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Stationary processes and pure point diffraction

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Abstract. We consider the construction and classification of some new mathematical objects, called ergodic spatial stationary processes, on locally compact abelian groups. These objects provide a natural and very general setting for studying diffraction and the famous inverse problems associated with it. In particular, we can construct complete families of solutions to the inverse problem from any given positive pure point measure that is chosen to be the diffraction. In this case these processes can be classified by the dual of the group of relators based on the set of Bragg peaks, and this gives an abstract solution to the homometry problem for pure point diffraction.

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1. *Outline and notation*

This paper is concerned with the mathematics of diffraction. More specifically, we are interested in the famous inverse problem for diffraction: given something that is putatively the diffraction of something, what are all the somethings that could have produced this diffraction?

Diffraction has been a mainstay in crystallography for about a hundred years, beginning with the famous Knipping–Laue X-ray experiments of 1912 that initiated the subject. The fact that the diffraction contains vital information about the structure of the crystal structure being observed, yet at the same time lacks all the phase information that would uniquely identify that structure, is both the source of its power and the source of the significant difficulties of utilizing it effectively. Some dozen Nobel Prizes awarded for diffraction itself or from discoveries in which it played a key role bear this out; see [**36**].

With the proliferation of extraordinary new materials with varying degrees of order and disorder, the importance of diffraction in revealing internal structure continues to be central. The precision, complexity, and variety of modern diffraction images is striking; see for instance the recent review article [**45**]. Nonetheless, in spite of many advances, the fundamental question of diffraction, the inverse problem of deducing physical structure from diffraction images, remains as challenging as ever.

The discovery of aperiodic tilings and quasicrystals, which revealed from both the physical and mathematical points of view just how much we still have to learn about diffraction, revived interest in the mathematics of diffraction, particularly since the types of diffraction images generated by such structures—essentially or exactly pure point diffraction together with symmetries not occurring in ordinary crystals—had not been foreseen by mathematicians, crystallographers, or materials scientists†. It also made plain some genuine inadequacies in the usual mathematical approaches to diffraction, which could not directly be made rigorous. Starting with [**18**], the resulting new techniques created in order to understand mathematical diffraction have been considerable. Among them we mention the introduction of ideas from the harmonic analysis of translation bounded measures [**6**, **7**, **40**], ergodic dynamical systems [**8**, **22**, **23**, **32**–**34**, **38**], and stochastic point processes [**1**, **11**, **16**].

The diffraction of a structure is defined as the Fourier transform of its autocorrelation. The latter is a positive-definite measure in the ambient space of the structure—typically $\mathbb{R}^3$, but mathematically any locally compact abelian group $\mathbb{G}$—and the diffraction is then

† Indeed, the discovery of quasicrystals by D. Shechtman via diffraction experiments met with substantial disbelief for a period of about two years. His determination to communicate his findings to a skeptical scientific community was particularly stressed by the committee awarding him the Nobel prize in Chemistry in 2011 for this discovery.

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a centrally symmetric positive measure in the corresponding Fourier reciprocal space—either $\widehat{\mathbb{R}^3} \simeq \mathbb{R}^3$ or generally $\widehat{\mathbb{G}}$ as the case may be.

In this paper we examine three basic questions that arise from this theory. The first question asks whether *every* positive centrally symmetric measure is actually the diffraction of something. The second asks about the classification of all the various 'somethings' that have this given diffraction. The third asks what kinds of structures the 'somethings' can be. In the case of pure point diffraction (when the diffraction measure is a pure point measure), we can give a satisfactory answer to these problems.

We will be in the setting of locally compact abelian groups. The difficulties of the questions, at least as we examine them here, have little to do with the generality of the setting. They are just as hard for $\mathbb{R}^3$. Indeed, the second question is a very old one in crystallography, called the *homometry problem*, and is part of *the* fundamental problem of diffraction theory already alluded to above: how to unravel the nature of a structure that has created a given diffraction pattern. For mathematical insights into this we mention the revealing paper of Grünbaum and Moore [**17**], work stemming from this present paper in [**43**], and the encyclopedic introduction to aperiodic order [**4**].

Our first question immediately raises the third question. Exactly what do we mean by a structure that can diffract? Typically, diffractive structures are conceived of as discrete measures, for instance point measures describing the positions of atoms, vertices in tilings, etc, weighted by appropriate scattering strengths, or as continuous measures describing the (scattering) distribution of the material structure in space. More recently, starting with the work of Gouéré [**15**, **16**], there has been a shift to discussing the diffraction of certain point processes, which in effect are random point measures, and various distortions of these (see e.g. [**1**, **11**, **26**]). In this paper we are led to introduce new structures which we call *spatial stationary processes*. We shall show that these always lead to autocorrelation and diffraction measures and contain the typical theories of diffraction discussed above†. In terms of these, we get an attractive answer to our three questions, at least in the case of pure point diffraction. However, the answer to the third question is interesting, because it does not describe the underlying structure explicitly, but rather in terms of the ways that it appears to compactly supported continuous functions on the ambient space. In this respect it resembles the description of measures given by the Riesz representation theorem or the theory of distributions with their spaces of test functions. In our case, the convergence conditions required of measures are not generally valid. This in itself is not a defect. It simply shows that from a mathematical point of view there is a theory of diffraction that includes in its solutions to the inverse problem density distributions that cannot be described in terms of measures.

Let $\mathbb{G}$ be a locally compact abelian group and $\widehat{\mathbb{G}}$ its dual group. We treat these groups in additive notation. The paper starts with an abstract notion of a stationary process for $\mathbb{G}$ and then shifts to the more concrete notion of a spatial stationary process for $\mathbb{G}$ (§§2 and 3.3). As for terminology, let us note that outside of a motivational discussion of the usual stochastic processes, the word 'stochastic' is not used in our development of processes and stationary processes.

† There is a technical requirement about the existence of second moments.

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A spatial stationary process basically consists of a $\mathbb{G}$-invariant mapping

$$N : C_c(\mathbb{G}) \longrightarrow L^2(X, \mu),$$

where (X, μ) is a probability space on which there is a measure-preserving action of $\mathbb{G}$.

The idea here derives directly from the theory of stochastic point processes, and it is perhaps useful to discuss this briefly. We follow [**19**] here. A stochastic point process, say in $\mathbb{R}^d$, is a random variable M on a probability space $(\Omega, \mathcal{F}, P)$ with values in the space $\mathcal{M}_p$ of point measures ξ on $\mathbb{R}^d$ for which $\xi(B) \in \mathbb{Z}_{\geq 0}$ for all bounded subsets B of $\mathbb{R}^d$. As these are point measures, they can be written in the form $\xi = \sum_{j=1}^{K} \delta_{t_j}$, where K can be a positive integer or infinity and the points t_j are (not necessarily distinct) points of $\mathbb{R}^d$. Usually, the space $\mathcal{M}_p$ is far larger than needed. For one thing, it allows points in $\mathbb{R}^d$ to appear with multiplicities, and for another it does not require any minimal separation between them (a hard core condition) that would usually be imposed in crystallography or in tiling theories. We assume then that we are really only interested in some subset $X \subset \mathcal{M}_p$ of permissible outcomes for the point process, and that almost surely the point process produces measures in X. Typically, we wish X to be invariant under translation since the actual positions of our point sets are not particularly relevant, and we assume that the law μ of the process (the probability measure μ induced on X by the random variable) is invariant under translation (i.e. the process is stationary).

Now the point is this. If $f \in C_c(\mathbb{R}^d)$, then we obtain a random variable on $(\Omega, \mathcal{F}, P)$ by $\omega \mapsto N_f(\xi) := \sum_{j=1}^{K} f(t_j)$, where $\xi = M(\omega) \in X$ is the measure indicated above. In effect, N can be viewed as a mapping from $C_c(\mathbb{R}^d)$ into mappings on X. Under mild assumptions, $N : C_c(\mathbb{R}^d) \longrightarrow L^2(X, \mu)$. As is often the case with random variables, we ignore the underlying probability space $(\Omega, \mathcal{F}, P)$ since we have everything we need from the probability space (X, μ) and the mapping N. Then N itself can be referred to as the stochastic point process.

In this paper $\mathbb{R}^d$ is replaced by any locally compact abelian group $\mathbb{G}$. (Later, in §3.3, where we exhibit the autocorrelation as a limit, we will need the assumption of second countability of the topology; and from §4 on, where we study almost periodicity of our processes, we will need to assume σ-compactness.) Also, X is not assumed to have any particular form (e.g. a set of point sets or a set of measures). We do not wish to presume any particular mathematical structure for the outcomes of the processes we are studying. Our point of view is that we will start with a positive measure on $\widehat{\mathbb{G}}$ which we would like to show is the diffraction of something, but we do not know in advance what sort of mathematical objects could produce this diffraction (point sets, continuous distributions of density, Schwartz distributions, etc). We derive information about X only from the behaviour of the functions $N(F)$, $F \in C_c(\mathbb{G})$, upon it. From a physical point of view, this is rather appropriate. Indeed, in a physical situation one determines the structure of a physical object by measurements upon it, and the results of measurements are ultimately *all* that one can know about it.

We are particularly interested in pure point diffraction. However, the concept of stationary processes is interesting in its own right and we develop the theory of these a little, independent of the question of pure point diffraction. It is even useful initially to ignore the fact that the resulting process is *spatial*, that is, it is supposed to result from

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some structure in $\mathbb{G}$. So, at the beginning, we often only require that we have a $\mathbb{G}$-invariant mapping $N : C_c(\mathbb{G}) \longrightarrow \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space with conjugation. We call these *stationary processes*. These definitions lead to a natural concept of isomorphism of stationary processes (Definition 2.5), which later becomes of central importance.

Assuming that such a process has second moments, we can then find an 'autocorrelation measure' on $\mathbb{G}$ and a 'diffraction measure' on $\widehat{\mathbb{G}}$. The autocorrelation measure comes about by factoring the second moment by its natural translation invariance and the diffraction measure is just the Fourier transform of the autocorrelation measure†. The diffraction measure is always a centrally symmetric positive translation bounded measure, and through it we can define continuous and pure point diffraction. We show in §4 how pure point and continuous diffraction are tied to notions of almost periodicity of N. Also, we show how to decompose a sum of spatial processes into subprocesses which are respectively pure point and continuous, see §5.

Coming to the pure point part of the paper, §6, we assume that we are given a centrally symmetric positive pure point measure ω on $\widehat{\mathbb{G}}$ which is backwards transformable, that is, it can be expressed as a Fourier transform of some measure on $\mathbb{G}$. We wish to create a probability space (X, μ) on which there is an ergodic action of $\mathbb{G}$ and a continuous stationary process $N : C_c(\mathbb{G}) \longrightarrow L^2(X, \mu)$ whose diffraction is ω.

Not surprisingly, phase factors play a crucial role in this since it is precisely phase information that is lost in the process of diffraction. There is a natural combinatorial structure in the form of the group Z generated by the positions of the Bragg peaks. This group can be seen as an abelianized homotopy group of an associated Cayley graph. It is the dual group of Z, or rather the dual group of a natural factor $\mathcal{Z}$ of this group, that classifies all the spatial processes on $\mathbb{G}$ with diffraction ω, the classification being up to isomorphism or up to translational isomorphism, respectively.

We call these phase factors *phase forms*. Background on phase forms is given in §7. The construction of a phase form from a stationary process with pure point diffraction is carried out in §8. In §10, we show how to use ω and a phase form a^* to construct a spatial process whose diffraction is ω. Uniqueness is already shown in §9. How all these ingredients give a solution to the homometry problem is discussed in §11.

Our solution to the pure point problem is in some sense an elaboration of the famous Halmos–von Neumann result about realizing ergodic pure point dynamical systems in terms of the character theory of compact abelian groups. There the objective was to classify pure pointedness at the level of the spectrum. In our case we wish to classify the diffraction, which amounts to not only knowing the spectrum but also the intensity of diffraction at each point of the spectrum. Our approach to the construction of a spatial process is to realize X as the dual to the discrete group generated by the set of Bragg peaks, but at the same time to include all the phase information which derives from the Bragg intensities. In this context we mention the recent work of Robinson [**35**] on how to realize systems with a given group of eigenvalues via so-called cut-and-project schemes.

Here is a short guideline to the paper.

† The use of the autocorrelation in diffraction theory was initially introduced by A. L. Patterson in 1935 and the autocorrelation is often called the Patterson *function*.

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- Any stationary process with second moment has an autocorrelation measure and associated diffraction measure (Proposition 3.1 and Definition 3.5).
- Every spatial process with second moment splits into the sum of two subprocesses whose autocorrelation measures are the strongly almost periodic and null weakly almost periodic parts of its autocorrelation, and whose diffraction measures are the pure and continuous parts of its diffraction (Proposition 5.6).
- Each pure point ergodic spatial process gives rise to a pure point diffraction measure ω and a phase form a^* and vice versa (Propositions 8.1 and 10.1).
- Spatial processes with the same pure point diffraction measure and the same phase form are naturally isomorphic (Definition 2.5 and Theorem 9.1).
- The set of all possible phase forms associated with a given pure point measure ω forms an abelian group $\mathcal{Z}(\omega)$ and, for each choice of $a^* \in \mathcal{Z}(\omega)$, there is an ergodic spatial process with diffraction ω and phase form a^* (§10 and Theorem 11.2).

The present paper is concerned with setting up an abstract theory of stationary processes geared towards dealing with the inverse problem of diffraction. In a companion work we intend to investigate concrete examples. We mention here that the material presented above has been used in recent investigations by Terauds dealing with the inverse problem of diffraction for the integer lattice [**42**, **43**].

We finish this section by gathering some notation used throughout.

The set $\mathbb{N} := \{1, 2, \dots, \}$. Let $\mathbb{G}$ be a locally compact abelian group. We let $C_c(\mathbb{G})$ denote the space of compactly supported complex-valued continuous functions on $\mathbb{G}$. For compact $K \subset \mathbb{G}$, $C_K(\mathbb{G})$ is the subspace of elements of $C_c(\mathbb{G})$ whose support is in K. For $F \in C_c(\mathbb{G})$, $\widetilde{F} \in C_c(\mathbb{G})$ is defined by $\widetilde{F}(x) = \overline{F(-x)}$. The translation action of $\mathbb{G}$ on itself is denoted by τ: $\tau_t(x) = t + x$ for all $t, x \in \mathbb{G}$. This action determines, in the usual way, an action on $C_c(\mathbb{G})$. By $l_{\mathbb{G}}$, we denote a (fixed) Haar measure on $\mathbb{G}$.

The convolution of two functions $F, G \in C_c(\mathbb{G})$ is defined to be the function $F * G \in C_c(\mathbb{G})$ given by

$$F * G(t) = \int_{\mathbb{G}} F(t - s)G(s)\, dl_{\mathbb{G}}(s).$$

The dual group of $\mathbb{G}$ is denoted by $\widehat{\mathbb{G}}$ and the *Fourier transform* of an $F \in C_c(\mathbb{G})$ is denoted by $\widehat{F}$, i.e.

$$\widehat{F}(k) = \int_{\mathbb{G}} \overline{(k, t)}F(t)\, dl_{\mathbb{G}}(t),$$

with (k, t) being the value of the character k at t.

A measure ν on $\mathbb{G}$ is called *transformable* if there exists a measure σ on $\widehat{\mathbb{G}}$ with

$$\int_{\widehat{\mathbb{G}}} |\widehat{F}|^2\, d\sigma = \int_{\mathbb{G}} F * \widetilde{F}\, d\nu$$

for all $F \in C_c(\mathbb{G})$. In this case σ is uniquely determined and called the *Fourier transform of* ν. In such a situation, we call σ *backward transformable*. Unlike all other notation introduced in this section, the concept of backward transformability is not standard. However, it is clearly very useful in our context as it is exactly the property shared by the diffraction measures we investigate.

A measure ν on $\mathbb{G}$ is called *positive definite* if $\nu(F * \widetilde{F}) \geq 0$ for all $F \in C_c(\mathbb{G})$. Any positive-definite measure is transformable; see e.g. [**14**].

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A sequence $\{A_n\}$ of compact subsets of $\mathbb{G}$ is called a *van Hove sequence* if for every compact $K \subset \mathbb{G}$,

$$\lim_{n\to\infty} \frac{l_{\mathbb{G}}(\partial^K A_n)}{l_{\mathbb{G}}(A_n)} = 0. \tag{1}$$

Here, for compact A, K, the *K-boundary* $\partial^K A$ of A is defined as

$$\partial^K A := ((A + K) \setminus A^\circ) \cup ((\overline{\mathbb{G} \setminus A} - K) \cap A).$$

The existence of van Hove sequences for all σ-compact locally compact abelian groups is shown in [**37**, p. 249]; see also §3.3 and Theorem (3.L) of [**41**, Appendix]†.

A map between two spaces, on which $\mathbb{G}$ acts, is a $\mathbb{G}$-*map* or $\mathbb{G}$-*invariant* if it intertwines the action of $\mathbb{G}$.

The characteristic function of a set A is denoted as 1_A.

2. *Stationary processes introduced*

In this section we introduce our concept of a stationary process on a locally compact abelian group $\mathbb{G}$. The concept is somewhat more general than is needed in the later part of the paper, but the increased generality has two virtues: it does not lead to more complicated proofs, but rather makes them more transparent, and for the study of mixed spectra it may prove to be especially useful since it allows splitting into pure point and continuous parts.

Let $\mathbb{G}$ be a locally compact abelian group and let $\mathcal{H}$ be a Hilbert space with inner product $\langle\cdot|\cdot\rangle$. We assume linearity in the first variable and conjugate linearity in the second. A *strongly continuous unitary representation* of the group $\mathbb{G}$ on $\mathcal{H}$ is a map T from $\mathbb{G}$ into the bounded operators on $\mathcal{H}$ such that $t \mapsto \langle T_t f, T_t f\rangle$ is constant on $\mathbb{G}$ for every $f \in \mathcal{H}$, T_0 is the identity on $\mathcal{H}$, $T_{t+s} = T_t T_s$ holds for all $s, t \in \mathbb{G}$, and $t \mapsto T_t f$ is continuous for every $f \in \mathcal{H}$. Then, obviously, each T_s is unitary (i.e. bijective and norm preserving). An $f \in \mathcal{H}$ is then called an *eigenfunction* of T with *eigenvalue* $k \in \widehat{\mathbb{G}}$ if $T_t f = \overline{(k, t)} f$ for every $t \in \mathbb{G}$. The closed subspace of $\mathcal{H}$ spanned by all eigenfunctions is denoted by $\mathcal{H}_p$. The representation T has *pure point spectrum* if $\mathcal{H} = \mathcal{H}_p$ or equivalently if $\mathcal{H}$ has an orthonormal basis consisting of eigenfunctions‡.

By Stone's theorem, compare [**29**, §36D], there exists a projection-valued measure

$$E_T\colon \text{ Borel sets of } \widehat{\mathbb{G}} \longrightarrow \text{ projections on } \mathcal{H}$$

with

$$\langle f \mid T_t f\rangle = \int_{\widehat{\mathbb{G}}} (k, t)\, d\rho_f(k) \tag{2}$$

for all $t \in \mathbb{G}$ and $f \in \mathcal{H}$, where ρ_f is the measure on $\widehat{\mathbb{G}}$ defined by $\rho_f(B) := \langle f \mid E_T(B) f\rangle$. The map E_T is called the *spectral family of* T and ρ_f is called the *spectral measure* of f. It is the unique measure on $\widehat{\mathbb{G}}$ satisfying (2).

† We note that in our considerations in §3.3, van Hove sequences are ultimately more suitable than the more common Følner sequences discussed in [**41**] (compare [**4**]).

