mathbb{N}. \tag{3.3}$$

Observe that (3.2) gives us

$$f_n(x) = 2nr\sqrt{\pi}I_0(2n^2 r\|x\|)e^{-n^2(\|x\|^2+r^2)} \qquad \forall x \in \mathbb{R}^2,\ \forall n \in \mathbb{N}.$$

Lemma 3.1 *For each $r > 0$, the sequence $\{f_n\}_{n\in\mathbb{N}}$ is an approximate r-circle with Fourier transform given by*

$$\widehat{f_n}(y) = \frac{2r\pi\sqrt{\pi}}{n}e^{-\pi^2\|y\|^2/n^2}J_0(2\pi r\|y\|) \qquad \forall y \in \mathbb{R}^2,\ \forall n \in \mathbb{N}. \tag{3.4}$$

Proof By Theorem 2.4, we have that $f_n \in \mathcal{S}(\mathbb{R}^2)$ for each $n \in \mathbb{N}$, since G_n is a Schwartz function and θ_r is compactly supported.

Next, observe that

$$\begin{aligned} f_n(x) &= \frac{2nr\sqrt{\pi}I_0(2n^2r\|x\|)}{e^{n^2(\|x\|^2+r^2)}} = \frac{2n\sqrt{r\pi\|x\|}I_0(2n^2r\|x\|)}{e^{2n^2r\|x\|}} \cdot \frac{\sqrt{r}e^{2n^2r\|x\|}}{\sqrt{\|x\|}e^{n^2(\|x\|^2+r^2)}} \\ &= u(2n^2r\|x\|)\sqrt{\frac{r}{\|x\|}}e^{-n^2(\|x\|-r)^2}, \end{aligned} \tag{3.5}$$

where $u(t) := e^{-t}\sqrt{2\pi t}I_0(t)$. We now show that the two conditions (C1) and (C2) of Definition 2.2 hold.

(C1): Since $I_0(0) = 1$, when $x = 0$ we have

$$\lim_{n\to\infty} f_n(0) = \lim_{n\to\infty} 2nr\sqrt{\pi}e^{-n^2r^2} = 0.$$

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Moreover, for $x \neq 0$, we get from (2.3) and (3.5) that

$$\lim_{n\to\infty} f_n(x) = \lim_{n\to\infty} \sqrt{\frac{r}{\|x\|}} e^{-n^2(\|x\|-r)^2} = \begin{cases} 1 & \|x\| = r \\ 0 & \|x\| \neq 0 \text{ and } \|x\| \neq r \,. \end{cases}$$

This proves (C1).

(C2): The function u is continuous on $[0,\infty)$ and satisfies $\lim_{t\to\infty} u(t) = 1$. This implies that there exists some constant A such that $|u(t)| \leq A$ for all $t \in [0,\infty)$. In particular, for all x and n, we have $|u(2n^2 r\|x\|)| \leq A$. Then, by (3.5), we have

$$|f_n(x)| \leq A\sqrt{\frac{r}{\|x\|}} e^{-n^2(\|x\|-r)^2} \leq A\sqrt{\frac{r}{\|x\|}} e^{-(\|x\|-r)^2} \,.$$

In particular, we get

$$|f_n(x)| \leq A\sqrt{2} e^{-(\|x\|-r)^2} =: \psi_1(x) \qquad \forall \|x\| \geq \frac{r}{2} \,. \tag{3.6}$$

Next, let $\|x\| \leq \frac{r}{2}$. Then, for any $y \in C_r$, we have $\|x-y\| \geq \frac{r}{2}$. From this, we see that

$$\begin{aligned} 0 \leq g_n * \theta_r(x) &= \int_{C_r} g_n(x-y)\, \mathrm{d}\theta_r(y) = 2rn\sqrt{\pi} \int_{C_r} e^{-n^2\|x-y\|^2}\, \mathrm{d}\theta_r(y) \\ &\leq 2rn\sqrt{\pi} \int_{C_r} e^{-n^2 r^2/4}\, \mathrm{d}\theta_r(y) = 2rn\sqrt{\pi} e^{-n^2 r^2/4} \leq 2r\sqrt{\pi} c_1 =: c_2 \,, \end{aligned}$$

where $c_1 := \sup\{ne^{-n^2 r^2/4} : n \in \mathbb{N}\} < \infty$.

Now, pick some nonnegative $\psi_2 \in C_c^\infty(\mathbb{R}^2)$ such that $\psi_2(x) \geq c_2$ for all $\|x\| \leq \frac{r}{2}$. This, together with (3.6) gives

$$|f_n(x)| \leq \psi_1(x) + \psi_2(x) =: F(x) \qquad \forall x \in \mathbb{R}^2 \,.$$

This shows condition (C2). Therefore, $\{f_n\}_{n\in\mathbb{N}}$ is an approximate r-circle.

