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Dynamical versus diffraction spectrum for structures with finite local complexity

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Abstract. It is well known that the dynamical spectrum of an ergodic measure dynamical system is related to the diffraction measure of a typical element of the system. This situation includes ergodic subshifts from symbolic dynamics as well as ergodic Delone dynamical systems, both via suitable embeddings. The connection is rather well understood when the spectrum is pure point, where the two spectral notions are essentially equivalent. In general, however, the dynamical spectrum is richer. Here, we consider (uniquely) ergodic systems of finite local complexity and establish the equivalence of the dynamical spectrum with a collection of diffraction spectra of the system and certain factors. This equivalence gives access to the dynamical spectrum via these diffraction spectra. It is particularly useful as the diffraction spectra are often simpler to determine and, in many cases, only very few of them need to be calculated.

1. *Introduction*

Dynamical systems as defined by the translation action of locally compact Abelian groups (LCAGs) form an important class of structures whose classification is only partially known. An important tool is the dynamical spectrum, which was introduced in [**31**] and then largely developed by von Neumann [**42**]. It was used by Halmos and von Neumann [**28**] to achieve the classification of ergodic systems with pure point dynamical spectrum up to metric isomorphism, together with giving canonical representatives in terms of group additions on compact Abelian groups; see [**16**, **23**] for further details.

In the more general case of a system with mixed dynamical spectrum, much less is known, although these spectra are practically relevant; compare [**52**] and references

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therein for recent examples, and [**3**, **8**] for some theoretical counterpart. The maximal equicontinuous factor, also known as the Kronecker factor, is a natural object for analysing the pure point part of the spectrum, but it is totally blind to continuous spectral components. In many concrete examples, it seems advantageous to drop the demand of equicontinuity and search for a maximal factor with pure point spectrum, preferably of the same type. This will be a (generally not one-to-one) cover of the Kronecker factor; see [**6**] and references therein for some recent results from tiling theory. It is known, however, that this approach is not always possible [**29**], while it is very efficient when it works; see [**5**, **6**, **9**] for examples.

A different object, of physical origin and seemingly unrelated at first sight, is the *diffraction measure* $\widehat{\gamma}$ of a translation bounded measure ω on an LCAG G. Here, ω may be viewed as a model of an individual many-particle configuration, which we assume to be a typical representative of an (ergodic) ensemble of such structures, so that all quantities under consideration are well defined. Then, the measure $\widehat{\gamma}$ is the Fourier transform of the positive-definite autocorrelation measure γ of ω. Interestingly, a closer inspection shows a deep connection between the diffraction measure of ω and the dynamical spectrum of the orbit closure of ω under the translation action of G. This connection was exploited in [**22**] and led to the important equivalence theorem between pure pointedness of dynamical and diffraction spectra for measure dynamical systems [**11**, **13**, **33**, **36**, **37**, **50**]. The relevance of measure dynamical systems stems from the fact that many dynamical systems, such as subshifts from symbolic dynamics or Delone dynamical systems, are naturally embedded into this class of dynamical systems; compare [**11**, **14**, **37**].

It was noticed quite early [**24**] that a similarly simple correspondence cannot hold for systems with singular continuous spectral components, and it was later shown that the same (negative) conclusion is generally also true in the presence of absolutely continuous parts [**4**]. In these systems beyond the pure point case, the dynamical spectrum is richer than the diffraction spectrum (which is the group generated by the Fourier–Bohr spectrum of γ when $\widehat{\gamma}$ is a pure point measure; see equation (2) below for a precise definition). A main insight of [**4**] is the observation that, in the examples appearing in [**4**, **24**] as well as in many others (compare [**10**] and references therein), the missing parts of the dynamical spectrum could be reconstructed from the diffraction measures of suitable factors of the original system.

The importance of factors is perhaps not surprising, for instance in light of Fraczek's theorem [**25**] which asserts that, under some mild assumption, the maximal spectral measure can be realized as that of a continuous function; see also [**1**]. This continuous function gives rise to a factor where the correspondence between the dynamical and the diffraction spectrum can be understood via a minor variant of Dworkin's argument [**22**]; see also [**19**]. However, the factor obtained in this way might have a rather complicated structure, as it generally cannot be obtained from a function of finite range; compare [**29**]. In particular, in the case of symbolic dynamics, such a factor will generally not be realized over a finite alphabet, but rather over the unit disc. The observation mentioned above indicates that there might be an alternative path via a collection of factors, but then significantly simpler ones.

Given this situation, it is a natural conjecture that, under reasonable assumptions on the type of the dynamical system, the dynamical spectrum is equivalent to the *collection*

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(or union) of diffraction spectra of the system and its factors, where the latter should be of a similar kind as the system itself (or simpler). This conjecture is also supported by the physical intuition that the autocorrelation essentially is a two-point correlation, while higher-order correlations may still contain important information on the system. Many of these correlations are not seen by the diffraction measure of the original system itself, but at least the generalized two-point correlations (between the positions of local patterns, say) should be accessible via suitable factors and their diffraction measures. Since all correlation functions together determine the entire system (again under suitable assumptions; see [**35**]), the above conjecture is plausible. The present paper is centred around this conjecture.