‡ Often the eigenfunction condition is written as $T_t f = (k, t) f$ for an eigenvalue $k \in \widehat{\mathbb{G}}$. For our purposes, things work out more smoothly by formulating it with the conjugate value.

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A mapping $\overline{(\cdot)}$ of a Hilbert space $(\mathcal{H}, \langle\cdot \mid \cdot\rangle)$ into itself is said to be a *conjugation* of $\mathcal{H}$ if:
(i) $\overline{(\cdot)}$ is conjugate-linear and $\overline{\overline{f}} = f$;
(ii) for all $f, g \in \mathcal{H}$, $\langle \overline{f} \mid \overline{g}\rangle = \langle g \mid f\rangle = \overline{\langle f \mid g\rangle}$.
An $f \in \mathcal{H}$ is called *real* if $f = \overline{f}$.

Definition 2.1. Let $\mathbb{G}$ be a locally compact abelian group. A *stationary process* or $\mathcal{H}$-*stationary process* on $\mathbb{G}$ is a triple $\mathcal{N} = (N, \mathcal{H}, T)$ consisting of a Hilbert space $\mathcal{H}$ with conjugation, a strongly continuous unitary representation T of $\mathbb{G}$ on $\mathcal{H}$, and a linear $\mathbb{G}$-map $N : C_c(\mathbb{G}) \longrightarrow \mathcal{H}$ such that for all $F \in C_c(\mathbb{G})$, $N(\overline{F}) = \overline{N(F)}$. A stationary process is called *ergodic* if the eigenspace of T for the eigenvalue 0 is one dimensional.

The origins of the preceding definition lie in the theory of stochastic point processes, hence the name. We will often simply write *process* instead of *stationary process*. We do not use the word *stochastic*, although our definition allows for processes that are stochastic in nature.

The set of all $\mathcal{H}$-stationary processes on $\mathbb{G}$ forms a real vector space in the obvious way by taking linear combinations of mappings. There is also a canonical notion of isomorphism between stochastic processes: the processes $(N_1, \mathcal{H}_1, T_1)$ and $(N_2, \mathcal{H}_2, T_2)$ are called *isomorphic* if there exists an invertible unitary map $U : \mathcal{H}_1 \longrightarrow \mathcal{H}_2$ which intertwines T_1 and T_2 and satisfies $N_2 = UN_1$.

We will be interested in the spectral theory of stationary processes. An important notion is given next.

Definition 2.2. A stationary process $\mathcal{N} = (N, \mathcal{H}, T)$ is said to have *pure point spectrum* if the representation T of $\mathbb{G}$ on $\mathcal{H}$ has pure point spectrum.

Definition 2.3. A stationary process $\mathcal{N} = (N, \mathcal{H}, T)$ on a locally compact abelian group $\mathbb{G}$ is called a *spatial stationary process* if there are a probability space (X, μ) and an action $T : \mathbb{G} \times X \longrightarrow X$, $(t, x) \mapsto t \cdot x$, such that μ is invariant under the $\mathbb{G}$-action on X through T, $\mathcal{H} = L^2(X, \mu)$ with the usual inner product $\langle f \mid g\rangle = \int_X f\overline{g}\, d\mu$, and the action of T is extended to an action on $\mathcal{H}$ by $T_t f(\cdot) = f((-t)(\cdot))$ for all $t \in \mathbb{G}$, $f \in L^2(X, \mu)$. The conjugation on $\mathcal{H}$ is the natural one: complex conjugation of functions on X. We write $\mathcal{N} = (N, X, \mu, T)$. The stationary spatial process is called *full* if the algebra generated by functions of the form $\psi \circ N(F)$, $\psi \in C_c(\mathbb{C})$, $F \in C_c(\mathbb{G})$, is dense in $L^2(X, \mu)$. (Here $\circ$ denotes the composition of functions.)

Remark 2.4. In some sense the assumption of fullness is only a convention. More precisely, given any spatial stationary process, we may create a full process with essentially the same properties by a variant of the Gelfand construction. Details are given below in Theorem 5.4.

For the sake of economy, we have used the same notation, T, for the action of $\mathbb{G}$ on X and the corresponding action of $\mathbb{G}$ on $\mathcal{H} := L^2(X, \mu)$. We often omit the word 'stationary' in the sequel, but we will always understand it to be in force.

The definition of stationary processes implicitly defines them as *real* processes: $N(F)$ is real for all real-valued functions F on $\mathbb{G}$ in the sense that $\overline{N(F)} = N(F)$. In the case of

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spatial processes, all real-valued functions on $\mathbb{G}$ are mapped by N to real-valued functions on X. One could relax the conditions to allow complex-valued processes, but we shall not do that here.

Definition 2.5. Two stationary spatial processes $\mathcal{N} = (N, X, \mu, T)$ and $\mathcal{N}' = (N', X', \mu', T')$ on $\mathbb{G}$ are *spatially isomorphic* if there is an invertible unitary mapping $M : L^2(X, \mu) \longrightarrow L^2(X', \mu')$ with:

- $M \circ N = N'$;
- $M \circ T_t = T'_t \circ M$ for all $t \in \mathbb{G}$;
- $M(fg) = M(f)M(g)$ for all $f, g \in L^\infty(X, \mu)$ and $M^{-1}(f'g') = M^{-1}(f')M^{-1}(g')$ for all $f', g' \in L^\infty(X', \mu')$.

The map M is then called a spatial isomorphism between the processes.

The isomorphism class of $\mathcal{N} = (N, X, \mu, T)$ is denoted by $[\mathcal{N}] = [(N, X, \mu, T)]$.

Remark 2.6. (a) The first two points of the definition just say that the processes are isomorphic. The special requirement for spatial isomorphy is the third point. As shown in the next proposition, the spatial isomorphisms are exactly those isomorphisms which are compatible with the L^∞-module structure of L^2 in the sense that $M(fg) = M(f)M(g)$ for all $f \in L^\infty$ and $g \in L^2$.

(b) Our definition of spatial isomorphism parallels the notion of spectral isomorphism for measure-preserving group actions on probability spaces. Our conditions on M imply that spatial isomorphism implies conjugacy in the sense that there is a measure isomorphism between the Borel sets of X and those of X' [**44**, Theorem 2.4]. If in addition X, X' are complete separable metric spaces, then this can be improved to being an isomorphism between X and X', that is, a bijective intertwining mapping between two subsets of full measure in X and X', respectively [**44**, Theorem 2.6].

PROPOSITION 2.7. *Let $\mathcal{N} = (N, X, \mu, T)$ and $\mathcal{N}' = (N', X', \mu', T')$ be spatially isomorphic processes with spatial isomorphism M. Then M maps $L^\infty(X, \mu)$ into $L^\infty(X', \mu')$ and $M(fg) = M(f)M(g)$ holds for all $f \in L^\infty(X, \mu)$ and $g \in L^2(X, \mu)$. The corresponding statements hold for M^{-1} as well.*

Proof. It suffices to consider the statements on M. By assumption, we have that for $f, g \in L^\infty(X)$ the product $M(f)M(g)$ belongs to $L^2(X')$ and in fact equals $M(fg)$ (and similarly for M^{-1}). By a simple limit argument, we then see that for any $f \in L^\infty(X)$, the equation $M(fg) = M(f)M(g)$ must hold for any $g \in L^2(X)$. This shows that the operator of multiplication by $M(f)$ is defined on the whole of $L^2(X')$ (as M is onto). Furthermore, the graph of every multiplication operator can easily be seen to be closed. Thus, the closed graph theorem gives that the operator of multiplication by $M(f)$ is a bounded operator on $L^2(X')$. This in turn yields that $M(f)$ belongs to $L^\infty(X')$. □

3. *Diffraction theory for stationary processes*

In this section we show how each stationary process with a second moment comes with a positive-definite measure γ on $\mathbb{G}$ called the autocorrelation, a positive measure ω on $\widehat{\mathbb{G}}$ called the diffraction measure, and the diffraction to dynamics map θ. We then discuss

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how the autocorrelation comes about as a limit and characterize existence of a second moment. Throughout, all stationary processes are assumed to be on a locally compact abelian group $\mathbb{G}$.

3.1. *Autocorrelation and diffraction.* Let a stationary process $\mathcal{N} = (N, \mathcal{H}, T)$ be given.

We say that $\mathcal{N}$ has a *second moment* (or is *with second moment*) if there is a measure $\mu^{(2)} := \mu_N^{(2)}$ on $C_c^{\mathbb{R}}(\mathbb{G} \times \mathbb{G})$ (necessarily unique if it exists) satisfying

$$\mu^{(2)}(F \otimes G) = \langle N(F) \mid N(G) \rangle \tag{3}$$

for all real-valued $F, G \in C_c(\mathbb{G})$. Much of this paper is based on the assumption that the second moment measure exists. Since N is real valued on real-valued functions, so too is the measure $\mu^{(2)}$. Furthermore, $\mu^{(2)}$ is evidently translation bounded since N is $\mathbb{G}$-invariant†.

As shown in the next proposition, the second moment will give rise to a measure on $\mathbb{G}$ via a suitable quotient. In the theory of point processes on Euclidean spaces, similar considerations are carried out in the context of so-called factorial second moments and Palm measures [**1**, **5**, **10**, **15**].

PROPOSITION 3.1. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a process. Then $\mathcal{N}$ has a second moment if and only if there is a measure $\gamma = \gamma_N$ on $\mathbb{G}$ satisfying*

$$\gamma(F * \widetilde{G}) = \langle N(F) \mid N(G) \rangle \tag{4}$$

for all $F, G \in C_c(\mathbb{G})$. In the case that such a measure exists, it is unique and furthermore it is real (i.e. assigns real values to real-valued functions), positive definite, and translation bounded.

Proof. (See also [**10**, §10.4], where a reduction of this form is discussed.) It suffices to restrict attention to real-valued F and G in $C_c(\mathbb{G})$ as N is invariant under a conjugation and hence both $F * \widetilde{G}$ and $\langle N(F) \mid N(G) \rangle$ are linear in F and antilinear in G. Let $\psi := \mu^{(2)}$ above. The assumption of stationarity of N shows that ψ is invariant under simultaneous translation of both of its two variables. Define the mapping

$$\begin{aligned} \mathbb{G} \times \mathbb{G} &\longrightarrow \mathbb{G} \times \mathbb{G}, \\ (s, t) &\mapsto (s - t, t) =: (u, v). \end{aligned} \tag{5}$$

For $F_1, F_2 \in C_c^{\mathbb{R}}(\mathbb{G})$, we define $H \in C_c(\mathbb{G} \times \mathbb{G})$ by $H(u, v) = H(s - t, t) = F_1(s)F_2(t)$. This change of variables defines a new measure ψ^* via

$$\int_{\mathbb{G}} \int_{\mathbb{G}} F_1(s)F_2(t)\, d\psi(s, t) = \int_{\mathbb{G}} \int_{\mathbb{G}} H(u, v)\, d\psi^*(u, v).$$

Since $(\tau_r s, \tau_r y) \leftrightarrow (u, \tau_r v)$, the translation invariance of ψ translates to translation invariance of the second variable of ψ^*. Thus, for measurable sets $A, B \subset \mathbb{G}$, we have

† The mth moment of $\mathcal{N}$ will be defined by $\mu^{(m)}(F_1 \otimes \cdots \otimes F_m) = \int_X N(F_1) \cdots N(F_m)\, d\mu$, which is different from what we get from the inner product $\langle \cdot \mid \cdot \rangle$ when $m = 2$ unless we restrict to real-valued functions. This is why we restrict to real-valued functions in this definition.

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$\psi^*(A \times B) = \psi^*(A \times (r + B))$ for all $r \in \mathbb{G}$. For A fixed, this leads to a translation-invariant measure on $\mathbb{G}$ which is hence a multiple $c(A)$ of Haar measure $l_{\mathbb{G}}$:

$$\psi^*(A \times B) = c(A) l_{\mathbb{G}}(B).$$

The mapping $A \mapsto c(A)$ is a measure on $\mathbb{G}$ and this measure is the reduction ψ^{red} of ψ:

$$\psi^*(A \times B) = \psi^{\mathrm{red}}(A)\, l_{\mathbb{G}}(B).$$

Now, for $H(u, v) = F_1(u + v)F_2(v)$,

$$\begin{aligned}\int\int H(u, v)\, d\psi^*(u, v) &= \int\int F_1(u + v)F_2(v)\, d\psi^{\mathrm{red}}(u)\, dl_{\mathbb{G}}(v)\\ &= \int\left(\int F_1(u + v)F_2(v)\, dl_{\mathbb{G}}(v)\right) d\psi^{\mathrm{red}}(u)\\ &= \int (F_1 * \widetilde{F}_2)(u)\, d\psi^{\mathrm{red}}(u),\end{aligned}$$

so finally

$$\psi(F_1 \otimes F_2) = \psi^{\mathrm{red}}(F_1 * \widetilde{F}_2)$$

and ψ^{red} is the desired measure, which we now denote by γ.

It is positive definite since $\gamma(F * \widetilde{F}) = \mu^{(2)}(F \otimes F) = \|N(F)\|^2 \geq 0$. All positive-definite measures are translation bounded [**9**]. Since $\psi := \mu^{(2)}$ is a real measure, one sees that γ is also a real measure. The denseness of the set of functions $F * \widetilde{G}$ in $C_c(\mathbb{G})$ shows that γ is unique.

We can reverse all the steps of this proof and, from the existence of the real positive-definite measure γ satisfying (4), derive the corresponding second moment measure (3). □

Existence of a second moment immediately implies some continuity properties of N.

COROLLARY 3.2. *Let $(N, \mathcal{H}, T)$ be a stationary process with second moment. Let $1 \leq p, q \leq \infty$ be given with $1/p + 1/q = 1$. Then, for any compact $K \subset \mathbb{G}$, there exists a $C_K \geq 0$ with*

$$|\langle N(F) \mid N(G)\rangle| \leq C_K \|F\|_{L^p(\mathbb{G})} \|G\|_{L^q(\mathbb{G})}$$

for all $F, G \in C_c(\mathbb{G})$ with support contained in K. In particular, for each compact $K \subset \mathbb{G}$, the map $N : C_K(\mathbb{G}) \longrightarrow \mathcal{H}$ is continuous with respect to the L^2-norm on $C_K(\mathbb{G})$. Furthermore, $N : C_c(\mathbb{G}) \longrightarrow \mathcal{H}$ is continuous with respect to the inductive limit topology on $C_c(\mathbb{G})$ (i.e. the restriction of N to any $C_K(\mathbb{G})$, $K \subset \mathbb{G}$ compact, is continuous with respect to the supremum norm).

Proof. For $F, G \in C_c(\mathbb{G})$ with support contained in K, the support of $F * \widetilde{G}$ is contained in $K - K$ and $\|F * \widetilde{G}\|_\infty \leq \|F\|_{L^p(\mathbb{G})}\|G\|_{L^q(\mathbb{G})}$. As $|\langle N(F), N(G)\rangle| = |\gamma(F * \widetilde{G})|$, this easily gives the first statement. Now the second statement follows by taking $p = q = 2$. Finally, for $F \in C_K(\mathbb{G})$, $\|F\|_{L^2(\mathbb{G})} \leq \|F\|_\infty (l_{\mathbb{G}}(K))^{1/2}$. □

The continuity property of the preceding corollary allows one to extend the map N.

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COROLLARY 3.3. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with second moment. The map N can be uniquely extended to the vector space consisting of all measurable functions f on $\mathbb{G}$ that vanish outside of some fixed compact set and that are square integrable with respect to the Haar measure on $\mathbb{G}$. This extension (again denoted by N) is $\mathbb{G}$-equivariant and satisfies*

$$\int_{\mathbb{G}} F * \widetilde{F}\, d\gamma = \langle N(F) | N(F) \rangle,$$

meaning in particular that the integral exists and is finite.

Proof. It suffices to show that N can be uniquely extended to $L^2(U, l_U)$ for any open U in $\mathbb{G}$ with compact closure. Let such a U be given.

Let $F \in L^2(U, l_U)$. As U is open, we can find a sequence $\{F_n\}$ in $C_c(U)$ converging to F in the sense of $L^2(U, l_U)$. By the previous corollary, we infer that $\{N(F_n)\}$ must be a Cauchy sequence, and its limit does not depend on the choice of the approximating sequence $\{F_n\}$. This shows that N can be extended to $L^2(U, l_U)$.

By construction of $N(F)$ and the definition of γ, we have furthermore

$$\langle N(F) \mid N(F) \rangle = \lim_{n\to\infty} \int_{\mathbb{G}} F_n * \widetilde{F}_n\, d\gamma.$$

Moreover, a direct application of the Cauchy–Schwarz inequality shows that $F_n * \widetilde{F}_n$ converges to $F * \widetilde{F}$ with respect to the supremum norm and has support contained in $\overline{U} - \overline{U}$. This easily gives that

$$\lim_{n\to\infty} \int_{\mathbb{G}} F_n * \widetilde{F}_n\, d\gamma = \int_{\mathbb{G}} F * \widetilde{F}\, d\gamma.$$

This finishes the proof. □

Remark 3.4. Note that any bounded measurable function with compact support belongs to $L^2(U, d\, l_{\mathbb{G}})$ for any open U containing the support. Thus, N can in particular be extended to bounded measurable functions with compact support.

The above discussion shows that any stationary process with a second moment gives rise to a real positive-definite measure γ. As γ is positive definite, it is transformable into a (positive) measure, i.e. its Fourier transform ω exists [**9**, **31**]. Furthermore, ω is a translation-bounded measure [**14**, **31**] and, since γ is a real measure, it is centrally symmetric ($\omega(A) = \omega(-A)$ for all measurable sets A). The measures γ and ω lie at the heart of our investigation.

Definition 3.5. Let $(N, \mathcal{H}, T)$ be a stationary process with second moment. Then $\gamma := \gamma_N$ is called the *autocorrelation* of the stationary process. Its Fourier transform $\omega := \omega_N := \widehat{\gamma_N}$ is called the *diffraction* or *diffraction measure* of the stationary process.

Definition 3.6. A stationary process $(N, \mathcal{H}, T)$ with second moment is said to have *pure point diffraction* (respectively *continuous diffraction*) if the diffraction measure ω is a pure point measure (respectively a continuous measure).

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The definition of ω yields that it is a centrally symmetric positive measure and is the unique measure satisfying

$$\int_{\widehat{\mathbb{G}}} |\widehat{F}|^2 \, d\omega = \int_{\mathbb{G}} F * \widetilde{F} \, d\gamma \tag{6}$$

or, equivalently, by linearizing this,

$$\int_{\widehat{\mathbb{G}}} \widehat{F}\overline{\widehat{G}} \, d\omega = \int_{\mathbb{G}} F * \widetilde{G} \, d\gamma$$

for all $F, G \in C_c(\mathbb{G})$. Considering the Hilbert space $L^2(\widehat{\mathbb{G}}, \omega)$ with the corresponding inner product being written $\langle \cdot \mid \cdot \rangle_{\widehat{\mathbb{G}}}$ and using the definition of γ, we obtain for any $F, G \in C_c(\mathbb{G})$,

$$\langle \widehat{F} \mid \widehat{G} \rangle_{\widehat{\mathbb{G}}} = \int_{\widehat{\mathbb{G}}} \widehat{F}\overline{\widehat{G}} \, d\omega = \int_{\mathbb{G}} F * \widetilde{G} \, d\gamma = \langle N(F) \mid N(G) \rangle. \tag{7}$$

This shows that the map $\widehat{F} \mapsto N(F)$ is an isometry.