Now, it is easy to see that for all $y \in \mathbb{R}^2$ we have $\widehat{G_n}(y) = \frac{\pi}{n^2} e^{-\pi^2\|y\|^2/n^2}$.

The claim follows from (2.2) and the convolution theorem. ∎

By Corollary 2.6 and Lemma 3.1, we get the following theorem.

Theorem 3.2 (Intensity of C_r) *Let $\mu \in \mathcal{SM}(\mathbb{R}^2)$ and let $r > 0$. Then*

$$\widehat{\mu}(C_r) = \lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, d\mu(y) \,. \tag{3.7}$$

Moreover, in the case of the autocorrelation measure, we get the following corollary.

Corollary 3.3 *Let $\omega \subseteq \mathbb{R}^2$ be any translation-bounded measure and let γ be an autocorrelation of ω. Given $r > 0$ and an approximate r-circle $\{f_n\}_{n\in\mathbb{N}}$, we have*

$$\widehat{\gamma}(C_r) = \lim_{n\to\infty} \int_{\mathbb{R}^2} \widehat{f_n}(y)\, d\gamma(y) \,.$$

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In particular,

$$\widehat{\gamma}(C_r) = \lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, d\gamma(y)\,.$$

We now consider the above formula when the autocorrelation is expressed as a limit of finite approximants. More specifically, let $\gamma_m := \frac{1}{\mathrm{vol}(A_m)} \omega_m * \widetilde{\omega_m}$, where $\{A_m\}_{m\in\mathbb{N}}$ is the van Hove sequence along which the autocorrelation γ is calculated and $\omega_m := \omega|_{A_m}$. Then, since $\gamma_m \to \gamma$ as tempered distributions, we have

$$\widehat{\gamma}(C_r) = \lim_{n\to\infty} \int_{\mathbb{R}^2} \widehat{f_n}(y)\, \mathrm{d}\gamma_m(y) = \lim_{n\to\infty} \lim_{m\to\infty} \int_{\mathbb{R}^2} \widehat{f_n}(y)\, \mathrm{d}\gamma_m(y)\,. \tag{3.8}$$

When calculating the intensity of Bragg peaks, we get a formula that is similar in appearance. In that case, when it is possible to interchange the two limits, we get the Consistent Phase Property, which gives us the intensity of a Bragg peak as a formula in terms of ω (i.e., the intensity of the Bragg peak is the square absolute value of the Fourier–Bohr coefficient). Thus, it is natural to ask what we get when the two limits (3.8) can be interchanged.

In the case of the approximate r-circle defined as in (3.3), we have

$$\begin{aligned}&\lim_{n\to\infty} \int_{\mathbb{R}^2} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, \mathrm{d}\gamma_m(y)\\ &= \lim_{n\to\infty} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \frac{2r\pi\sqrt{\pi}}{n} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, \mathrm{d}\gamma_m(y) = 0\,,\end{aligned}$$

where the last equality follows from the dominated convergence theorem.

Therefore, for this choice of f_n, when the two limits in (3.8) can be interchanged, we get $\widehat{\gamma}(C_r) = 0$. In fact, we can show that the same holds for any approximate r-circle.

Indeed, let us note here that if $\{f_n\}_{n\in\mathbb{N}}$ is any approximate r-circle, we have

$$\int_{\mathbb{R}^2} \widehat{f_n}(y)\, \mathrm{d}\gamma_m(y) = \int_{\mathbb{R}^2} f_n(x)\mathrm{d}\widetilde{\gamma_m}(x) = \frac{1}{\mathrm{vol}(A_m)} \int_{\mathbb{R}^2} f_n(x)\, |\widehat{\omega_m}(x)|^2\, \mathrm{d}x\,. \tag{3.9}$$

Therefore, we get the following.

Corollary 3.4 *Let $\omega \subseteq \mathbb{R}^2$ be any translation-bounded measure, let γ be an autocorrelation of ω with respect to a van Hove sequence $\{A_m\}_{m\in\mathbb{N}}$, and let $\{f_n\}_{n\in\mathbb{N}}$ be an approximate r-circle. Then*

(a) $\widehat{\gamma}(C_r) = \lim_{n\to\infty} \lim_{m\to\infty} \frac{1}{\mathrm{vol}(A_m)} \int_{\mathbb{R}^2} f_n(x)\, |\widehat{\omega_m}(x)|^2 dx$;

(b) $\lim_{m\to\infty} \lim_{n\to\infty} \frac{1}{\mathrm{vol}(A_m)} \int_{\mathbb{R}^2} f_n(x)\, |\widehat{\omega_m}(x)|^2\, dx = 0$.