We define an action $\hat{T}$ of $\mathbb{G}$ on $L^2(\widehat{\mathbb{G}}, \omega)$ by defining $\hat{T}_t f$ for all $f \in L^2(\widehat{\mathbb{G}}, \omega)$ through

$$\hat{T}_t f(k) = \overline{(k, t)} f(k) \tag{8}$$

for all $t \in \mathbb{G}$ and all $k \in \widehat{\mathbb{G}}$. Then $\hat{T}$ is clearly a strongly continuous unitary representation on $L^2(\widehat{\mathbb{G}}, \omega)$. Its spectral family $E_{\hat{T}}$ is given by

$$E_{\hat{T}}(A) f = 1_A f$$

for any measurable $A \subset \widehat{\mathbb{G}}$. Indeed, we obviously have

$$\langle f, \hat{T}_t f \rangle_{\widehat{\mathbb{G}}} = \int (k, t) |f|^2 \, d\omega$$

for any $f \in L^2(\widehat{\mathbb{G}}, \omega)$. Hence, the spectral measure of f must be given by $|f|^2\omega$ and this satisfies

$$\int 1_A |f|^2 \, d\omega = \langle f, 1_A f \rangle.$$

Remark 3.7. We note that if N is a $\mathcal{H}$-stationary process on $\mathbb{G}$ with second moment, then, for all $c \in \mathbb{R}$, cN is another such process. The corresponding autocorrelation and diffraction measures are then scaled by $|c|^2$.

3.2. *The diffraction to dynamics map.* Any process with a second moment comes with an isometric $\mathbb{G}$-map θ from $L^2(\widehat{\mathbb{G}}, \omega)$ to $\mathcal{H}$. This allows one to transfer certain questions from $\mathcal{H}$ to $L^2(\widehat{\mathbb{G}}, \omega)$. Also, it means that for certain eigenvalues there are canonical eigenfunctions available. These topics are studied next.

PROPOSITION 3.8. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with second moment. Then $\{\widehat{F} : F \in C_c(\mathbb{G})\}$ is dense in $L^2(\widehat{\mathbb{G}}, \omega)$ and there exists a unique isometric embedding*

$$\theta = \theta_N : L^2(\widehat{\mathbb{G}}, \omega) \longrightarrow \mathcal{H} \tag{9}$$

with $\widehat{F} \mapsto N(F)$ for each $F \in C_c(\mathbb{G})$. This mapping is a $\mathbb{G}$-map and, furthermore, for all $D \in L^2(\widehat{\mathbb{G}}, \omega)$,

$$\theta(\widetilde{D}) = \overline{\theta(D)}.$$

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Proof. We begin with the denseness statement. Let L be the closure of $\{\widehat{F} : F \in C_c(\mathbb{G})\}$ in $L^2(\widehat{\mathbb{G}}, \omega)$. We wish to show that $L = L^2(\widehat{\mathbb{G}}, \omega)$. As ω is a translation-bounded measure, the space $C_c(\widehat{\mathbb{G}})$ is dense in $L^2(\widehat{\mathbb{G}}, \omega)$. Thus, it suffices to show that $C_c(\widehat{\mathbb{G}})$ belongs to L. As the convolutions of elements from $C_c(\mathbb{G})$ belong to $C_c(\mathbb{G})$ as well, we infer that for all $G_1, \dots, G_m \in C_c(\mathbb{G})$,

$$\widehat{F_1} \cdots \widehat{F_n} \cdot \widehat{G_1} \cdots \widehat{G_m} \in L$$

for all $F_i \in C_c(\mathbb{G})$. Now $\widehat{F_j}$ belongs to the set $C_0(\widehat{\mathbb{G}})$ of continuous functions on $\widehat{\mathbb{G}}$ vanishing at infinity. An application of the Stone–Weierstrass theorem then shows that

$$f\widehat{G_1} \cdots \widehat{G_m} \in L$$

for each $f \in C_0(\widehat{\mathbb{G}})$. Fixing $f \in C_c(\widehat{\mathbb{G}})$, we can then use another application of the Stone–Weierstrass theorem to infer that

$$fg \in L$$

for all $f \in C_c(\widehat{\mathbb{G}})$ and $g \in C_0(\widehat{\mathbb{G}})$. This yields $C_c(\widehat{\mathbb{G}}) \subset L$, as we intended to show.

The existence of θ now follows by defining it initially by $\theta : \widehat{F} \mapsto N(F)$ for all $F \in C_c(\mathbb{G})$, using the fact that it is an isometric mapping by (7), and then extending it to the L^2-closure L, which is $L^2(\widehat{\mathbb{G}}, \omega)$.

As for the second statement, first we note that the $\mathbb{G}$-action on $L^2(\widehat{\mathbb{G}}, \omega)$ is designed to make the mapping $\hat{F} \mapsto F$ into a $\mathbb{G}$-map, while $F \mapsto N(F)$ is already a $\mathbb{G}$-map and, second, for all $F \in C_c(\mathbb{G})$, $\widetilde{\widehat{F}} = \overline{\widehat{F}}$, from which

$$\theta(\widetilde{\widehat{F}}) = \theta(\overline{\widehat{F}}) = N(\overline{F}) = \overline{N(F)} = \overline{\theta(\widehat{F})}.$$

We finish using the denseness of the first part. □

Definition 3.9. The map $\theta = \theta_N$ associated to a stationary process $\mathcal{N} = (N, \mathcal{H}, T)$ with second moment is called the *diffraction to dynamics map*.

The relevance of θ for spectral-theoretic considerations comes from the following consequence of the previous proposition.

THEOREM 3.10. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with second moment and θ the associated diffraction to dynamics map. Then, for any $H \in L^2(\widehat{\mathbb{G}}, \omega)$, we have*

$$(E_T(A) \circ \theta)(H) = \theta(1_A H)$$

for any measurable $A \subset \widehat{\mathbb{G}}$ and the spectral measure $\rho_{\theta(H)}$ is given by

$$\rho_{\theta(H)} = |H|^2 \omega.$$

Proof. As θ is an isometric $\mathbb{G}$-map, it establishes a unitary equivalence between the action of $\hat{T}$ on $L^2(\widehat{\mathbb{G}}, \omega)$ and the restriction of T to the subspace $\theta(L^2(\widehat{\mathbb{G}}, \omega))$. This directly gives $E_T(A) \circ \theta = \theta \circ E_{\hat{T}}(A)$ for all measurable $A \subset \widehat{\mathbb{G}}$ as well as $\rho_{\theta(H)} = \rho_H^{(\hat{T})}$ for all $H \in L^2(\widehat{\mathbb{G}}, \omega)$, where $\rho_H^{(\hat{T})}$ denotes the spectral measure with respect to $\hat{T}$. Now, as already discussed above in the text following (8), we have $E_{\hat{T}}(A)H = 1_A H$ and the spectral measure $\rho_H^{(\hat{T})}$ is given by $|H|^2\omega$. This finishes the proof. □

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From the previous theorem, it is clear that if $\mathcal{N} = (N, \mathcal{H}, T)$ has pure point spectrum, then ω is discrete and the diffraction is pure point. However, we can expect (e.g. [**24**]) that this will work in the other direction too: pure point diffraction implies pure point spectrum. We shall see that it is so: each implies the other in the case of spatial processes. More specifically, the diffraction to dynamics map connects pure point diffraction to eigenvectors of the $\mathbb{G}$ action on $\mathcal{H}$. Later, we shall see that in the case of spatial processes, this allows us to make a complete correspondence between pure point diffraction and pure point dynamics.

For an arbitrary stationary process with diffraction measure ω, we define the set of its *atoms* by

$$\mathcal{S} = \mathcal{S}(\omega) := \{k \in \widehat{\mathbb{G}} : \omega(\{k\}) \neq 0\} = \{k \in \widehat{\mathbb{G}} : \omega(\{k\}) > 0\}.$$

The set $\mathcal{S}$ is often called the *Bragg spectrum* of the process, and its elements are sometimes called *Bragg peaks*. Then, for $k \in \mathcal{S}$, the value $\omega(\{k\})$ is referred to as the *intensity of the Bragg peak*†.

In the sequel, we will often omit the brackets when dealing with singleton sets $\{k\}$. In particular, we will set $\omega(k) := \omega(\{k\})$ for $k \in \widehat{\mathbb{G}}$.

Let 1_k be the characteristic function of the set $\{k\} \subset \widehat{\mathbb{G}}$, i.e. $1_k(k')$ is 1 or 0 according as k' equals k or not. It is easy to see that these functions are the only possible eigenfunctions for our action of $\mathbb{G}$ on $L^2(\widehat{\mathbb{G}}, \omega)$. Define f_k, $k \in \mathcal{S}$, by $f_k = \theta(1_k)$. Then each f_k is an eigenfunction in $\mathcal{H}$ for the eigenvalue k, in the sense that $T_t f_k = \overline{(k, t)} f_k$.

LEMMA 3.11. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with second moment. Then, for all $k \in \mathcal{S}$, $-k \in \mathcal{S}$, $f_{-k} = \overline{f_k}$ and $\|f_{-k}\| = \|f_k\| = \omega(k)^{1/2}$.*

Proof. Since ω is centrally symmetric, $\omega(\{-k\}) = \omega(\{k\})$, which gives the first statement. For the second, using Proposition 3.8, we have $f_{-k} = \theta(1_{-k}) = \theta(\widetilde{1_k}) = \overline{\theta(1_k)} = \overline{f_k}$. Then $\|f_{-k}\|^2 = \langle f_{-k} \mid f_{-k}\rangle = \langle f_k \mid f_k\rangle = \|f_k\|^2 = \langle 1_k, 1_k\rangle_{\widehat{\mathbb{G}}} = \omega(k)$. □

We can use the preceding considerations to compute the map N in the case of pure point diffraction.

PROPOSITION 3.12. *Let $(N, \mathcal{H}, T)$ be a stationary process with pure point diffraction and associated Bragg spectrum $\mathcal{S}$. Let θ be the associated diffraction to dynamics map and $f_k = \theta(1_k)$, $k \in \mathcal{S}$. Then*

$$N(F) = \sum_{k \in \mathcal{S}} \widehat{F}(k) f_k$$

for all $F \in C_c(\mathbb{G})$.

Proof. By definition of θ, we have $N(F) = \theta(\widehat{F})$. Obviously, $\widehat{F} = \sum_{k \in \mathcal{S}} \widehat{F}(k) 1_k$ and the claim follows. □

3.3. *Spatial stationary processes: two-point correlation.* In this section we show how the autocorrelation can be given a meaning that agrees with 'classical' two-point correlation associated to stationary point processes.

† Sometimes, the term Bragg peak is also taken to mean both the position k of the atom and its intensity $\omega(\{k\})$.

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Assume that we are given an ergodic spatial stationary process $\mathcal{N} = (N, X, \mu, T)$. As discussed in Corollary 3.3, we can assume that N is defined on all measurable bounded functions with compact support. We also assume that $\mathbb{G}$ has a countable basis of topology and is hence metrizable. Let $\{A_n\}_{n=1}^{\infty}$ be a van Hove sequence for $\mathbb{G}$ (as discussed at the end of the introduction). We assume that this is fixed once and for all.

Definition 3.13. For $x \in X$, we define the *two-point correlation or autocorrelation* of x at any $F \in C_c(\mathbb{G})$ as

$$\lim_{B\to 0} \frac{1}{l_{\mathbb{G}}(B)} \left(\lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \int_{A_n} (N(1_B)N(F))(T_{-t}x)\, dl_{\mathbb{G}}(t) \right)$$

whenever the limit exists.

This needs some comments: the limits in the definition are taken in the order indicated: first the inner and then the outer. Here B is an open (or measurable) neighbourhood of 0 in $\mathbb{G}$. The statement $B \to 0$ means that we take a nested descending sequence $\{B_m\}$ of such neighbourhoods, all within some fixed compact set K, and that $l_{\mathbb{G}}(B_m) \to 0$. We shall use the notation dt to stand for the longer $dl_{\mathbb{G}}(t)$. The definition requires that we give meaning to $N(1_B)$ as a measurable function on $\mathbb{G}$. This uses the extension of N from $C_c(\mathbb{G})$ to L^2-functions with compact support given in Corollary 3.3.

The intuition behind the definition is as follows. Assume first that the elements of X can be considered as functions x on $\mathbb{G}$ providing densities with respect to the Haar measure. Then the two-point correlation at $x \in X$ for $F \in C_c(\mathbb{G})$ should look something like

$$\begin{aligned} &\lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \int_{A_n} \int_{A_n} x(t)x(s)F(-t+s)\, dt\, ds \\ &\quad = \lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \int_{A_n} x(t) \int_{\mathbb{G}} x(s)(T_t F)(s)\, ds\, dt, \end{aligned}$$

where the right-hand side arises by using the usual trick from van Hove sequences and the compactness of the support of F (that is, the difference of the two sides of the equation is due to the difference between $-A_n$ and $-A_n + \mathrm{supp}(F)$, which by the van Hove assumption is irrelevant in the limit). Of course in our case x is not a function of t and the integrands do not make sense. But the inner integral on the right-hand side is what should be $N(T_t F)(x) = N(F)(T_{-t}x)$ and we can rewrite this 'autocorrelation' as

$$\lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \int_{A_n} (T_{-t}x)(0) N(F)(T_{-t}x)\, dl_{\mathbb{G}}(t).$$

The term $(T_{-t}x)(0)$ has no meaning. But Palm theory tells us how to go around this. We instead average over a small neighbourhood B of 0, and this brings us to Definition 3.13.

THEOREM 3.14. *Let $\mathbb{G}$ be a locally compact group whose topology has a countable basis and let (N, X, μ, T) be an ergodic spatial stationary process on $\mathbb{G}$ with second moment. The two-point correlation of $x \in X$ exists μ-almost surely and its value at $F \in C_c(\mathbb{G})$ is $\gamma(F)$.*

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Proof. The function $(N(1_B)N(F))(T_{-t}x)$ is measurable as a function of $t \in \mathbb{G}$ and the Birkhoff theorem says that almost surely

$$\lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \int_{A_n} (N(1_B)N(F))(T_{-t}x)\ dt = \int_X N(1_B)N(F)\, d\mu, \tag{10}$$

meaning that the limit will exist and equal the right-hand side. We shall prove that

$$\lim_{B\to 0} \frac{1}{l_{\mathbb{G}}(B)} \int_X N(1_B)N(F)\, d\mu = \gamma(F), \tag{11}$$

proving that Definition 3.13 works μ-almost surely in x for each $F \in C_c(\mathbb{G})$ and that γ does have the meaning of an autocorrelation.

This has to be made to work simultaneously for all F in $C_c(\mathbb{G})$, which can be done in the usual way from a countable basis of $C_c(\mathbb{G})$. This will then prove Theorem 3.14.

Here are the details: it is enough to prove (11) for real-valued F. Using (7), we have for all $F, G \in C_c^{\mathbb{R}}(\mathbb{G})$,

$$\int_{\mathbb{G}} F * \widetilde{G}\, d\gamma = \langle N(F) \mid N(G)\rangle.$$

Let $F \in C_c^{\mathbb{R}}(\mathbb{G})$ and choose $\epsilon > 0$. Let B be a measurable subset of $\mathbb{G}$ with compact closure. Then, by Proposition 3.3, $N(B) := N(1_B)$ is defined and is a measurable L^2-function on X. By linearization, we have

$$\begin{aligned}\int_X N(1_B)N(F)\, d\mu &= \int_{\mathbb{G}} 1_B * \widetilde{F}\, d\gamma \\ &= \int_{\mathbb{G}}\int_{\mathbb{G}} 1_B(t)\widetilde{F}(s-t)\, dt\, d\gamma(s) = \int_{\mathbb{G}}\int_{\mathbb{G}} 1_B(t)F(t-s)\, dt\, d\gamma(s).\end{aligned}$$

Since F is uniformly continuous on $\mathbb{G}$, for any sufficiently small neighbourhood B of 0, $|F(t-s) - F(-s)| < \epsilon$ for all $t \in B$ and for all $s \in \mathbb{G}$. Then

$$\left|\int_{\mathbb{G}} 1_B(t)F(t-s)\, dt - l_{\mathbb{G}}(B)F(-s)\right| \le \int_{\mathbb{G}} 1_B(t)|F(t-s) - F(-s)|\, dt < \epsilon\, l_{\mathbb{G}}(B)$$

for all $s \in \mathbb{G}$, so

$$\begin{aligned}&\frac{1}{l_{\mathbb{G}}(B)}\left|\int_X N(B)N(F)\, d\mu - l_{\mathbb{G}}(B)\int_{\mathbb{G}} F(-s)\, d\gamma(s)\right| \\ &\quad= \frac{1}{l_{\mathbb{G}}(B)}\left|\int_{\mathbb{G}}\int_{\mathbb{G}} 1_B(t)F(t-s)\, dt\, d\gamma(s) - l_{\mathbb{G}}(B)\int_{\mathbb{G}} F(-s)\, d\gamma(s)\right| \\ &\quad\le \frac{1}{l_{\mathbb{G}}(B)}\int_{\mathbb{G}}\int_{\mathbb{G}} 1_B(t)|F(t-s) - F(-s)|\, dt\, d\gamma(s) \\ &\quad\le \frac{1}{l_{\mathbb{G}}(B)}\epsilon\, l_{\mathbb{G}}(B)|\gamma|(-\mathrm{supp}(F) + B).\end{aligned}$$

Since $\gamma(s) = \gamma(-s)$ (γ is positive definite and real, by Proposition 3.1), we see that as $B \to 0$ (and correspondingly $\epsilon \to 0$) we have a proof of (11). Together with (10), we have the desired interpretation of Definition 3.13 as the autocorrelation at x and its almost sure equality with $\gamma(F)$, and Proposition 3.14 is proved. □

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Remark 3.15. This type of result was first established for certain uniformly discrete point processes on Euclidean space by Hof [**18**] (see [**37**] for the case of general locally compact abelian groups). This was then extended to rather general point processes by Gouéré [**16**] and to certain measure processes by Baake and Lenz [**6**]. A unified treatment was then given by Lenz and Strungaru [**28**]. Our result contains all these results (provided the underlying process is real).

3.4. *A second glance at second moments.* The discussion above has shown that existence of second moments has strong consequences. It implies existence of the diffraction to dynamics map by Proposition 3.8 and further continuity properties by Corollary 3.2. It turns out that a converse of sorts holds. This is investigated in this section. Along the way, we will also show that continuity of N implies an intertwining property of the map N and this will be crucial for our considerations in this section.

Any process $(N, \mathcal{H}, T)$ gives rise to two representations of $C_c(\mathbb{G})$ (and in fact even of $L^1(\mathbb{G})$). The first representation L acts by

$$L_G F = G * F$$

for $F, G \in C_c(\mathbb{G})$. The second representation T (extending the action T and therefore denoted by the same letter) acts by

$$T_G f := \int G(t) T_t f \, dl_{\mathbb{G}}(t)$$

for $G \in C_c(\mathbb{G})$ and $f \in \mathcal{H}$. Call N *continuous* if the restriction of N to $C_K(\mathbb{G})$ is continuous for any compact $K \subset \mathbb{G}$ (where $C_K(\mathbb{G})$ is equipped with the supremum norm). Note that Corollary 3.2 establishes this continuity for any stationary process with a second moment. This continuity yields an intertwining property.

LEMMA 3.16. *Let $(N, \mathcal{H}, T)$ be a process with a continuous N. Then*

$$N \circ L_G = T_G \circ N$$

for all $G \in C_c(\mathbb{G})$.

Proof. For $F \in C_c(\mathbb{G})$, we have

$$N(L_G(F)) = N(G * F) = N\left(\int_{\mathbb{G}} G(t) T_t F \, dl_{\mathbb{G}}(t) \right).$$

By the linearity and continuity of N, it commutes with taking integrals and

$$N\left(\int_{\mathbb{G}} G(t) T_t F \, dl_{\mathbb{G}}(t) \right) = \int_{\mathbb{G}} G(t) N(T_t F) \, dl_{\mathbb{G}}(t) = \int_{\mathbb{G}} G(t) T_t N(F) \, dl_{\mathbb{G}}(t)$$

holds, which finishes the proof. □

We will need a somewhat stronger continuity property of N.

Definition 3.17. Let $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$ be given. The process $(N, \mathcal{H}, T)$ is said to be weakly (p, q)-continuous if for any compact $K \subset \mathbb{G}$, there exists a C_K with

$$|\langle N(F) \mid N(G) \rangle| \leq C_K \|F\|_{L^p(\mathbb{G})} \|G\|_{L^q(\mathbb{G})}$$

for all $F, G \in C_c(\mathbb{G})$ with support contained in K (compare with Corollary 3.2).

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Remark 3.18.

(a) Note that continuity of N is exactly weak $(2, 2)$-continuity.

(b) By standard interpolation theory, we can conclude that weak $(2, 2)$-continuity together with weak $(1, \infty)$-continuity implies weak (p, q)-continuity for all p, q with $1 \leq p, q \leq \infty$ and $1/p + 1/q = 1$.

THEOREM 3.19. *Let $(N, \mathcal{H}, T)$ be a stationary process. Then the following assertions are equivalent:*

(i) *N has a second moment.*

(ii) *N is weakly (p, q)-continuous for all $1 \leq p, q \leq \infty$ with $1/p + 1/q = 1$.*

In this case N is continuous and has the intertwining property that

$$N \circ L_G(F) = T_G N(F)$$

for all $F, G \in C_c(\mathbb{G})$.

Proof. (i) $\Longrightarrow$ (ii): This follows immediately from Corollary 3.2.

(ii) $\Longrightarrow$ (i): As N is weakly $(2, 2)$ continuous, it is continuous and the intertwining property follows from the previous lemma. By Proposition 3.1, it suffices to show existence of a measure γ on $\mathbb{G}$ with

$$\langle N(F) \mid N(G) \rangle = \gamma(F * \widetilde{G})$$

for all $F, G \in C_c(\mathbb{G})$. A short calculation shows that for such a γ, the equality

$$\langle N(F) \mid N(G) \rangle = \int F(s)(\gamma * G)(s)\, dl_{\mathbb{G}}(s)$$

must hold for all $F, G \in C_c(\mathbb{G})$. The idea is now to 'reverse' this reasoning to conclude existence of γ. The main issue is to show continuity of the object H_G replacing the not yet defined $\gamma * G$. This is shown using the intertwining property. Here are the details: it suffices to only consider real-valued functions. We choose an arbitrary compact K in $\mathbb{G}$ and assume without loss of generality that $0 \in K$. Let U be an open neighborhood of 0 with compact closure and set K_1 to be the closure of $K + U$. Set $L = K_1 - K_1 + K_1 - K_1$.

As N is weakly $(1, \infty)$-continuous, and $L^\infty(L)$ is the dual of $L^1(L)$, we can find to each $G \in C_c(\mathbb{G})$ with support in K_1 a function H_G in $L^\infty(L)$ with

$$\langle N(F) \mid N(G) \rangle = \int F(s) H_G(s)\, dl_{\mathbb{G}}(s)$$

for all $F \in C_c(\mathbb{G})$ with support in L and

$$\|H_G\|_\infty \leq C \|G\|_\infty, \tag{12}$$

where $C = C_L$. As N has the intertwining property, a short argument shows that

$$H_{G_1 * G_2}(t) = \int G_1(s) H_{G_2}(t - s)\, dl_{\mathbb{G}}(y)$$

for $t \in K$ for all $G_2 \in C_c(\mathbb{G})$ with support contained in K and all $G_1 \in C_c(\mathbb{G})$ with support contained in U. This gives, in particular, that $H_{G_1 * G_2}$ is a continuous function (on K) for all such G_1, G_2. Now (12) yields

$$\|(H_{D*G} - H_G)\|_\infty = \|H_{D*G-G}\|_\infty \leq C \|D * G - G\|_\infty.$$

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Taking an approximate unit for D, we see that H_G can be approximated uniformly by continuous functions. This shows continuity of H_G. Moreover, by (12) again, the map

$$G \mapsto H_G(t)$$

is continuous for each x. Thus, we can indeed define the measure γ with

$$\gamma * G(t) = H_G(t).$$

By construction, γ has the desired properties. □

3.5. *A remark on mean density.* A familiar concept in the theory of point processes is that of the mean density of a point process. Here we introduce the corresponding concept for stationary processes. Our considerations provide an analogue (with a somewhat alternative point of view) to [**4**, Proposition 9.2].

Definition 3.20. Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with second moment. Then the *mean density* of N is defined to be

$$\operatorname{den}(\mathcal{N}) = \lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \|N(1_{A_n})\|,$$

where $\{A_n\}$ is any van Hove sequence in $\mathbb{G}$ and $\|\cdot\|$ is the norm on the Hilbert space $\mathcal{H}$.

The question of existence of the limit and its independence from the choice of van Hove sequence, along with its basic connection to the diffraction, is treated in the following proposition.

PROPOSITION 3.21. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with second moment. Then the mean density* $\operatorname{den}(\mathcal{N})$ *exists and is equal to* $\omega(0)^{1/2}$.

Proof. The proof is inspired by related considerations in (the proof of) Corollary 5 of [**25**]. Set $H_n := 1/(l_{\mathbb{G}}(A_n))1_{A_n}$. We will show that $N(H_n) \to \theta(1_{\{0\}})$ as $n \to \infty$, and the desired statement follows from Lemma 3.11.

Choose $F \in C_c(\mathbb{G})$ with $F \geq 0$ and $\int F\, dx = 1$ (and hence $\widehat{F}(0) = 1$). Note that $F * F$ (like F) is continuous, has compact support, and satisfies $\int F * F\, dx = 1$. Set $G_n := H_n * F$. Then H_n and $G_n * F = H_n * (F * F)$ agree except on the 'boundary' of A_n, where they are of size $(1/l(A_n))$. Thus, using the linearity of N, Proposition 3.1, and the facts that γ is translation bounded and (A_n) is van Hove, we easily find (compare also [**25**, Lemma 6])

$$\begin{aligned}\|N(H_n) - N(G_n * F)\|^2 &= \|N(H_n - G_n * F)\|^2 \\ &= \gamma((H_n - G_n * F) * (\widetilde{H_n - G_n} * F)) \to 0,\ n \to \infty.\end{aligned}$$

Thus, it suffices to show that

$$\lim_{n\to\infty} N(G_n * F) = \theta(1_{\{0\}}).$$

By the intertwining property given in Theorem 3.19, we have

$$N(G_n * F) = N(L_{G_n} F) = T_{G_n} N(F).$$

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By von Neumann's ergodic theorem, see e.g. [**20**, Theorem 6.4.1], we obtain

$$T_{H_n} N(F) \to E_T(0) N(F), \quad n \to \infty,$$

with the spectral family E_T defined above. As G_n and H_n agree up to a boundary term, we obtain $T_{G_n} N(F) \to E_T(0) N(F)$, $n \to \infty$. Putting this together, we arrive at

$$N(G_n * F) \to E_T(0) N(F), \quad n \to \infty.$$

So, it remains to show that $E_T(0) N(F) = \theta(1_{\{0\}})$. Now, by definition of θ, we have $N(F) = \theta(\widehat{F})$. Moreover, by Theorem 3.10, we have $E_T(0)\theta(H) = \theta(1_{\{0\}} H)$ (for any $H \in L^2(\widehat{\mathbb{G}}, \omega)$), so we obtain the desired statement

$$E_T(0) N(F) = E_T(0)\theta(\widehat{F}) = \theta(1_{\{0\}} \widehat{F}) = \theta(1_{\{0\}}),$$

where we used $\widehat{F}(0) = 1$ in the last step. □

Remark 3.22.

(a) The proof shows that $N(H_n) \to \theta(1_{\{0\}})$, $n \to \infty$ with $H_n = 1/(l_{\mathbb{G}}(A_n)) 1_{A_n}$. Thus, we obtain in particular also the following formula for the mean density:

$$\lim_{n\to\infty} \langle N(F), N(H_n) \rangle = \langle N(F), \theta(1_{\{0\}}) \rangle = \langle \widehat{F}, 1_{\{0\}} \rangle_{\widehat{\mathbb{G}}} = \omega(0) = \operatorname{den}(\mathcal{N})^2$$

for any $F \in C_c(\mathbb{G})$ with $\int F \, dx = 1$.

(b) Let $k \in \widehat{\mathbb{G}}$ be arbitrary and define $H_n^{(k)} := k/(l_{\mathbb{G}}(A_n)) 1_{A_n}$. Then the proof can easily be adapted to show that

$$N(H_n^{(k)}) \to \theta(1_{\{k\}}), \quad n \to \infty \text{ and } \|N(H_n^{(k)})\|^2 \to \omega(k), \quad n \to \infty$$

(see [**25**] for a related reasoning). So, the intensity of any Bragg peak can be calculated by this approximation.

(c) It may be worth noting that the considerations of this section do not require the underlying process to be spatial.

4. *Almost periodicity*

Almost periodicity is closely linked to nature of diffraction via the Fourier transform. This concept allows one to compare properties of the autocorrelation and the diffraction measure. In particular, it can be used to characterize pure point and continuous diffraction. The considerations of this section play a role in subsequent parts of the paper: they are used in §5 to decompose an arbitrary process into a part with pure point diffraction and a part with continuous diffraction and in §6 to prove the equivalence of pure point diffraction spectrum and pure point spectrum. The material of this section derives from [**14**] and, in a more accessible account, [**31**] and from [**27**, **28**] as well. For further studies of aspects of almost periodicity in our context, we refer to [**16**, **21**, **38**].

We shall assume in this and subsequent sections that $\mathbb{G}$ is a σ-compact locally compact abelian group.

Almost periodicity is most commonly defined by a compactness condition: $f \in C_u(\mathbb{G})$ is almost periodic if the translation orbit $\mathbb{G}.f$ of f is compact. Here $C_u(\mathbb{G})$ is the space of uniformly continuous $\mathbb{C}$-valued functions on $\mathbb{G}$. The key point, however, is in which

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topology is the translation orbit to be compact? In the case of the supremum norm topology the concept defines *strong almost periodicity*. In the case that the topology is defined by the family of seminorms induced by the set of all continuous linear functionals on $C_u(\mathbb{G})$, it is called *weak almost periodicity*. Strong almost periodicity coincides with H. Bohr's original concept of almost periodicity: $f \in C_u(\mathbb{G})$ is strongly periodic if and only if for every $\epsilon > 0$ the set of $t \in \mathbb{G}$ for which $\|T_t f - f\|_{\sup} < \epsilon$ is relatively dense. It is harder to get an intuitive feel for weak almost periodicity. Fortunately what one needs to know about it is fairly straightforward:

- all positive-definite functions on $\mathbb{G}$ are weakly almost periodic;
- for every weakly almost periodic function f, the *mean* of f, defined as

$$\lim_{n\to\infty} \frac{1}{l_{\mathbb{G}}(A_n)} \int_{A_n} f(x+t)\, dl_{\mathbb{G}}(t),$$

  exists for any van Hove (more generally Følner) sequence $\{A_n\}$ in $\mathbb{G}$ and for any $x \in \mathbb{G}$, and its value is independent of both x and the choice of van Hove sequence.

One says that a weakly almost periodic function f is *null weakly almost periodic* if its mean is 0. These concepts lift to measures in a simple way: a Borel measure ϕ on $\mathbb{G}$ is called *strongly* (respectively *weakly*, *null weakly*) *almost periodic* if $f * \phi$ is a strongly (respectively weakly, null weakly) almost periodic function for every $f \in C_c(\mathbb{G})$.

Positive-definite measures on $\mathbb{G}$ turn out to be weakly almost periodic and are also, as we have noted already, Fourier transformable.

THEOREM 4.1. [**14**] *Every weakly almost periodic measure ϕ is uniquely expressible as the sum of a strongly almost periodic measure and a null weakly almost periodic measure. If the measure ϕ is Fourier transformable, then so too are the strong and null weak components, and furthermore the Fourier transforms of these components are the pure point and continuous parts of $\widehat{\phi}$.* □

Remark 4.2. The decomposition of ϕ given in the theorem is sometimes known as *Eberlein decomposition*; see [**31**] for further investigation and references.

These considerations can be applied to strongly continuous unitary representations and hence to processes as well. This is discussed next. The crucial connection is given by the following (well-known) lemma.

LEMMA 4.3. *Let T be a strongly continuous unitary representation of $\mathbb{G}$ on a Hilbert space $\mathcal{H}$. Then, for any $f \in \mathcal{H}$, the function $t \mapsto \langle f \mid T_t f\rangle =: F_f(t)$ is positive definite and hence weakly almost periodic and Fourier transformable. Its Fourier transform is the spectral measure ρ_f.*

Proof. As T is unitary, we have for any $t_1, \ldots, t_n \in \mathbb{G}$ and $c_1, \ldots, c_n \in \mathbb{C}$,

$$\sum_{k,l=1}^{n} c_k \overline{c_l} F_f(t_k - t_l) = \left\| \sum_{l=1}^{n} c_l F_f(t_l) \right\|^2 \geq 0$$

and F_f is shown to be positive definite. The remaining statements follow from (2) and the preceding discussion. □

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Combining the previous lemma and the previous theorem, we infer the following corollary.

COROLLARY 4.4. *Let T be a strongly continuous unitary representation of $\mathbb{G}$ on a Hilbert space $\mathcal{H}$. Then, for any $f \in \mathcal{H}$, the function $t \mapsto \langle f \mid T_t f \rangle$ is the sum of a strongly almost periodic function and a null weakly almost periodic function. This strongly almost periodic function is given by the (inverse) Fourier transform of the pure point part of the spectral measure ρ_f and the null weakly almost periodic function is given by the (inverse) Fourier transform of the continuous part of the spectral measure ρ_f.*

Of particular relevance is the question whether the spectral measures are pure point. Here the following holds as shown in [**28**, Lemma 2.1].

LEMMA 4.5. *Let T be a strongly continuous unitary representation of $\mathbb{G}$ on $\mathcal{H}$. Then the following assertions are equivalent for $f \in \mathcal{H}$.*

(i) *The map $\mathbb{G} \longrightarrow \mathcal{H}$, $t \mapsto T_t f$, is almost periodic in the sense that for any $\varepsilon > 0$, the set $\{t \in \mathbb{G} : \|T_t f - f\| \leq \varepsilon\}$ is relatively dense in $\mathbb{G}$.*
(ii) *The hull $\{T_t f : t \in \mathbb{G}\}$ is relatively compact.*
(iii) *The map $\mathbb{G} \longrightarrow \mathbb{C}$, $t \mapsto \langle f \mid T_t f \rangle$, is strongly almost periodic.*
(iv) *ρ_f is a pure point measure.*
(v) *f belongs to $\mathcal{H}_p$.*

The preceding equivalence allows one to show some stability properties of $\mathcal{H}_p$. This is discussed next (see [**28**] as well for a proof of (a) of the following theorem). There, we say that a *measure μ is supported on a measurable set S* if the μ-measure of the complement of S is zero.

THEOREM 4.6. *Let T be a strongly continuous unitary representation of $\mathbb{G}$ on $\mathcal{H}$.*

(a) *Let $C : \mathcal{H} \longrightarrow \mathcal{H}$ be continuous with $T_t C f = C T_t f$ for each $t \in \mathbb{G}$ and $f \in \mathcal{H}$. Then C maps $\mathcal{H}_p$ into $\mathcal{H}_p$. If f belongs to $\mathcal{H}_p$ and ρ_f is supported on the subgroup S of $\widehat{\mathbb{G}}$, then so is ρ_{Cf}.*
(b) *Let $M : \mathcal{H} \times \mathcal{H} \longrightarrow \mathcal{H}$ be continuous with $T_t M(f, g) = M(T_t f, T_t g)$. Then M maps $\mathcal{H}_p \times \mathcal{H}_p$ into $\mathcal{H}_p$.*

Proof. The statements on C and M are clear from the equivalence of (v) and (ii) in Lemma 4.5 and the continuity and intertwining property of C and M. The statement on the support in (a) is proven in [**28**]. □

We now further restrict attention to processes with second moments. Then Theorem 4.1 together with Corollary 4.4 can directly be applied to give the following result (which parallels results from [**7**, **16**, **28**, **30**]).

PROPOSITION 4.7. *A stationary process $(N, \mathcal{H}, T)$ with second moment is pure point diffractive if and only if its autocorrelation is strongly almost periodic. It has continuous diffraction if and only if the autocorrelation is null weakly almost periodic.* □

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Remark 4.8. Note that one has a (trivial) Bragg peak at zero if and only if the mean density of the process does not vanish; see Proposition 3.21. Thus, the case of (purely) continuous diffraction can occur only for processes with vanishing mean density.

We can then combine the above results to obtain the following.

PROPOSITION 4.9. *For any stationary process $(N, \mathcal{H}, T)$ with second moment, the mapping $t \mapsto \langle N(F) \mid T_t N(F)\rangle$ is a weakly almost periodic function on $\mathbb{G}$ for all $F \in C_c(\mathbb{G})$. The process $(N, \mathcal{H}, T)$ then has pure point (respectively continuous) diffraction if and only if $t \mapsto \langle N(F) \mid T_t N(F)\rangle$ is a strongly (respectively null weakly) almost periodic function on $\mathbb{G}$ for all $F \in C_c(\mathbb{G})$. Furthermore, the diffraction is pure point if and only if for all $F \in C_c(\mathbb{G})$, $t \mapsto T_t N(F)$ is a strongly almost periodic function on $\mathbb{G}$ with respect to the norm on $\mathcal{H}$.*

Proof. The first statement comes from Lemma 4.3. We now turn to the second statement. By Theorem 4.1 and the definition of the diffraction spectrum, we have pure point (respectively continuous) diffraction if and only if γ is strongly (respectively null weakly) almost periodic. Now, from Proposition 3.1 and a straightforward calculation, we obtain for all $F, G \in C_c^{\mathbb{R}}(\mathbb{G})$ and all $t \in \mathbb{G}$,

$$G * \widetilde{F} * \gamma(t) = \gamma(G * \widetilde{T_t F}) = \langle N(G) \mid T_t N(F)\rangle. \tag{13}$$

With G set equal to F, we then get the required almost periodicity properties of $t \mapsto \langle N(F) \mid T_t N(F)\rangle$ from the corresponding almost periodicity properties of γ, by our definition of these concepts. In the reverse direction, upon linearizing the expressions $\langle N(F) \mid T_t N(F)\rangle$, we obtain (13). From the almost periodicity properties of $t \mapsto \langle N(G) \mid T_t N(F)\rangle$, we then obtain the desired almost periodicity properties for all convolutions of the form $G' * \widetilde{F} * \gamma(-t)$. An approximate unit argument allows us to get the strong (respectively null weak) almost periodicity of γ from this; see [**31**, Corollary 9]. Here we use that these almost periodicity properties are stable under uniform convergence.

The last statement is a consequence of Lemma 4.5. This finishes the proof. □

We finish this section with a discussion of stability properties of almost periodicity in the case of spatial processes. We will need the following proposition on continuity of composition with a fixed function. The proposition is not hard to prove and can be found in [**28**].

PROPOSITION 4.10. *Let $\{h_n\}$ be a sequence in $L^2(X, \mu)$ converging to $h \in L^2(X, \mu)$. Let $\varphi : \mathbb{C} \longrightarrow \mathbb{C}$ be continuous with compact support. Then $\varphi \circ h_n$ converges to $\varphi \circ h$.* □

Now we turn to the following consequence of Theorem 4.6 (see [**28**] as well).