In particular, when the two above limits can be interchanged, we have $\widehat{\gamma}(C_r) = 0$.

Proof (a) By (3.8) and (3.9), we have

$$\widehat{\gamma}(C_r) = \lim_{n\to\infty} \lim_{m\to\infty} \int_{\mathbb{R}^2} \widehat{f_n}(y)\, \mathrm{d}\gamma_m(y) = \lim_{n\to\infty} \lim_{m\to\infty} \frac{1}{\mathrm{vol}(A_m)} \int_{\mathbb{R}^2} f_n(x)\, |\widehat{\omega_m}(x)|^2\, \mathrm{d}x\,.$$

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(b) By Lemma 2.5, we have

$$\lim_{n\to\infty} \frac{1}{\mathrm{vol}(A_m)} \int_{\mathbb{R}^2} f_n(x)\, |\widehat{\omega_m}(x)|^2 \, \mathrm{d}x = (|\widehat{\omega_m}|^2 \lambda)(C_r) = 0\,.$$

The claim follows. ∎

4 Applications

In this section, we provide applications of Theorem 3.2 and highlight some interesting observations that could lead to further applications. We start with some simple examples with measures μ where $\widehat{\mu}(C_r)$ is easily evaluated.

Example 4.1

(a) If $\mu \in \mathcal{SM}(\mathbb{R}^2)$ is such that $\widehat{\mu}$ is absolutely continuous, then

$$\lim_{n\to\infty} \frac{1}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, \mathrm{d}\mu(y) = 0\,.$$

(b) If λ is the Lebesgue measure on $\mathbb{R}^2$, then $\widehat{\mu} = \delta_0$ and

$$\lim_{n\to\infty} \frac{1}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, \mathrm{d}y = 0 \qquad \forall r > 0\,.$$

(c) Let $x \in \mathbb{R}^2\backslash\{0\}$ and let μ be the absolutely continuous measure with density function $y \mapsto e^{-2\pi i x\cdot y}$. Then $\widehat{\mu} = \delta_x$ and

$$\lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-2\pi i x\cdot y} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, \mathrm{d}y = \begin{cases} 1 & \|x\| = r \\ 0 & \|x\| \neq r\,. \end{cases}$$

Next, we consider the case where $\widehat{\mu} = \theta_{r'}$ for some $r' > 0$. This example is of particular interest because it leads to an orthogonality relation for Bessel functions of the form $J_0(2\pi r\|\cdot\|)$. Applying Corollary 2.6 with $\mu = J_0(2\pi r\|\cdot\|)$, we get the following.

Corollary 4.2 *Let $r, r' > 0$. If $\{f_n\}_{n\in\mathbb{N}}$ is an approximate r-circle, then the following identity holds:*

$$\lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} \widehat{f_n}(y) J_0(2\pi r'\|y\|)\, dy = \begin{cases} 1 & r' = r \\ 0 & r' \neq r\,. \end{cases}$$

In particular, when $f_n = 2nr\sqrt{\pi} G_n * \theta_r$, we have

$$\begin{aligned} (4.1)\qquad & \lim_{n\to\infty} \frac{r\sqrt{\pi}}{n} \int_0^\infty e^{-z^2/4n^2} J_0(rz) J_0(r'z)\, z\, dz \\ & = \lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|) J_0(2\pi r'\|y\|)\, dy = \begin{cases} 1 & r' = r \\ 0 & r' \neq r\,. \end{cases} \end{aligned}$$

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4.1 Measures with pure-point Fourier transform

Lastly, we consider some examples with pure-point diffraction. In this case, the left-hand side of (3.7) is the sum of the intensities of the Bragg peaks that lie on the circle C_r.

Proposition 4.3 *Let $r > 0$ and let $\mu \in \mathcal{SM}(\mathbb{R}^2)$ be such that $\widehat{\mu}$ is pure point, that is, $\widehat{\mu}$ is concentrated on a countable subset of $\mathbb{R}^2$. Let $\{f_n\}_{n\in\mathbb{N}}$ be any approximate r-circle. Then*

$$\lim_{n\to\infty} \int_{\mathbb{R}^2} \widehat{f_n}(y)\, d\mu(y) = \sum_{\substack{x\in\mathbb{R}^2 \\ \|x\|=r}} \widehat{\mu}(\{x\})\,.$$

In particular, when $f_n = 2nr\sqrt{\pi}G_n * \theta_r$, we have

$$\lim_{n\to\infty} \frac{2r\pi\sqrt{\pi}}{n} \int_{\mathbb{R}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi r\|y\|)\, d\mu(y) = \sum_{\substack{x\in\mathbb{R}^2 \\ \|x\|=r}} \widehat{\mu}(\{x\})\,.$$

This result leads to an interesting formula for the sum of two squares function from number theory (see, e.g., [Gro85]), which is the function $r_2 : \mathbb{N} \to \mathbb{N}$ defined as

$$r_2(n) := \operatorname{card}\{(k,l) \in \mathbb{Z}^2 : k^2 + l^2 = n\}\,. \tag{4.2}$$

Remark 4.4

(a) In [BG03, BGJR00], $r_2(n)$ is called the *shelling function*;
(b) The function $r_2(n)$ also appears as the coefficients in the power series representation of the Jacobi theta function $\vartheta_3^2(x)$.