COROLLARY 4.11. *Let $(N, \mathcal{H}, T)$ be a spatial process with $\mathcal{H} = L^2(X, \mu)$. Let $\varphi, \psi : \mathbb{C} \longrightarrow \mathbb{C}$ be continuous functions with compact support and $f, g \in \mathcal{H}_p$ be given. Then we have the following.*

(a) *The function $\varphi \circ f$ belongs to $\mathcal{H}_p$ and the spectral measure $\rho_{\varphi \circ f}$ is supported in the subgroup S of $\widehat{\mathbb{G}}$ if ρ_f is supported in this subgroup.*

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(b) *The function* $(\varphi \circ f)(\psi \circ g)$ *belongs to* $\mathcal{H}_p$. *If both* ρ_f *and* ρ_g *are supported in the subgroup* S *of* $\widehat{\mathbb{G}}$, *then so is* $\rho_{(\varphi\circ f)(\psi\circ g)}$.

Proof. By the previous proposition, the maps $C : \mathcal{H} \longrightarrow \mathcal{H}$, $f \mapsto \varphi \circ f$, and $M : \mathcal{H} \times \mathcal{H} \longrightarrow \mathcal{H}$, $M(f, g) := (\varphi \circ f)(\psi \circ g)$ are continuous. They obviously commute with the action of $\mathbb{G}$. Thus, both (a) and the first statement of (b) follow from Theorem 4.6. It remains to show the second statement of (b): let $\mathcal{H}_p^S$ be the subspace of $\mathcal{H}_p$ consisting of elements whose spectral measure is supported on S. Then it is not hard to see that $\mathcal{H}_p^S$ is a closed subspace of $\mathcal{H}$. By (a) and the assumption on f and g, the spectral measures of both $\varphi \circ f$ and $\varphi \circ g$ belong to $\mathcal{H}_p^S$. Moreover, $\varphi \circ f$ and $\varphi \circ g$ are bounded functions. Thus, it suffices to show that $\mathcal{H}_p^S \cap L^\infty(X, \mu)$ is an algebra. This can be shown by mimicking the proof of Lemma 1 in [**6**] (see [**24**] as well). For the convenience of the reader, we sketch a proof.

Note first that every eigenfunction can be approximated by bounded eigenfunctions via a simple cut-off procedure, namely, if e is an eigenfunction, then, for an arbitrary $m > 0$, the function

$$e^{(m)}(x) := \begin{cases} e(x) & \text{for } |e(x)| \le m, \\ 0 & \text{otherwise,} \end{cases} \tag{14}$$

is again an eigenfunction (to the same eigenvalue). Evidently, the $e^{(m)}$ converge to e in L^2 as $m \to \infty$. Now let non-zero functions $a, b \in \mathcal{H}_p^S \cap L^\infty(X, \mu)$ be given and choose $\varepsilon > 0$ arbitrarily. As a belongs to $\mathcal{H}_p^S$, there exists a finite linear combination $a' = \sum a_i e_i$ of eigenfunctions to eigenvalues in S with

$$\Big\| a - \sum a_i e_i \Big\|_2 \;\le\; \frac{\varepsilon}{\|b\|_\infty}.$$

By the conclusion after equation (14), we can assume that all e_i are bounded functions. Thus, in particular, $\|a'\|_\infty < \infty$.

Similarly, we can choose another finite linear combination $b' = \sum b_j e_j$ of bounded eigenfunctions to eigenvalues in S with

$$\Big\| b - \sum b_j e_j \Big\|_2 \;\le\; \frac{\varepsilon}{\|a'\|_\infty}.$$

Then

$$\|ab - a'b'\|_2 \;\le\; \|a'\|_\infty \, \|b - b'\|_2 + \|b\|_\infty \, \|a - a'\|_2 \;\le\; 2\varepsilon.$$

The product of bounded eigenfunctions to eigenvalues in S is again a bounded eigenfunction to an eigenvalue in S (as S is a group) and the claim follows. □

5. *The pure point–continuous split and the Gelfand construction*

In this section we first discuss how any stationary process canonically splits into two subprocesses, one of which has pure point spectrum and one of which has continuous spectrum. If the original process has a second moment, then so have the two subprocesses and their diffraction measure will be pure point and purely continuous, respectively (Theorem 5.1). If furthermore the original process is spatial, then its pure point part is canonically isomorphic to a spatial pure point process (Theorem 5.6). This last result is based on the Gelfand construction of commutative Banach algebras.

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As we will require the results of the previous section, we will assume in this and subsequent sections that the group $\mathbb{G}$ is σ-compact.

Whenever T is a strongly continuous unitary representation of $\mathbb{G}$ on the Hilbert space $\mathcal{H}$ and U is a T-invariant closed subspace of $\mathcal{H}$ with corresponding orthogonal projection P_U, we can form the restriction T_U of T to U and this will be a strongly continuous unitary representation as well. The orthogonal complement $U^\perp$ of U in $\mathcal{H}$ is also T-invariant and we can form the restriction $T_{U^\perp}$ as well. We will now focus on the special decomposition into its continuous and point parts†. More precisely, we can define the continuous Hilbert space $\mathcal{H}_c$ and the point Hilbert space $\mathcal{H}_p$ by

$$\mathcal{H}_p := \{f \in \mathcal{H} : \rho_f \text{ is a pure point measure}\}, \quad \mathcal{H}_c := \{f \in \mathcal{H} : \rho_f \text{ is continuous}\}.$$

Here ρ_f is the spectral measure associated to f above. Then both $\mathcal{H}_p$ and $\mathcal{H}_c$ are closed T-invariant with

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_c.$$

With the projections P_c and P_p onto $\mathcal{H}_p$ and $\mathcal{H}_c$, we then have $P_c \oplus P_p = id$ and $P_* T_t = T_t P_* =: T_t^*$ for $* = p, c$. This gives the decomposition of the representation T as $T = T_p \oplus T_c$ with $T_* := P_* T$, $* = p, c$. Obviously, all spectral measures associated to T_p are purely discrete and all spectral measures associated to T_c are purely continuous. Accordingly, we call T_p the *point part of the representation* T and T_c the *continuous part of the representation* T.

We now turn to the case that we are given a stationary process $(N, \mathcal{H}, T)$. Of course, T is then a strongly continuous unitary representation of $\mathbb{G}$ on $\mathcal{H}$. So, any T-invariant subspace U gives rise to a decomposition of T. Moreover, the $\mathbb{G}$-invariance of N then implies that N can as well be decomposed into $N_U := P_U N$ and $N_{U^\perp} = P_{U^\perp} N$. Accordingly, the process $\mathcal{N}$ can be decomposed into the two processes $\mathcal{N}_U := (N_U, U, T_U)$ and $\mathcal{N}_{U^\perp} := (N_{U^\perp}, U^\perp, T_{U^\perp})$ and we write $\mathcal{N} = \mathcal{N}_U \oplus \mathcal{N}_{U^\perp}$.

As just discussed, T can be decomposed into its pure point part and its continuous part $N = N_p \oplus N_c$ with $N_* = P_* N$, $* = p, c$. Hence, any process $\mathcal{N} := (N, \mathcal{H}, T)$ can be decomposed into the two processes $\mathcal{N}_p := (N_p, \mathcal{H}_p, T_p)$ and $\mathcal{N}_c := (N_c, \mathcal{H}_c, T_c)$, which are called the *point part* and the *continuous part* of $\mathcal{N}$, respectively.

Now assume that the original process has a second moment and associated autocorrelation measure γ and diffraction measure $\omega = \widehat{\gamma}$. By Theorem 4.1, this γ can be decomposed uniquely into its strongly almost periodic part γ_{sap} and its null weakly almost periodic part $\gamma_{0\text{wap}}$ and the Fourier transform of γ_{sap} is the pure point part ω_p of ω and the Fourier transform of $\gamma_{0\text{wap}}$ is the continuous part ω_c of ω. It turns out that these are just the autocorrelation and diffraction measures of the pure point part and the continuous part of $\mathcal{N}$. This is the content of the next theorem.

THEOREM 5.1. *Let $\mathcal{N} = (N, \mathcal{H}, T)$ be a stationary process with a second moment and associated autocorrelation γ, diffraction measure ω, and diffraction to dynamics map θ. Let γ_{sap} and $\gamma_{0\text{wap}}$ be the strongly almost periodic part and the null weakly almost periodic part of γ and ω_p and ω_c the respective Fourier transforms. Then the point part $\mathcal{N}_p$ of $\mathcal{N}$*

† This decomposition is of spectral nature. It should not be confused with the extraction of some sort of point process out of a spatial process.

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has a second moment with autocorrelation given by γ_{sap} and diffraction measure given by ω_p and the continuous part $\mathcal{N}_c$ of $\mathcal{N}$ with autocorrelation given by $\gamma_{0\mathrm{wap}}$ and diffraction measure given by ω_c.

Proof. By Proposition 3.1, it suffices to show that

$$\gamma_{\mathrm{sap}}(F * \widetilde{G}) = \langle P_p N(F) \mid P_p N(G)\rangle \quad \text{and} \quad \gamma_{0\mathrm{wap}}(F * \widetilde{G}) = \langle P_c N(F) \mid P_c N(G)\rangle \tag{15}$$

for all $F, G \in C_c(\mathbb{G})$. By linearity, it suffices to consider the case $F = G$. Let F_t be the function $T_t F = F(\cdot - t)$ and consider the function $t \mapsto \gamma(F * \widetilde{F_t})$. We will decompose this function into a strongly almost periodic part and a null weakly almost periodic part in two ways and then conclude the desired statement from the uniqueness of the decomposition. Here are the details: by definition of γ_{sap} and $\gamma_{0\mathrm{wap}}$, we can decompose this function as

$$\gamma(F * \widetilde{F_t}) = \gamma_{\mathrm{sap}}(F * \widetilde{F_t}) + \gamma_{0\mathrm{wap}}(F * \widetilde{F_t})$$

with a strongly almost periodic function $t \mapsto \gamma_{\mathrm{sap}}(F * \widetilde{F_t})$ and a null weakly almost periodic function $t \mapsto \gamma_{0\mathrm{wap}}(F * \widetilde{F_t})$. On the other hand, by definition of γ and the fact that P_c and P_p are orthogonal, we also obtain the decomposition

$$\gamma(F * \widetilde{F_t}) = \langle N(F) \mid T_t N(F)\rangle = \langle P_p N(F) \mid T_t P_p N(F)\rangle + \langle P_c N(F) \mid T_t P_c N(F)\rangle.$$

Now $t \mapsto \langle P_p N(F) \mid T_t P_p N(F)\rangle = \int (t, k)\, d\rho_{P_p N(F)}(k)$ is strongly almost periodic as it is the inverse Fourier transform of a pure point measure and $t \mapsto \langle P_c N(F) \mid T_t P_c N(F)\rangle = \int (k, t)\, d\rho_{P_c N(F)}(k)$ is null weakly almost periodic as it is the inverse Fourier transform of a continuous measure. From Theorem 4.1, we conclude that

$$\gamma_{\mathrm{sap}}(F * \widetilde{F_t}) = \langle P_p N(F) \mid T_t P_p N(F)\rangle \quad \text{and} \quad \gamma_{0\mathrm{wap}}(F * \widetilde{F_t}) = \langle P_c N(F) \mid T_t P_c N(F)\rangle$$

for all $t \in \mathbb{G}$. Setting $t = 0$, we obtain (15). □

In the situation of the previous theorem, we can easily see that the diffraction to dynamics map $\theta : L^2(\widehat{\mathbb{G}}, \omega) \longrightarrow \mathcal{H}$ can be decomposed as

$$\theta = \theta_p \oplus \theta_c. \tag{16}$$

Here θ_p and θ_c are the diffraction to dynamics maps of $\mathcal{N}_p$ and $\mathcal{N}_c$ respectively and the natural decompositions $L^2(\widehat{\mathbb{G}}, \omega) = L^2(\widehat{\mathbb{G}}, \omega_p) \oplus L^2(\widehat{\mathbb{G}}, \omega_c)$ and $\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_c$ are implicitly used.

We now restrict attention to spatial processes. In this situation we can induce subprocesses via subalgebras of L^∞. This is discussed next. We will use the main result of Gelfand theory that any commutative C^*-algebra $\mathcal{A}$ with a unit is canonically isomorphic to the algebra $C(X_{\mathcal{A}})$ of continuous functions on the compact space $X_{\mathcal{A}}$ given by the maximal ideals of $\mathcal{A}$. We will denote the space of all continuous bounded complex-valued functions on the complex plane by $C_b(\mathbb{C})$.

PROPOSITION 5.2. *Let $\mathcal{N} := (N, \mathcal{H}, T)$ be a spatial process with Hilbert space $\mathcal{H} = L^2(X, \mu)$. Let $\mathcal{A}$ be a $\mathbb{G}$-invariant subalgebra of $L^\infty(X, \mu)$ which is closed under complex conjugation, contains the constant functions, and is closed with respect to the supremum norm. Let $U = U(\mathcal{A})$ be the closed subspace of $\mathcal{H}$ generated by $\mathcal{A}$ and let*

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$X_{\mathcal{A}}$ be the maximal ideal space of $\mathcal{A}$. Then $X_{\mathcal{A}}$ can be equipped in a unique way with a $\mathbb{G}$-action and a $\mathbb{G}$-invariant measure $\mu_{\mathcal{A}}$ such that the canonical Gelfand isomorphism $J : C(X_{\mathcal{A}}) \longrightarrow \mathcal{A}$ extends to a unitary $\mathbb{G}$-map (also called J)

$$J : L^2(X_{\mathcal{A}}, \mu_{\mathcal{A}}) \longrightarrow U.$$

The map J is compatible with the algebraic structure in that it satisfies:

- *$J(fg) = J(f)J(g)$ for all $f \in L^\infty(X_{\mathcal{A}}, \mu_{\mathcal{A}})$ and $g \in L^2(X_{\mathcal{A}}, \mu_{\mathcal{A}})$; and*
- *$J(\phi(f)) = \phi(J(f))$ for all $f \in L^2$ and for all continuous bounded $\phi : \mathbb{C} \longrightarrow \mathbb{C}$.*

The subspace U is a $\mathbb{G}$-invariant subspace and $\mathcal{N}$ can be decomposed as

$$\mathcal{N} = \mathcal{N}_U \oplus \mathcal{N}_{U^\perp},$$

where $\mathcal{N}_U$ is isomorphic via J to the spatial process $\mathcal{N}_{\mathcal{A}}$ with $N_{\mathcal{A}} = J^{-1} P_U N$, $\mathcal{H}_{\mathcal{A}} = L^2(X_{\mathcal{A}}, \mu_{\mathcal{A}})$. If $\mathcal{N}$ is ergodic, so is $\mathcal{N}_U$.

Proof. All statements are rather straightforward up to the compatibility of J with the algebraic structure and the ergodicity.

This compatibility with algebraic structure will be discussed next: by definition, J is an algebra isomorphism from $C(X_{\mathcal{A}})$ and $\mathcal{A}$. In particular, $J(fg) = J(f)J(g)$ for $f, g \in C(X_{\mathcal{A}})$. By a simple approximation argument, we then obtain $J(fg) = J(f)J(g)$ for all $f \in L^\infty(X_{\mathcal{A}})$ and $g \in L^2(X_{\mathcal{A}})$. Here we use that $\{fg_n\}$ converges to fg in $L^2(X_{\mathcal{A}})$ whenever $\{g_n\}$ converges to g in $L^2(X_{\mathcal{A}})$ and f is bounded. This shows that J is compatible with multiplication.

As J is an isomorphism of algebras, we also have $J(q(f)) = q(J(f))$ for any polynomial q and any $f \in C(X_{\mathcal{A}})$. By a Stone–Weierstrass type argument, this gives $J(\phi(f)) = \phi(J(f))$ for any $\phi \in C_b(\mathbb{C})$ and $f \in C(X_{\mathcal{A}})$. Consider now the set

$$\mathcal{C} := \{f \in L^2(X_{\mathcal{A}}, \mu_{\mathcal{A}}) : \phi(J(f)) = J(\phi(f)) \forall \phi \in C_b(\mathbb{C})\}.$$

Then $C(X_{\mathcal{A}}) \subset \mathcal{C}$ by what we have just shown. Moreover, $\mathcal{C}$ is closed in L^2 by Proposition 4.10. Thus, $\mathcal{C}$ must agree with $L^2(X_{\mathcal{A}}, \mu_{\mathcal{A}})$ as $C(X_{\mathcal{A}})$ is dense in $L^2(X_{\mathcal{A}}, \mu_{\mathcal{A}})$ (as $\{\phi(h_n)\}$ converges to $\phi(h)$ whenever $\{h_n\}$ converges to h).

It remains to show the statement on ergodicity. By definition, ergodicity means that the eigenspace of T for the eigenvalue 1 is one dimensional. This is obviously stable under the above constructions. □

Definition 5.3. The process $\mathcal{N}_{\mathcal{A}}$ constructed in the previous proposition is called the subprocess of $\mathcal{N}$ induced by $\mathcal{A}$.

THEOREM 5.4. *Let $\mathcal{N} := (N, \mathcal{H}, T)$ be a spatial process with Hilbert space $\mathcal{H} = L^2(X, \mu)$. Let $\mathcal{A}$ be the closure with respect to the supremum norm of the subalgebra of $L^\infty(X, \mu)$ generated by $\psi_1 \circ N(F_1) \cdots \psi_n \circ N(F_n)$ with $n \in \mathbb{N}$, $F_j \in C_c(\mathbb{G})$ and ψ_j continuous bounded functions from $\mathbb{C}$ to $\mathbb{C}$. Let $U = U(\mathcal{A})$ be the subspace of $\mathcal{H}$ generated by $\mathcal{A}$. Then U contains the range of N and the subprocess $\mathcal{N}_U$ is isomorphic to the full spatial process $\mathcal{N}_{\mathcal{A}}$. The process $\mathcal{N}_{\mathcal{A}}$ is ergodic if $\mathcal{N}$ is ergodic. Moreover,*

$$\langle N_{\mathcal{A}}(F) \mid N_{\mathcal{A}}(G) \rangle = \langle N(F) \mid N(G) \rangle$$

holds for all $F, G \in C_c(\mathbb{G})$. In particular, $\mathcal{N}$ has a second moment if and only if $\mathcal{N}_{\mathcal{A}}$ has a second moment and their autocorrelations agree in this case.

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Proof. By definition of $\mathcal{A}$, the range of N is obviously contained in the subspace U. Thus, $P_U N = N$ and therefore

$$\langle N_U(F) \mid N_U(G)\rangle = \langle N(F) \mid N(G)\rangle$$

holds for all $F, G \in C_c(\mathbb{G})$. Given this, all statements of the theorem follow immediately from the previous proposition. □

Remark 5.5. The theorem says that to any (ergodic) stationary process $\mathcal{N}$ we can find an (ergodic) stationary subprocess $\mathcal{N}_U$ which is full and has the same second moment. In the situation of the theorem, fullness of the original process $\mathcal{N}$ then just means that $\mathcal{N} = \mathcal{N}_U$.

Now let $(N, \mathcal{H}, T)$ be a spatial process with $\mathcal{H} = L^2(X, \mu)$. Let $V \subset L^2(X, \mu)$ be the closure of the linear span of products of the form

$$\psi_1 \circ N_p(F_1) \cdots \psi_n \circ N_p(F_n), \quad n \in \mathbb{N}, \psi_j \in C_b(\mathbb{C}), F_j \in C_c(\mathbb{G}).$$

Then V is a closed T-invariant subspace of $L^2(X, \mu)$. Let P_V be the orthogonal projection onto V. Then P_V commutes with T. Then (N_V, V, T_V) with $N_V = P_V N$ and $T_V = P_V T = T P_V$ is a stationary process. We call (N_V, V, T_V) the *augmented point part* of the stationary process $(N, \mathcal{H}, T)$. Let $V^\perp$ be the orthogonal complement of V in $\mathcal{H}$. Then $V^\perp$ gives rise to a stationary process $(N_{V^\perp}, V^\perp, T_{V^\perp})$ and $\mathcal{N}$ is the sum of these processes.

THEOREM 5.6. *Let $\mathcal{N} := (N, \mathcal{H}, T)$ be a spatial process with Hilbert space $\mathcal{H} = L^2(X, \mu)$ and associated augmented point part $\mathcal{N}_V := (N_V, V, T_V)$. Then the following hold:*

- *$\mathcal{N} = \mathcal{N}_V \oplus \mathcal{N}_{V^\perp}$;*
- *$\mathcal{N}_V$ is isomorphic to a full spatial process;*
- *$\langle P_V N(F) \mid P_V N(G)\rangle = \langle P_p N(F) \mid P_p N(G)\rangle$ and $\langle P_{V^\perp} N(F) \mid P_{V^\perp} N(G)\rangle = \langle P_c N(F) \mid P_c N(G)\rangle$ hold for all $F, G \in C_c(\mathbb{G})$.*

If $\mathcal{N}$ has a second moment with autocorrelation γ and diffraction ω, furthermore the following are true:

- *$\mathcal{N}_V$ has a second moment with autocorrelation γ_{sap} and diffraction measure given by the pure point part of ω;*
- *$\mathcal{N}_{V^\perp}$ has a second moment with autocorrelation $\gamma_{0\text{wap}}$ and the diffraction measure given by the continuous part of ω.*

Proof. Let $\mathcal{N}'_p = (N_p, \mathcal{H}, T)$. Let the algebra $\mathcal{A}$ be the closure with respect to the sup-norm of the linear span of products of the form

$$\psi_1 \circ N_p(F_1) \ldots \psi_n \circ N_p(F_n), \quad n \in \mathbb{N}, \psi_j \in C_b(\mathbb{C}), F_j \in C_c(\mathbb{G}).$$

Then V is just the subspace of $\mathcal{H}$ generated by $\mathcal{A}$.

We can then apply the previous theorem to $\mathcal{N}'_p$ and the algebra $\mathcal{A}$. This gives a decomposition $\mathcal{N}'_p = \mathcal{N}'_V \oplus \mathcal{N}'_{V^\perp}$, where $\mathcal{N}'_V$ is isomorphic to a full spatial process and

$$\langle N'_V(F), N'_V(G)\rangle = \langle N_p(F), N_p(G)\rangle = \langle P_p N(F) \mid P_p N(G)\rangle$$

holds for all $F, G \in C_c(\mathbb{G})$. Here the last equality follows by definition of N_p as $P_p N$.

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It remains to show that $P_V N(F) = P_p N(F)$ (then all remaining statements follow easily). To do so, we first note that the range of $N_p = P_p N$ is contained in the range of U by construction. Moreover, by general principles the algebra $\mathcal{A}$ and hence the subspace V is contained in the pure point part of T [**6**, **24**]. Thus, $P_V N = P_p N$ holds.

Similar remarks apply to N_c. Note that $P_{V^\perp} N = N - P_V N = N - P_p N = P_c N$. □

The considerations of this section and in particular the preceding theorem have the following consequence: whenever we are given a spatial process we can restrict attention to its point part and obtain a full spatial process with pure point spectrum. In particular, the whole theory developed below for full spatial processes with pure point spectrum will apply to the point part of any spatial process.

6. *Spatial processes with pure point diffraction*

In this section we discuss spatial processes with pure point diffraction. It is these processes that we will be able to classify. We show that for these processes the two notions of pure pointedness of the spectrum defined above, viz. pure point diffraction spectrum and pure point dynamical spectrum, actually agree. As noted in Theorem 5.6, any spatial process with second moment can be decomposed into a full spatial process with pure point diffraction and a general stationary process with continuous diffraction. Thus, the results of this section apply to the corresponding parts of any spatial process.

Let (N, X, μ, T) be a stationary process with pure point diffraction as discussed in §2. Thus, its diffraction measure ω is a pure point measure and the set of its atoms denoted by $\mathcal{S} = \mathcal{S}(\omega)$ is given by

$$\mathcal{S} = \{k \in \widehat{\mathbb{G}} : \omega(k) > 0\}.$$

Let

$$\theta : L^2(\widehat{\mathbb{G}}, \omega) \longrightarrow L^2(X, \mu)$$

be the associated diffraction to dynamics map and $f_k := \theta(1_k)$, $k \in \mathcal{S}$.

While the subspace $\theta(L^2(\widehat{\mathbb{G}}, \omega))$ of $L^2(X, \mu)$ may be small in some sense, in another sense it controls the whole Hilbert space $L^2(X, \mu)$ due to our assumption of pure point spectrum. A precise version is given next.

THEOREM 6.1. *Let $\mathcal{N} = (N, X, \mu, T)$ be a spatial stationary process, which is full and possesses a second moment. Then the following assertions are equivalent.*

(i) *The diffraction measure ω of (N, X, μ, T) is a pure point measure.*

(ii) *The representation T has pure point spectrum.*

In this case, the group $\mathcal{E}$ of eigenvalues of T is generated by the set $\mathcal{S}(\omega)$, and any eigenfunction is a (multiple of a) product of eigenfunctions of the form f_k, $k \in \mathcal{S}(\omega)$.

Proof. We mimic the argument of [**28**] (see [**6**, **24**] as well). By definition of the spectral measures ρ_f given in (2), we have

$$\langle N(F) \mid T_t N(F) \rangle = \int_{\widehat{\mathbb{G}}} (k, t)\, d\rho_{N(F)}(k)$$

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for all $F \in C_c(\mathbb{G})$. Moreover, by definition of ω and γ and the fact that N is a $\mathbb{G}$-mapping, we find

$$\langle N(F) \mid T_t N(F)\rangle = \gamma(F * \widetilde{F(T_{-t}\cdot)}) = \int_{\widehat{\mathbb{G}}} (k,t)|\widehat{F}|^2 \, d\omega(k)$$

first for real-valued $F \in C_c(\mathbb{G})$ and then by linearity for all $F \in C_c(\mathbb{G})$. Taking inverse Fourier transforms, we infer that

$$\rho_{N(F)} = |\widehat{F}|^2 d\omega \tag{17}$$

for all $F \in C_c(\mathbb{G})$.

The implication (ii) $\Longrightarrow$ (i) is now clear from (17). (We also saw this earlier from the properties of θ.) We next show (i) $\Longrightarrow$ (ii) as the diffraction measure is a pure point measure, the spectral measures associated to $N(F)$ are pure point measures (supported on $\mathcal{S}$) by (17). Thus, by part (a) of Corollary 4.11, the spectral measures of $\psi \circ N(F)$ for $\psi \in C_c(\mathbb{C})$, $F \in C_c(\mathbb{G})$, are then also pure point measures supported on the group generated by $\mathcal{S}$. By the fullness assumption and part (b) of Corollary 4.11, we then infer that T has pure point spectrum with eigenvalues contained in the group generated by $\mathcal{S}$.

Now, multiplying eigenfunctions f_k, $k \in \mathcal{S}$, we obtain eigenfunctions for arbitrary elements in the group generated by $\mathcal{S}$. This shows that the group generated by $\mathcal{S}$ is indeed the group of eigenvalues. At the same time it gives an eigenfunction for each eigenvalue. By ergodicity, the multiplicity of each eigenvalue is one and these eigenfunctions are all eigenfunctions. □

Remark 6.2.

(a) There is quite some history to Theorem 6.1: the implication (ii) $\Longrightarrow$ (i) is sometimes known as the Dworkin argument. It was first established by Dworkin [**12**] with later extensions by Hof [**18**] and Schlottmann [**37**] (see [**34**, **39**] for remarkable applications as well). In special situations, equivalence was then shown by Lee *et al* in [**24**]. This was then generalized in various directions by Gouéré [**16**], Baake and Lenz [**6**], Deng and Moody [**11**], and Lenz and Strungaru [**28**] (the latter result containing all earlier ones). The above result contains all these results (provided the underlying process is real).

(b) The equivalence between diffraction and dynamical spectrum cannot hold for the complete spectrum, as discussed by van Enter and Miękisz [**13**]. Indeed, Ref. [**13**] gives an example of a mixed spectrum where the pure point part of the dynamical spectrum is completely missing in the diffraction (up to the constant eigenfunction). For recent developments on how to recover—in certain cases—the whole dynamical spectrum via diffraction of factors, we refer the reader to [**2**, **3**].

Due to the previous theorem, we do not need to distinguish between pure point diffraction and pure point dynamical spectrum when dealing with full processes with second moments. This suggests the following definition.

Definition 6.3. A spatial stationary process (N, X, μ, T) is called *pure point* if it is full, possesses a second moment, and its diffraction measure is a pure point measure.

If $0 \in \mathcal{S}$ in the situation of Proposition 3.12, then by Lemma 3.11 f_0 is a real function belonging to the $k = 0$-eigenspace of $L^2(X, m)$ and $\|f_0\| = \omega(0)^{1/2}$. Since the constant

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function $1_X : x \mapsto 1$ for all $x \in X$ is an eigenfunction for $k = 0$ and the dynamical system is ergodic, it spans the $k = 0$-eigenspace of $L^2(X, m)$. Thus, $f_0 = \pm\omega(0)^{1/2}1_X$. Now we have already pointed out that if N is a stationary process, then so is any non-zero real multiple of it. In particular, $\pm N$ are stationary processes and one of them has the corresponding function $f_0 = \omega(0)^{1/2}1_X$. It causes unnecessary awkwardness later on in the discussion of phase forms to deal with the case $f_0 = -\omega(0)^{1/2}1_X$, so we wish to normalize N to avoid this situation.

Assumption 6.4. In the pure point ergodic case we shall always assume that $f_0 = \omega(0)^{1/2}1_X$.

7. *Relators and associated phase forms*

As mentioned already, our aim is to describe all stationary processes with a given pure point diffraction measure ω. This description will be given in terms of a set of objects called *relators* arising out of the Bragg spectrum of ω. While the later sections need the material of this section, it can be read independently of the previous ones.

Let $\widehat{\mathbb{G}}$ be a locally compact abelian group. Let $\mathcal{S} \subset \widehat{\mathbb{G}}$ be given with $\mathcal{S} = -\mathcal{S}$ and let $\mathcal{E}$ be the subgroup of $\widehat{\mathbb{G}}$ generated by $\mathcal{S}$. We shall give this group the discrete topology and, in order to keep this clear, we shall usually write $\mathcal{E}_d$ instead of $\mathcal{E}$.

In the sequel, we often use m-tuples $(k_1, \ldots, k_m) \in \mathcal{S}^m$ (for various m) of elements of $\mathcal{S}$ or of $\mathcal{E}_d$ and we often simply denote these by bold letters $\boldsymbol{k}$. The *length* of $\boldsymbol{k} = (k_1, \ldots, k_m)$ is m. If $\boldsymbol{k} = (k_1, \ldots, k_m)$, $\boldsymbol{l} = (l_1, \ldots, l_n)$, then $\boldsymbol{kl}$ is the concatenation

$$\boldsymbol{kl} = (k_1, \ldots, k_m, l_1, \ldots, l_n)$$

and

$$[\boldsymbol{k}] := k_1 + \cdots + k_m \in \mathcal{E}_d.$$

In this way $\mathbb{S} := \bigcup_{m=0}^{\infty} \mathcal{S}^m$ becomes a monoid under concatenation, with the empty 0-tuple $\emptyset$ as the identity element.

A *relator* is any m-tuple $\boldsymbol{k} = (k_1, \ldots, k_m) \in \mathcal{S}^m$ with

$$[\boldsymbol{k}] = k_1 + \cdots + k_m = 0.$$

The empty tuple is also taken to be a relator. Thus, the relators are a subset of $\mathbb{S}$. Let

$$\begin{aligned} Z_n &:= \{\boldsymbol{k} = (k_1, \ldots, k_n) \in \mathcal{S}^n : [\mathbf{k}] = 0\}, \quad n \geq 1, \\ Z_0 &:= \{\emptyset\}, \\ Z &:= \bigcup_{n=0}^{\infty} Z_n. \end{aligned}$$

Note that $Z_1 = \{(0)\}$ if $0 \in \mathcal{S}$, otherwise it is empty.

Concatenations of relators are relators and this makes Z a submonoid of $\mathbb{S}$.

We introduce an equivalence relation on $\mathbb{S}$ by transitive extension of the three rules:

(R1) $\boldsymbol{k} \sim \boldsymbol{l}$ if $\boldsymbol{l}$ is a permutation of the symbols of $\boldsymbol{k}$;

(R2) if $\boldsymbol{k} = (k_1, \ldots, k_m) \in \mathbb{S}$ and $0 \in \mathcal{S}$, then $(k_1, \ldots, k_m, 0) \sim (k_1, \ldots, k_m)$ (along with the first rule, this means that when $0 \in \mathcal{S}$, zeros can be dropped or added wherever they appear);

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(R3) $\boldsymbol{k} \sim \boldsymbol{l}$ if $\boldsymbol{l}$ can be obtained from $\boldsymbol{k}$ by inserting or removing pairs $\{k, -k\}$, $k \in \mathcal{S}$.

The second item here is related to our Assumption 6.4, see below.

It is easy to see that $\boldsymbol{k} \sim \boldsymbol{k}'$, $\boldsymbol{l} \sim \boldsymbol{l}' \Rightarrow \boldsymbol{kl} \sim \boldsymbol{k}'\boldsymbol{l}'$, so multiplication descends from $\mathbb{S}$ to $\mathbb{S}^{\sim} := \mathbb{S}/\sim$, whereupon $\mathbb{S}^{\sim}$ becomes an abelian group under this multiplication with $\emptyset^{\sim}$ as the identity element. Note that if $0 \in \mathcal{S}$, then $0^{\sim} = \emptyset^{\sim}$. We give $\mathbb{S}^{\sim}$ the discrete topology, so in particular it is a locally compact abelian group.

Since the sum $[\boldsymbol{k}] = k_1 + \cdots + k_m$ of an element of $\mathcal{S}^m$ is constant on the entire equivalence class $\boldsymbol{k}^{\sim}$, we see that Z is the union of all equivalence classes with component sum equal to 0, and we obtain $\mathcal{Z} := Z/\sim$ as a subgroup of $\mathbb{S}^{\sim}$. In addition, we see that there is a surjective homomorphism

$$\phi : \mathbb{S}^{\sim} \longrightarrow \mathcal{E}_d \quad \text{with } \boldsymbol{k} \mapsto [\boldsymbol{k}]$$

and its kernel is precisely $\mathcal{Z}$.

Definition 7.1. The group $\mathcal{Z} = \mathcal{Z}(\mathcal{S})$ is called the *relator group*. The elements of its dual group $\widehat{\mathcal{Z}}$ are called *phase forms*. Thus, a phase form is a group homomorphism

$$a^* : \mathcal{Z} \longrightarrow U(1)$$

(the latter being the unit circle in $\mathbb{C}$).

Remark 7.2.

(a) It is useful to think of relators in terms of the cycle structure of the Cayley graph of the group of eigenvalues with respect to the generators $\mathcal{S}$. In this way the group $\mathcal{Z}$ may then be seen as a kind of abelianized homotopy group or a first cohomology group of the graph. This works in the following way: we begin with $\mathcal{E}$ and the set $\mathcal{S}$ which satisfies $\mathcal{S} = -\mathcal{S}$ and generates $\mathcal{E}$. The Cayley graph has vertices $\mathcal{E}$ and edges consisting of all pairs $(x, x + k)$, where $x \in \mathcal{E}$ and $k \in \mathcal{S}$. Since for each edge $(x, x + k)$ we have the reverse edge $(x + k, x + k - k = x)$, we can think of the graph as being non-directed. Since $\mathcal{S}$ generates $\mathcal{E}$, the graph is connected. Each $\boldsymbol{k} = (k_1, \ldots, k_m)$ can be thought of as an edge sequence. Given any $x \in \mathcal{E}$, we obtain a path $x, x + k_1, x + k_1 + k_2, \ldots, x + k_1 + \cdots + k_m$ from it. This path is a cycle if and only if $\boldsymbol{k}$ is a relator, that is, $[\boldsymbol{k}] = 0$.
There is a sort of homotopy of edge sequences, which is generated by rules corresponding to (R1), (R2), and (R3) above. The first amounts to saying that for all $x \in \mathcal{E}$ and for all $k, l \in \mathcal{S}$, the paths $x, x + k, x + k + l$ and $x, x + l, x + l + k$ are homotopic; the second says that if $0 \in \mathcal{S}$, then the path $x, x + 0$ is homotopic with the empty path from x; and the third says that the path $x, x + k, x + k + (-k)$ is homotopic to the empty path from x. The group $\mathcal{Z}$ may be thought of as a sort of homotopy group for cycles originating (and terminating) at 0.

(b) It should be noted that the homotopy group $\mathcal{Z}$ may be infinite even when the group $\mathbb{G}$ and hence the associated graph is finite.

The phase forms play a central role in the homometry problem. Indeed, they will later be shown to play the role of parametrizing homometric processes. Here we note already that they depend only on $\mathcal{S}$, not on the actual values of the diffraction measure ω. We shall

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find it convenient to sometimes relax the notation and write things like $a^*(k_1, \ldots, k_m)$, where we mean $a^*((k_1, \ldots, k_m)^\sim)$ when using the phase form a^*.

Of the various $\boldsymbol{k} = (k_1, \ldots, k_m)$ that can represent a given element in $\mathcal{Z}$, there is (at least) one of minimal length n. This minimal length is denoted by $\mathrm{len}(\boldsymbol{k})$ and is called the *reduced length* of $\boldsymbol{k}$. Here, of course, the length of $(k_1, \ldots, k_m)$ is given by m.

Define $\mathcal{Z}_n$ to be the set of elements in $\mathcal{Z}$ which have reduced length less than or equal to n. We have

$$\mathcal{Z} = \bigcup_{n=0}^{\infty} \mathcal{Z}_n,$$
$$\mathcal{Z}_n \mathcal{Z}_p \subset \mathcal{Z}_{n+p} \quad \text{for all non-negative integers } n \text{ and } p.$$

We let $\mathcal{F}(\mathcal{S})$ be the abelian group (with discrete topology) generated by symbols $e(k)$, $k \in \mathcal{S}$, subject only to the relations† $e(0) = 1$ (if $0 \in \mathcal{S}$) and $e(-k)e(k) = 1$ for all $k \in \mathcal{S}$.

PROPOSITION 7.3. *The mapping $\varphi : e(k) \mapsto (k)^\sim$ for all $k \in \mathcal{S}$ extends to an isomorphism $\varphi : \mathcal{F}(\mathcal{S}) \longrightarrow \mathbb{S}^\sim$.*

Proof. The existence of φ as a surjective homomorphism is clear since $\mathbb{S}^\sim$ is the abelian group freely generated by the symbols $(k)^\sim$ subject only to the relations defining $\mathcal{F}(\mathcal{S})$. These correspond precisely to $(k)^\sim(-k)^\sim = (k, -k)^\sim = \emptyset^\sim$ and $(0)^\sim = \emptyset^\sim$ when $0 \in \mathcal{S}$, which hold in $\mathbb{S}^\sim$.