By the Poisson summation formula, we have that $\widehat{\delta_{\mathbb{Z}^2}} = \delta_{\mathbb{Z}^2}$. Therefore, we get the following formula for r_2 in terms of Bessel functions. Similar formulas can be deduced by using other approximate r-circles.

Proposition 4.5 *For all $k > 0$, the sum of two squares function r_2 satisfies*

$$\lim_{n\to\infty} \frac{2\pi\sqrt{\pi k}}{n} \sum_{m=0}^{\infty} r_2(m) e^{-\frac{\pi^2 m}{n^2}} J_0(2\pi\sqrt{km}) = \begin{cases} r_2(k) & k \in \mathbb{N} \\ 0 & k \notin \mathbb{N}\,. \end{cases}$$

Proof For each $k > 0$, by applying Proposition 4.3 with $\mu = \delta_{\mathbb{Z}^2}$ and $r = \sqrt{k}$, we have

$$\lim_{n\to\infty} \frac{2\pi\sqrt{\pi k}}{n} \sum_{y\in\mathbb{Z}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi\sqrt{k}\|y\|) = \delta_{\mathbb{Z}^2}(C_{\sqrt{k}}) = \begin{cases} r_2(k) & k \in \mathbb{N} \\ 0 & k \notin \mathbb{N}\,. \end{cases}$$

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Next, grouping the elements in $\mathbb{Z}^2$ by their norm, we get

$$\sum_{y\in\mathbb{Z}^2} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi\sqrt{k}\|y\|) = \sum_{m=0}^{\infty} \sum_{\substack{y\in\mathbb{Z}^2 \\ \|y\|^2=m}} e^{-\pi^2\|y\|^2/n^2} J_0(2\pi\sqrt{k}\|y\|)$$

$$= \sum_{m=0}^{\infty} \sum_{\substack{y\in\mathbb{Z}^2 \\ \|y\|^2=m}} e^{-\pi^2 m/n^2} J_0(2\pi\sqrt{km}) = \sum_{m=0}^{\infty} r_2(m) e^{-\pi^2 m/n^2} J_0(2\pi\sqrt{km}) .$$

■

Remark 4.6 Proposition 4.5 seems to be related to the Hardy–Landau summation formula. Recall from [DF34, Equation (2.3)] that, if h satisfies some simple restrictions, then

$$\sum_{j=0}^{\infty} r_2(j)h(j) = \pi \sum_{m=0}^{\infty} r_2(m) \int_0^{\infty} h(y) J_0(2\pi\sqrt{my}) \mathrm{d}y . \tag{4.3}$$

Now, for $k > 0$, if h is supported inside a sufficiently small interval around k and satisfies $h(k) = 1$, then

$$\sum_{j=0}^{\infty} r_2(j)h(j) = \begin{cases} r_2(k) & k \in \mathbb{N} \\ 0 & k \notin \mathbb{N} . \end{cases}$$

On the other hand, the right-hand side of (4.3) contains the term $\int_0^{\infty} h(y) J_0(2\pi\sqrt{my})\mathrm{d}y$, which can be challenging to compute. Proposition 4.5 contains a similar formula, where the integral is replaced by a certain limit.

Proposition 4.5 can easily be extended to arbitrary lattices in $\mathbb{R}^2$. For a locally finite point set Λ in $\mathbb{R}^2$, denote by $r_\Lambda : [0,\infty) \to \mathbb{R}$ the function

$$r_\Lambda(k) := \mathrm{card}\{(s,t) \in \Lambda : s^2 + t^2 = k\} = \delta_\Lambda(C_{\sqrt{k}}) .$$

Proposition 4.7 *Let $L \subseteq \mathbb{R}^2$ be a lattice with dual lattice L^0. Then, for all $k > 0$, we have*

$$r_L(k) = \frac{1}{\det(L)} \lim_{n\to\infty} \frac{2\pi\sqrt{\pi k}}{n} \sum_{m\in[0,\infty)} r_{L^0}(m) e^{-\frac{\pi^2 m}{n^2}} J_0(2\pi\sqrt{mk}) .$$

Acknowledgements The authors are grateful to Michael Baake, Jan Mazáč, Noel Murasko, and the anonymous reviewers for numerous comments and suggestions.

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