A typical element $e(k_1) \cdots e(k_m)$ of $\mathcal{F}(\mathcal{S})$ is in the kernel of φ if and only if $(k_1)^\sim \cdots (k_m)^\sim = (k_1, \ldots, k_m)^\sim = \emptyset$. This happens only if the non-zero components of $(k_1, \ldots, k_m)$ cancel in pairs $k, -k$. Then also the corresponding terms in $e(k_1) \cdots e(k_m)$ cancel in pairs. Since also $e(0) = 1$ in $\mathcal{F}(\mathcal{S})$ when $0 \in \mathcal{S}$, we see that $e(k_1) \cdots e(k_m)$ reduces to the identity element. □

We find it convenient to identify $\mathcal{F}(\mathcal{S})$ and $\mathbb{S}^\sim$ through Proposition 7.3. Having done this, we obtain from $\phi : \mathbb{S}^\sim \longrightarrow \mathcal{E}_d$, defined above, the homomorphism

$$\varphi : \mathcal{F}(\mathcal{S}) \longrightarrow \mathcal{E}_d \quad \text{with } e(k) \mapsto k,$$

whose kernel can be identified with $\mathcal{Z}$.

Thus, we have the following exact sequence of groups (all given the discrete topology):

$$1 \longrightarrow \mathcal{Z} \longrightarrow \mathcal{F}(\mathcal{S}) \longrightarrow \mathcal{E}_d \longrightarrow 1. \tag{18}$$

Dualization then gives the exact sequence

$$1 \longleftarrow \widehat{\mathcal{Z}} \longleftarrow \widehat{\mathcal{F}(\mathcal{S})} \longleftarrow \mathbb{T} \longleftarrow 1, \tag{19}$$

where $\mathbb{T} := \widehat{\mathcal{E}_d}$ is a compact abelian group by Pontryagin duality. Note that we get surjectivity from the continuity of the mappings and the compactness of these groups. In fact, surjectivity of the map $\widehat{\mathcal{F}(\mathcal{S})} \longrightarrow \widehat{\mathcal{Z}}$ is crucial for our subsequent considerations.

† The second of these relations comes from the underlying assumption that we are dealing with *real* stationary processes. If this condition were dropped, then these relations would also be dropped.

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Definition 7.4. The mapping $a : \mathcal{S} \longrightarrow U(1)$ satisfies the *m-moment condition* if

$$a(k_1)a(k_2)\cdots a(k_m) = 1 \tag{20}$$

whenever $k_1, \ldots, k_m \in \mathcal{S}$ and $k_1 + \cdots + k_m = 0$.

Remark 7.5. The above conditions allow one to completely recover the moments of the underlying measure in certain cases. While this is not hard to see, it does not contribute to our investigation here. For this reason, we refrain from further discussion. Still it is for this reason that we chose the name.

Notice that the first moment condition is empty (and so trivially holds) unless $0 \in \mathcal{S}$, in which case it says that $a(0) = 1$. The second moment condition is equivalent to the statement that $a(-k) = \overline{a(k)}$ for all $k \in \mathcal{S}$. If $0 \in \mathcal{S}$, then the second moment condition alone gives $a(0)a(0) = 1$, so $a(0) = \pm 1$, see Assumption 6.4. If the first moment condition is not empty and holds, then $a(0) = 1$ and then the m-moment condition includes the n-moment condition for all $1 < n < m$ since additional slots can be filled with zeros.

Obviously, any mapping $a : \mathcal{S} \longrightarrow U(1)$ satisfying the first and second moment conditions determines a character of $\mathcal{F}(\mathcal{S})$, i.e. an element of $\widehat{\mathcal{F}(\mathcal{S})}$, via $e(k) \mapsto a(k)$ for all $k \in \mathcal{S}$. Conversely, every character of $\mathcal{F}(\mathcal{S})$ clearly determines a mapping a satisfying the first and second moment conditions. (Notice that when $0 \in \mathcal{S}$, then $e(0)$ is the identity element of $\mathcal{F}(\mathcal{S})$ and also $a(0) = 1$.) In the sequel, we will use these two concepts interchangeably and use the symbol a both as a mapping on $\mathcal{S}$ and as the corresponding character on $\mathcal{F}(\mathcal{S})$. When thought of as elements of $\widehat{\mathcal{F}(\mathcal{S})}$, they are called *elementary phase forms*.

By restriction, any elementary phase form a determines a phase form a^*, that is, an element of $\widehat{\mathcal{Z}}$. The exact sequence (19) shows that every phase form arises by restriction from an elementary phase form and two elementary phase forms restrict to the same phase form if and only their ratio is in $\mathbb{T}$, that is to say, if and only if their ratio is a character on $\mathcal{E}_d$. This is the essential part of determining equivalence of pure point processes.

PROPOSITION 7.6.

(i) *Any mapping $a : \mathcal{S} \longrightarrow U(1)$ satisfying the first and second moment conditions determines a unique elementary phase form and every elementary phase form arises in this way.*

(ii) *Any phase form is the restriction of an elementary phase form. The ratio of any two elementary phase forms giving the same phase form is an element of $\mathbb{T}$.*

(iii) *An elementary phase form satisfies the m-moment conditions for $m = 1, \ldots, n$ if and only if it annihilates $\mathcal{Z}_n$.*

(iv) *An elementary phase form a determines a character on $\mathcal{E}_d$, i.e. lies in $\mathbb{T}$, if and only if it satisfies all m-moment conditions, $m = 1, 2, \ldots$.*

Proof. Parts (i) and (ii) are already done above.

The set $\mathcal{Z}_n$ is generated by all the $\boldsymbol{k} = (k_1, \ldots, k_m)$ with $k_1 + \cdots + k_m = 0$, $m \leq n$. An elementary phase form a annihilates the equivalence class of $\boldsymbol{k}$ in $\mathcal{F}(S)$ if and only if

$$a(k_1)\cdots a(k_m) = 1.$$

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This gives (iii). An elementary phase form a annihilates all of $\mathcal{Z}$ if and only if a^* is trivial, which happens if and only if $a \in \mathbb{T} = \widehat{\mathcal{E}_d}$, which gives (iv). □

Of particular interest to us is the case where the group $\mathcal{Z}$ is generated by $\mathcal{Z}_n$ for some $n \geq 2$. This can be understood on the level of phase forms in the following way.

LEMMA 7.7. *Let $n \geq 2$. Then the following assertions are equivalent.*

(i) $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$.

(ii) *Any mapping $a : \mathcal{S} \longrightarrow U(1)$ satisfying the m-moment conditions for $1 \leq m \leq n$ extends to a character on $\mathcal{E}_d$ (i.e. lies in $\mathbb{T}$).*

Proof. (ii)$\Longrightarrow$ (i) The fact that $a : \mathcal{S} \longrightarrow U(1)$ satisfies the m-moment conditions for $1 \leq m \leq n$ is equivalent to saying that the corresponding character a on $\mathcal{F}(\mathcal{S})$ annihilates $\mathcal{Z}_n$ or, equivalently, annihilates the subgroup $\langle \mathcal{Z}_n \rangle$ that it generates. But Proposition 7.6 says that a extends to a character on $\mathcal{E}_d$ if and only if a annihilates $\mathcal{Z}$. Suppose that the fact that the mapping $a : S \longrightarrow U(1)$ satisfies the m-moment conditions for $1 \leq m \leq n$ is sufficient to guarantee that whenever a annihilates $\langle \mathcal{Z}_n \rangle$, it must also kill $\mathcal{Z}$. Then $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$ because $\langle \mathcal{Z}_n \rangle \subset \mathcal{Z}$, both are closed subgroups of $\mathcal{F}(\mathcal{S})$, and the Pontryagin duality theory says that the characters can distinguish distinct closed subgroups.

The implication (i) $\Longrightarrow$ (ii) is clear. □

Define

$$n_0 := n_0(\mathcal{Z}) := \inf\{n \in \mathbb{N} : \mathcal{Z} \text{ generated by } \mathcal{Z}_n\}.$$

Here the infimum of the empty set is defined to be ∞.

Remark 7.8. If $\mathcal{E} = \mathcal{S} + \cdots + \mathcal{S}$ (with r summands), then any relator can be written as a product of relators of length at most $2r + 1$, so $\mathcal{Z}_{2r+1}$ generates $\mathcal{Z}$. Thus, in this case $n_0 \leq 2r + 1$ [**26**].

Definition 7.9. The restriction of a phase form or an elementary phase form to Z_m is called its mth moment.

PROPOSITION 7.10. *Two elementary phase forms a and b give rise to the same mth moment if and only if their ratio $u = b/a$ satisfies the mth-moment condition.*

Proof. Elementary phase forms a, b give rise to equal mth moments if and only if $a(k_1, \ldots, k_m) = b(k_1, \ldots, k_m)$ whenever $k_1, \ldots, k_m \in \mathcal{S}$ with $k_1 + \cdots + k_m = 0$. However, being elementary phase forms, these equations can be written as $a(k_1) \cdots a(k_m) = b(k_1) \cdots b(k_m)$, which leads to the equivalent statement that

$$u(k_1) \cdots u(k_m) = 1$$

whenever $k_1, \ldots, k_m \in \mathcal{S}$ with $k_1 + \cdots + k_m = 0$. This is the mth-moment condition. □

Two elementary phase forms a, b give rise to the same phase form a^* if and only if their ratio is an element of $\mathbb{T}$ and so satisfies all moment conditions. By Proposition 7.10, this means that all their moments are the same, so that there is no ambiguity in speaking of the mth *moments of phase forms*.

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LEMMA 7.11. *Assume that* $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$ *for some* $n \geq 2$. *Then two phase forms agree if and only if they have the same* m*th moments for* $m = 1, \ldots, n$. *In particular, two elementary phase forms restrict to the same phase form if and only if they have the same* m*th moments for* $m = 1, \ldots, n$.

Proof. The first statement is clear. The second statement is a direct consequence of the first statement. □

Remark 7.12. Any of the phase forms a that we are interested in from the point of view of diffraction satisfy the first and second moment conditions by assumption. The relevance of the previous lemma is the following. If two stationary processes have the same pure point diffraction and their associated group of relators satisfies $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$, then the processes are isomorphic if they have the same mth moments for $m = 1, \ldots, n$ (see Corollaries 9.2 and 10.3 for precise statements).

8. *From spatial stationary processes with pure point diffraction to phase factors*

In this section we assume that we are given an ergodic spatial stationary process with pure point diffraction. We will discuss how this process gives rise to a diffraction measure ω, a set $\mathcal{S}$ which generates a group $\mathcal{E}$, canonical eigenfunctions f_k, for all $k \in \mathcal{S}$, and a phase form a^*. In the next section we will see that (ω, a^*) in some sense uniquely determines the process.

Let (N, X, μ, T) be an ergodic stationary spatial process with pure point diffraction. From the considerations of §2, we then obtain the following: the diffraction measure ω of (N, X, μ, T) is a pure point measure and the set of its atoms, which we called the Bragg spectrum, is denoted by $\mathcal{S} = \mathcal{S}(\omega)$, i.e.

$$\mathcal{S} = \mathcal{S}(\omega) := \{k \in \widehat{\mathbb{G}} : \omega(k) > 0\},$$

and satisfies $\mathcal{S} = -\mathcal{S}$. We let $\mathcal{E}$ be the subgroup of $\widehat{\mathbb{G}}$ generated by $\mathcal{S}$ and let $\mathcal{E}_d$ denote this group when it is given the discrete topology. We are now clearly in the situation of the previous section. In particular, there is an associated relator group $\mathcal{Z} = \mathcal{Z}(\mathcal{S}) = \mathcal{Z}(\omega)$ at our disposal. Let

$$\theta : L^2(\widehat{\mathbb{G}}, \omega) \longrightarrow L^2(X, m)$$

be the associated diffraction to dynamics map and, for each $k \in \widehat{\mathbb{G}}$, let 1_k be the characteristic function on $\mathbb{G}$ defined by the set $\{k\}$. Recall the action $\hat{T}$ defined of $\mathbb{G}$ acting on $L^2(\widehat{\mathbb{G}}, \omega)$ by

$$\hat{T}_t h(k) := \overline{(k, t)} h(k)$$

(see (8)) and observe that whenever $\omega(k) \neq 0$, 1_k is a k eigenfunction for this action. It is easy to see that up to scaling these are the only eigenfunctions of $L^2(\widehat{\mathbb{G}}, \omega)$. By the orthogonality of eigenfunctions, we have

$$\langle 1_k \mid 1_{k'} \rangle_{\widehat{\mathbb{G}}} = \omega(k) \delta_{k,k'}$$

and

$$\langle F \mid G \rangle_{\widehat{\mathbb{G}}} = \sum_{k \in \mathcal{S}} F(k) \overline{G(k)} \omega(k)$$

for all $F, G \in L^2(\widehat{\mathbb{G}}, \omega)$.

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To each element of $\mathcal{S}$ there exists a corresponding canonical eigenfunction. More specifically, we define f_k, $k \in \mathcal{S}$, by $f_k = \theta(1_k)$. Then each f_k is an eigenfunction in $L^2(X, \mu)$ for the eigenvalue k and $\|f_k\|_2 = \|1_k\|_{\widehat{\mathbb{G}}} = \omega(k)^{1/2}$. Since $|f_k|$ is a constant function (due to ergodicity) and μ is a probability measure, $|f_k| = \omega(k)^{1/2}$. Then, for all $k_1, \ldots, k_m \in \mathcal{S}$,

$$\begin{aligned}\|f_{k_1} \cdots f_{k_m}\|^2 &= \int_X f_{k_1} \cdots f_{k_m} \overline{f_{k_1} \cdots f_{k_m}}\, d\mu \\ &= \int_X |f_{k_1}|^2 \cdots |f_{k_m}|^2\, d\mu = \omega(k_1) \cdots \omega(k_m).\end{aligned}$$

At this point we invoke Assumption 6.4, which says that if $0 \in \mathcal{S}$, then $f_0 = \omega(0)^{1/2} 1_X$.

For $\boldsymbol{k} = (k_1, \ldots, k_m)$ with $k_j \in \mathcal{S}$ and $[\boldsymbol{k}] = 0$, the product $f_{k_1} \ldots f_{k_m}$ is an eigenfunction to 0 and hence (by ergodicity) a multiple of 1_X, which yields

$$f_{k_1} \cdots f_{k_m} = a^*(k_1, \ldots, k_m)\omega(k_1)^{1/2} \cdots \omega(k_m)^{1/2} \tag{21}$$

for some $a^*(\boldsymbol{k}) = a^*(k_1, \ldots, k_m) \in U(1)$. In this way we have a mapping $a^* : Z = Z(\mathcal{S}) \longrightarrow U(1)$. It clearly respects the multiplication by concatenation on Z. In the sequel, we shall usually write $Z(\omega)$ instead of $Z(\mathcal{S})$ since $\mathcal{S}$ is completely determined by ω. In view of our assumption on f_0 and Lemma 3.11, we have $f_{-k} = \overline{f_k}$, which shows that a^* is well defined on the equivalence classes of $Z = Z(\mathcal{S})$ defined in §7, and in this way we obtain a phase form

$$a^* : \mathcal{Z} \longrightarrow U(1). \tag{22}$$

These considerations show that any pure point stationary spatial process comes with a natural measure ω and a phase form a^*. This is summarized in the following proposition, where we have used the notation developed above.

PROPOSITION 8.1. *Each ergodic pure point stationary spatial process (N, X, μ, T) gives rise to a pair (ω, a^*) consisting of a pure point measure ω on $\widehat{\mathbb{G}}$ characterized by*

$$\int_{\widehat{\mathbb{G}}} \widehat{F}\overline{\widehat{G}}\, d\omega = \langle N(F) \mid N(G) \rangle$$

for all $F, G \in C_c(\mathbb{G})$ and the phase form a^* on the relator group $\mathcal{Z} = \mathcal{Z}(\omega)$ satisfying

$$f_{k_1} \cdots f_{k_m} = a^*(k_1, \ldots, k_m)\omega(k_1)^{1/2} \cdots \omega(k_m)^{1/2}.$$

Next we show that ω and a^* are a complete set of invariants for the underlying process.

9. *Isomorphism of pure point processes*

Recall that we have introduced a notion of isomorphism between spatial processes in §2. In this section we show that two pure point ergodic spatial stationary processes are isomorphic (in the sense of Definition 2.5) if they yield the same diffraction measure ω and the same phase form a^*.

We remind the reader that our concept of a pure point spatial stationary process given in Definition 6.3 entails that the process in question is full and possesses a diffraction measure (which is pure point).

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THEOREM 9.1. *Two pure point ergodic stationary spatial processes based on the same group $\mathbb{G}$ are isomorphic if and only if their associated diffraction measures and phase forms are the same.*

Proof. Assume that the full processes (N, X, μ, T) and (N', X', μ', T') are pure point ergodic and have the same diffraction measure ω and the same phase form a^*. Set $\mathcal{S} := \mathcal{S}(\omega) = \mathcal{S}(\omega')$. Let $f_k \in L^2(X, \mu)$ and $f'_k \in L^2(X', \mu')$, $k \in \mathcal{S}$, be the corresponding natural eigenfunctions. Thus, $N(F) = \sum_{k\in\mathcal{S}} \widehat{F}(k) f_k$ and $N'(F) = \sum_{k\in\mathcal{S}} \widehat{F}(k) f'_k$ for all $F \in C_c(\mathbb{G})$. Moreover, by Theorem 6.1, products of the f_k and the f'_k respectively provide orthonormal bases consisting of eigenfunctions of $L^2(X, \mu)$ and $L^2(X', \mu')$, respectively.

We construct an isomorphism M (see Definition 2.5) as follows: we define M to be the unique linear map with

$$f_{k_1} \dots f_{k_m} \mapsto f'_{k_1} \dots f'_{k_m}.$$

This mapping is well defined, for suppose that $f_{k_1} \dots f_{k_m}$ and $f_{l_1} \dots f_{l_n}$ are linearly dependent. Then $k_1 + \dots + k_m = l_1 + \dots + l_n$, so $k_1 + \dots + k_m - l_1 - \dots - l_n = 0$ and

$$\begin{aligned} f_{k_1} \dots f_{k_m} f_{-l_1} \dots f_{-l_n} = \omega(k_1)^{1/2} \dots \omega(k_m)\omega(l_1)^{1/2} \dots \omega(l_n)^{1/2} \\ \times a^*(k_1, \dots, k_m, -l_1, \dots, -l_n). \end{aligned}$$

Using Lemma 3.11, we obtain

$$\begin{aligned} f_{k_1} \dots f_{k_m} = \omega(k_1)^{1/2} \dots \omega(k_m)^{1/2}\omega(l_1)^{-1/2} \dots \omega(l_n)^{-1/2} \\ \times a^*(k_1, \dots, k_m, -l_1, \dots, -l_n) f_{l_1} \dots f_{l_n}. \end{aligned}$$

By our assumptions, we obtain the same relation when the fs are replaced with f's, so the same linear dependence occurs in $L^2(X', \mu')$.

As products of the f_k and the f'_k respectively give an orthogonal basis of $L^2(X, \mu)$ and $L^2(X', \mu')$, and as

$$\| f_{k_1} \dots f_{k_m} \|^2 = \omega(k_1) \dots \omega(k_m) = \| f'_{k_1} \dots f'_{k_m} \|^2,$$

our mapping is a unitary map. In particular, it is continuous.

The definition of M easily shows that it intertwines T and T' and maps $N(F)$ to $N'(F)$ for all $F \in C_c(\mathbb{G})$. Moreover, by definition, M satisfies

$$M(f_{k_1} \dots f_{k_n} f_{l_1} \dots f_{l_m}) = M(f_{k_1} \dots f_{k_n}) M(f_{l_1} \dots f_{l_m})$$

for all $k_1, \dots, k_n \in \mathcal{S}$ and $l_1, \dots, l_m \in \mathcal{S}$. Note that both $f_{k_1} \dots f_{k_n}$ and $M(f_{k_1} \dots f_{k_n}) = f'_{k_1} \dots f'_{k_n}$ are bounded functions. Thus, we can take linear combinations (in L^2) and their limits to obtain

$$M(f_{k_1} \dots f_{k_n} g) = M(f_{k_1} \dots f_{k_n}) M(g)$$

for all $g \in L^2(X, \mu)$ and $k_1, \dots, k_n \in \mathcal{S}$. In particular,

$$M(f_{k_1} \dots f_{k_n} g) = M(f_{k_1} \dots f_{k_n}) M(g)$$

holds for all $g \in L^\infty(X, \mu)$ and $k_1, \dots, k_n \in \mathcal{S}$. Another approximation argument now yields $M(fg) = M(f)M(g)$ for all $f, g \in L^\infty(X, \mu)$. This proves the isomorphism.

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Conversely, suppose that M is an isomorphism between the pure point ergodic stationary spatial processes (N, X, μ, T) and (N', X', μ', T') on $\mathbb{G}$. As M is a unitary mapping, one sees directly from the definitions that their correlation measures, and hence their diffraction measures, are the same (if second moments exist), and then that the diffraction to dynamics mappings are related by $\theta' = M \circ \theta$. Then, looking at the eigenfunctions, we have $M(f_k) = M(\theta(1_k)) = \theta'(1_k) = f'_k$. Since the f_k are bounded functions, the multiplicative property of M gives $M(f_{k_1} \dots f_{k_n}) = f'_{k_1} \dots f'_{k_n}$ for all $k_1, \dots, k_m \in \mathcal{S}$. Then the definition of the phase forms (21) and (22) shows that both processes have the same phase form. □

COROLLARY 9.2. *Let ω be a positive symmetric pure point measure on $\widehat{\mathbb{G}}$ and $\mathcal{Z}$ the associated group of relators. If $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$, then two stationary spatial processes with diffraction ω are spatially isomorphic if and only if the first n moments of their phase forms agree.*

Proof. This is a direct consequence of the previous theorem and Lemma 7.11. □

Remark 9.3.

(a) The above theorem deals with isomorphism between two processes. We can also characterize the automorphisms of a given pure point stationary spatial point process with Bragg peaks $\mathcal{S}$ and eigenfunctions f_k, $k \in \mathcal{S}$. These automorphisms are in one to one correspondence with elements from $\mathbb{T}$ in the following way: any character $\phi \in \mathbb{T}$ yields an automorphism of (N, X, μ, T) via $f_k \mapsto \phi(k) f_k$. Conversely, any automorphism of (N, X, μ, T) must necessarily map f_k to a multiple $\phi(k) f_k$ with $\phi(k) \in U(1)$. The arising function ϕ must then belong to $\mathbb{T}$ as (21) gives $\phi(k_1) \dots \phi(k_m) = 1$ whenever $k_1 + \dots + k_m = 0$.

(b) In the previous theorem, the isomorphism M between isomorphic pure point stationary spatial processes is not unique. However, if M_1, M_2 are two such isomorphisms, then $M := M_2^{-1} M_1$ is an automorphism of the first, say (N, X, μ, T). By (a) of this remark, we conclude that the isomorphisms are unique up to elements of $\mathbb{T}$.

10. *From phase forms to processes with pure point spectrum*

In this section we show how to construct an ergodic full stationary process with a given pure point measure as its diffraction measure ω and a given phase form a^* as its associated phase form. This yields a canonical model realizing a given diffraction measure.

We assume that we are given a locally compact abelian group $\mathbb{G}$ and a pure point positive symmetric backward transformable measure ω on $\widehat{\mathbb{G}}$. This data gives rise to

$$\mathcal{S} := \{k \in \widehat{\mathbb{G}} : \omega(k) > 0\}$$

and $\mathcal{E} = \langle \mathcal{S} \rangle_{\text{group}} \subset \widehat{\mathbb{G}}$. We consider $\mathcal{E}$ to have the induced topology from $\widehat{\mathbb{G}}$ and, as usual, let $\mathcal{E}_d$ denote the same group $\mathcal{E}$ but with the discrete topology. The dual of $\mathcal{E}_d$ is a compact abelian group $\mathbb{T}$. We denote the Haar measure of total volume 1 on $\mathbb{T}$ by $l_{\mathbb{T}}$ and the counting measure on $\mathcal{E}_d$ by l_d.

There is an associated group of relators $\mathcal{Z}(\omega)$ as discussed in §7. We are also given $a^* \in \widehat{\mathcal{Z}}$. We are going to construct a stationary process corresponding to (ω, a^*).

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From Proposition 7.6, we know that there is an elementary phase form $a : \mathcal{F}(\mathcal{S}) \longrightarrow U(1)$ (i.e. a character of $\mathcal{F}(\mathcal{S})$) which restricts to a^*: in other words, we can find a so that

$$a^*(k_1, \ldots, k_m) = a(k_1) \cdots a(k_m)$$

whenever $[\boldsymbol{k}] = 0$. (This a is not unique, but the ratio of any two of such elementary phase forms is a character on $\mathcal{E}_d$.) Thus, we can assume without loss of generality that a^* comes from an elementary phase form $a \in \widehat{\mathcal{F}(\mathcal{S})}$. Since ω is backward transformable, there is a measure γ on $\mathbb{G}$ so that for all $F \in C_c(\mathbb{G})$, we have

$$\int_{\widehat{\mathbb{G}}} |\widehat{F}|^2 \, d\omega = \int_{\mathbb{G}} F * \widetilde{F} \, d\gamma < \infty. \tag{23}$$

Then (23) can be reformulated as saying that

$$(k \mapsto \widehat{F}(k)\omega(k)^{1/2}) \in \ell^2(\mathcal{E}).$$

For $F \in C_c(\mathbb{G})$, define a function $n_a(F)$ on $\mathcal{E}_d$ by

$$n_a(F) = \sum_{k \in \mathcal{S}} \widehat{F}(k) a(k) \omega(k)^{1/2} 1_k,$$

where we take the positive square roots and 1_k is the function on $\mathcal{E}_d$ whose value at k is 1 and which takes the value 0 everywhere else. We have

$$\begin{aligned} \int_{\mathcal{E}_d} n_a(F)\overline{n_a(F)} \, dl_d &= \sum_{k \in \mathcal{S}} n_a(F)(k)\overline{n_a(F)(k)} = \sum_{k \in \mathcal{S}} |\widehat{F}(k)|^2 \omega(k) \\ &= \int_{\widehat{\mathbb{G}}} |\widehat{F}|^2 \, d\omega = \int_{\mathbb{G}} F * \widetilde{F} \, d\gamma < \infty, \end{aligned}$$

which implies in particular that $n_a(F) \in L^2(\mathcal{E}_d, l_d)$. The Fourier transform provides a fundamental isomorphism between $L^2(\mathcal{E}_d, l_d)$ and $L^2(\mathbb{T}, l_{\mathbb{T}})$ taking 1_{-k} to the character defined by k on $\mathbb{T}$. We usually denote this character by χ_k. Thus, we obtain, by applying the Fourier transform to $n_a(F)$,

$$N_a(F) := \sum_{k \in \mathcal{S}} \widehat{F}(k) a(k) \omega(k)^{1/2} \chi_k \in L^2(\mathbb{T}, l_{\mathbb{T}}) \tag{24}$$

with

$$\langle N_a(F) | N_a(F) \rangle = \int_{\mathbb{T}} N_a(F)\overline{N_a(F)} \, dl_{\mathbb{T}} = \int_{\mathcal{E}_d} n_a(F)\overline{n_a(F)} \, dl_d = \int_{\mathbb{G}} F * \widetilde{F} \, d\gamma. \tag{25}$$

This provides us with the mapping

$$N_a : C_c(\mathbb{G}) \longrightarrow L^2(\mathbb{T}, l_{\mathbb{T}}),$$

and shows that for any compact subset $K \subset \mathbb{G}$ we have $\|N_a(F)\|_2 \leq (|\gamma|(K + K))^{1/2} \|F\|_{\sup}$ for all $F \in C_c^{\mathbb{R}}(\mathbb{G})$ with support inside K, which shows that N_a is continuous.

The continuous embedding of $\mathcal{E}_d \to \widehat{\mathbb{G}}$ defined by inclusion leads to a dense homomorphism $\mathbb{G} \to \mathbb{T}$. Then each function on $\mathbb{T}$ 'restricts' to one on $\mathbb{G}$ and in particular

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we have an obvious meaning to the functions $t \mapsto \chi_k(t)$ for all $t \in \mathbb{G}$ and for all $k \in \mathcal{E}_d$. We also obtain a natural ergodic action of $\mathbb{G}$ on $\mathbb{T}$: for $t \in \mathbb{G}$ and $\xi \in \mathbb{T}$,

$$t \cdot \xi : k \mapsto \chi_k(t)\xi(k)$$

for all $k \in \mathcal{E}_d$. For $F \in C_c(\mathbb{G})$ and $k \in \mathcal{E}_d$,

$$\widehat{F}(k)\overline{\chi_k(t)} = \int_{\mathbb{G}} F(s)\overline{\chi_k(s)\chi_k(t)}\, dl_{\mathbb{G}}(s) = \int_{\mathbb{G}} (T_t F)(s)\overline{\chi_k(s)}\, dl_{\mathbb{G}}(s) = \widehat{T_t F}(k).$$

(Here we use the invariance of the measure $l_{\mathbb{G}}$.)

This leads by a straightforward calculation that $T_t N_a(F) = N_a(T_t F)$, which shows that N_a is a $\mathbb{G}$-equivariant map.

Thus, given (ω, a^*), we obtain an ergodic spatial stationary process $(N_a, \mathbb{T}, l_{\mathbb{T}})$. The above considerations also show that ω is the diffraction measure associated to N_a.

We will show next that N_a is full and has associated phase form a^*. To do so, we consider the map

$$\theta : L^2(\widehat{\mathbb{G}}, \omega) \longrightarrow L^2(\mathbb{T}, l_{\mathbb{T}}), \quad \theta(h) = \sum_{k \in \mathcal{S}} h(k)a(k)\omega(k)^{1/2}\chi_k.$$

Then θ is an isometry with $\theta(\widehat{F}) = N_a(F)$ for all $F \in C_c(\mathbb{G})$. By uniqueness of the dynamics to diffraction map, we infer that θ *is* the dynamics to diffraction map. This gives, in particular, that $\theta(1_k) = a(k)\omega(k)^{1/2}\chi_k$ for all $k \in \mathcal{S}$. These are the functions f_k of the previous sections. From this equality and the fact that a is a character on $\mathcal{F}(\mathcal{S})$, it follows easily that a^* is the phase form associated to N_a (see (21) and (22)). Moreover, Proposition 3.8 now shows that $a(k)\omega(k)^{1/2}\chi_k = \theta(1_k)$ belongs to the closure of the linear span of the $N(F)$, $F \in C_c(\mathbb{G})$, for any $k \in \mathcal{S}$. As products of these χ_k form an orthonormal basis of $L^2(\mathbb{T}, l_{\mathbb{T}})$, we obtain fullness of the stationary process N_a. We summarize the conclusions of this section.

PROPOSITION 10.1. *Let a pure point positive symmetric backward transformable measure ω on $\mathbb{G}$ be given and a^* be a phase form. Then, for any choice of elementary phase form a restricting to a^*, $(N_a, \mathbb{T}, l_{\mathbb{T}}, T)$ is an ergodic full stationary process on $\mathbb{G}$ with diffraction measure ω and phase form a^*.* □

The pure point process constructed in Proposition 10.1 depends on the choice of the elementary phase form a that we choose to represent the phase form a^*. What happens if we choose another representing elementary phase form, $b \in \widehat{\mathcal{F}(\mathcal{S})}$? We know already by Theorem 9.1 that the resulting process will be isomorphic and, since both use the same constructed dynamical system $X = \mathbb{T}$, this difference between the two processes is in effect an automorphism. Also, Proposition 7.6(ii) says that the ratio $u = b/a$ is an element of $\mathbb{T}$. From the perspective of N_a and N_b, then N_b is in effect a translation of N_a by $u \in \mathbb{T}$, i.e.

$$\begin{aligned} N_b(F) &= \sum_{k \in \mathcal{S}} \widehat{F}(k)b(k)\omega^{1/2}(k)\chi_k = \sum_{k \in \mathcal{S}} \widehat{F}(k)a(k)\omega^{1/2}(k)\chi_k(u)\chi_k \\ &= \sum_{k \in \mathcal{S}} \widehat{F}(k)a(k)\omega^{1/2}(k)T_{-u}(\chi_k) = (T_{-u}N_a)(F). \end{aligned} \tag{26}$$

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Remark 10.2. If $u = b/a$ above is actually continuous with respect to the original topology on $\mathcal{E}$, then u, being a character on $\mathcal{E}$, lifts to a character on $\overline{\mathcal{E}}$ and then by general character theory to all of $\widehat{\mathbb{G}}$. Thus, u can be identified with an element of $\mathbb{G}$. Now (26) becomes

$$N_b(F) = \sum_{k\in\mathcal{S}} \widehat{F}(k)b(k)\omega^{1/2}(k)\chi_k = \sum_{k\in\mathcal{S}} \widehat{F}(k)a(k)\omega^{1/2}(k)\chi_k(u)\chi_k$$
$$= \sum_{k\in\mathcal{S}} \widehat{T_{-u}F}(k)a(k)\omega^{1/2}(k)\chi_k = N_a(T_{-u}F). \tag{27}$$

This time the difference between N_a and N_b is a translation on $\mathbb{G}$. This situation occurs in the periodic situation, when $\mathbb{G}$ is compact and $\widehat{\mathbb{G}}$ is discrete.

COROLLARY 10.3. *Let ω be a positive backward transformable pure point measure on $\widehat{\mathbb{G}}$ and $\mathcal{Z}$ the associated group of relators. If $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$, then two mappings $a, b : \mathcal{S} \longrightarrow U(1)$ define isomorphic stationary pure point processes if and only if their first through nth moments are equal.*

Proof. This is a direct consequence of Corollary 9.2. □

11. *Solving the homometry problem*

In this section we discuss a main result of the paper, our solution to the homometry problem for pure point diffraction.

Definition 11.1. Given $\mathbb{G}$ and a measure ω on $\widehat{\mathbb{G}}$, we let $\mathcal{N}(\mathbb{G}, \omega)$ denote the set of all spatial isomorphism classes of ergodic full stationary spatial processes with diffraction ω satisfying Assumption 6.4.

The considerations of the previous sections rather directly prove the following result, which is in effect an abstract solution of the homometry problem for pure point diffraction.

THEOREM 11.2. *Let $\mathbb{G}$ be a locally compact abelian group. Let ω be a positive backward transformable pure point measure on $\widehat{\mathbb{G}}$ and $\mathcal{Z} = \mathcal{Z}(\omega)$ the associated group of relators. Then the map*

$$\widehat{\mathcal{Z}} \longrightarrow \mathcal{N}(\mathbb{G}, \omega),$$
$$a^* \mapsto [(N_a, \mathbb{T}, l_{\mathbb{T}}, T)],$$

where a is any elementary phase form representing a^*, is a bijection.

Proof. By Proposition 10.1, $(N_a, \mathbb{T}, l_{\mathbb{T}}, T)$ is an ergodic spatial stationary process with diffraction ω and phase a^*. Moreover, by Theorem 9.1, the map is well defined (i.e. independent of the choice of the elementary phase form representing a^*) and one to one. It is surjective by Proposition 8.1 and Theorem 9.1. □

Remark 11.3. Note that a positive backward transformable measure (such as ω) is necessarily translation bounded [**14**, **30**].

We note the following immediate consequence of the previous theorem and Corollary 9.2 (see Corollary 10.3 as well).

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COROLLARY 11.4. *Assume the situation of the theorem. If* $\langle \mathcal{Z}_n \rangle = \mathcal{Z}$, *then two ergodic spatial stationary processes over* $\mathbb{G}$ *with diffraction measure* ω *are spatially isomorphic if and only if their phase forms have the same* m*th moments for* $m = 1, \ldots, n$. □

Remark 11.5. Although it is obvious from the theory of pure point spatial processes that we have developed, it is worthwhile noting explicitly that the problem of classification of pure point spatial processes with a given ω depends only on the positions of the Bragg peaks, namely $\mathcal{S}$. Once one has $\mathcal{S}$, one has the group $\mathcal{Z}$, which depends only on the relationship of $\mathcal{S}$ to the subgroup $\mathcal{E}$ of $\widehat{\mathbb{G}}$ that it generates. And, in fact, this purely algebraic problem is in reality the entire homometry problem.

12. *The question of measures*

The general solution to the homometry problem for backwards transformable pure point measures, Theorem 11.2, is given in terms of ergodic spatial processes. Our underlying understanding of a spatial process $\mathcal{N} = (N, X, \mu, T)$ is that it represents some sort of family of 'densities' on the space $\mathbb{G}$. Each point $\xi \in X$ represents an instance of the yet unspecified structure ρ_ξ, which can be paired with elements of $C_c(\mathbb{G})$ to give

$$\langle \rho_\xi, F \rangle = N(F)(\xi).$$

Thus, $C_c(\mathbb{G})$ provides a set of test functions for some sort of distribution ρ_ξ at $\xi \in X$. Of course, $N(F)$ is not necessarily defined at all points of X (it is only an L^2-function on X), and even if it is defined it is not clear whether or not ρ_ξ could be interpreted as any particular kind of distribution. We do note, however, that from $\mathbb{G}$-invariance we have $N(F)(T_t\rho_\xi) = (T_{-t}N(F))(\xi) = N(T_{-t}F)(\xi)$, so $\langle T_t\rho_\xi, F\rangle = \langle \rho_\xi, T_{-t}F\rangle$ for all $t \in \mathbb{G}$.

An obvious question is whether or not this 'density' can be interpreted as a measure ρ_ξ on $X = \mathbb{G}$. Based on an earlier manuscript of the present paper, Terauds [**42**] (see [**43**] as well) looked into this question and a number of issues around it. The answer is that if the support of the diffraction is finite, then yes, one can always interpret ρ_ξ as a measure. However, when the support is infinite then there will always be solutions (in fact an uncountable number of solutions) in the form of ergodic spatial processes that are *not* measures [**42**, Theorem 3.4 and Corollary 3.7]. Here we simply give a key example from [**42**] based on the most familiar of all infinite diffraction patterns, $\delta_\mathbb{Z}$. One defines the symmetric, but non-periodic, set

$$L := 2\mathbb{Z} \cup \bigcup_{n\geq 1} (2{\cdot}4^n\mathbb{Z} + (4^n - 1)) \cup (2{\cdot}4^n\mathbb{Z} + (1 - 4^n)),$$

and the elementary phase form $a : \mathbb{Z} \longrightarrow \mathbb{T}$ defined by $a(k) = 1$ if $k \in L$, $a(k) = -1$ otherwise. The corresponding density turns out to be $2\widehat{\delta_L} - \delta_\mathbb{Z}$, and

$$\widehat{\delta_L} = \frac{1}{2}\delta_{\mathbb{Z}/2} + \sum_{n\geq 1} \frac{\cos(2\pi(4^n - 1)(\cdot))}{4^n}\delta_{\mathbb{Z}/2\cdot 4^n}$$

is not a measure. On the other hand, it is a tempered distribution, being the Fourier transform of a translation-bounded measure. It is an open question in which other cases (in which we are dealing with real spaces) the density ρ_ξ can also be interpreted as a tempered distribution.

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