For systems with pure point spectrum, little new insight seems gained at a first glance, as factors of such systems are pure point again [**12**]. Also, as mentioned before, we have equivalence of pure point diffraction and dynamical spectrum in those cases anyhow; see [**11**, **37**] and references therein. Still, as we shall see later, factors can shed some light on the structure of extinctions. In other examples, however, even simple factors may reveal coherent order, such as the period doubling chain (pure point) for the Thue–Morse chain (with singular spectrum of mixed type [**24**, **46**]). Here, the full dynamical spectrum can be reconstructed from the diffraction measure of the Thue–Morse chain and this one factor. In particular, one can represent the maximal spectral measure this way, which is implicit already in [**46**]. Several other examples are treated in [**10**]; see also [**5**, **6**, **9**] and references therein.

Below, we make the conjecture precise, and prove it for (uniquely ergodic) systems of finite local complexity (FLC), which includes symbolic dynamics on finite alphabets as well as FLC Delone dynamical systems. After some preliminary material on notions and methods (in §2), we treat those cases explicitly in one section each. While we focus on dynamical systems in $\mathbb{R}^d$ in those sections, a general abstract approach for the action of LCAGs is presented in §5, which also opens a path to drop the ergodicity and FLC assumptions. This is followed by some concluding remarks.

2. *Terminology and background*

Consider a (possibly unbounded) measure ω on $\mathbb{R}^d$, by which we mean a continuous linear functional on the space $C_{\mathsf{c}}(\mathbb{R}^d)$ of continuous functions with compact support. The corresponding weak-$*$ topology is called the *vague topology*. Due to the Riesz–Markov theorem, these measures can be identified with the regular Borel measures on $\mathbb{R}^d$. A measure ω is called *translation bounded* when $\sup_{t\in\mathbb{R}^d}|\omega|(t+K)<\infty$ holds for any compact $K\subset\mathbb{R}^d$; see [**10**, **15**, **30**, **50**] for background material. Given ω, the measure $\widetilde{\omega}$ is defined by $\widetilde{\omega}(g)=\overline{\omega(\widetilde{g})}$ for $g\in C_{\mathsf{c}}(\mathbb{R}^d)$, with $\widetilde{g}(x):=\overline{g(-x)}$.

Given a (translation bounded) measure ω on $\mathbb{R}^d$, its *autocorrelation measure* γ_ω, or autocorrelation for short, is defined as

$$\gamma_\omega := \omega \circledast \widetilde{\omega} := \lim_{r\to\infty} \frac{\omega|_r * \widetilde{\omega|_r}}{\mathrm{vol}(B_r(0))}, \tag{1}$$

where $\omega|_r$ denotes the restriction of ω to the open ball $B_r(0)$, and the limit is assumed to exist (no other situation will be considered below). The volume-weighted convolution $\circledast$

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of two unbounded measures is sometimes referred to as the *Eberlein convolution*. Note that the autocorrelation is often called the *Patterson function* in crystallography [**18**], even though it is a measure in our setting. This approach was introduced in [**30**]; see [**10**, Ch. 9] for a comprehensive exposition and [**8**] for an informal summary. Since γ_ω is positive definite by construction, its Fourier transform $\widehat{\gamma_\omega}$ exists [**15**] and is a positive measure. The latter is called the *diffraction measure* of ω, which can be seen as the generalization of the *structure factor* from classical crystallography [**18**].

Let us expand on the terminology around spectra by means of some additional definitions. A (translation-bounded) measure ω on $\mathbb{R}^d$ whose autocorrelation $\gamma = \omega \circledast \widetilde{\omega}$ exists is called *pure point diffractive* when $\widehat{\gamma}$ is a pure point measure. In this case, the supporting set

$$S_{\mathrm{FB}} := \{k \in \mathbb{R}^d \mid \widehat{\gamma}(\{k\}) > 0\} \tag{2}$$

is known as the *Fourier–Bohr spectrum* of γ. The set S_{FB} is also known as the set of Bragg peak locations in the physics literature. It is (at most) a countable set, but might (and generally will) be a dense subset of $\mathbb{R}^d$. Note that S_{FB} need not be a group, due to the possibility of extinctions [**18**, **35**].

Let ω be a translation bounded measure and consider $\mathbb{X} := \overline{\{\delta_t * \omega \mid t \in \mathbb{R}^d\}}$, with the closure taken in the vague topology. This defines a compact space that gives rise to a measure-theoretic dynamical system $(\mathbb{X}, \mathbb{R}^d, \mu)$, with the translation action of $\mathbb{R}^d$ and some invariant measure μ. The notion of the *dynamical spectrum* now emerges via the natural unitary (translation) action of $\mathbb{R}^d$ on the Hilbert space $L^2(\mathbb{X}, \mu)$; see [**16**, **41**, **46**] for general background and [**10**, Appendix B] for a brief summary. When $L^2(\mathbb{X}, \mu)$ possesses a basis of eigenfunctions for the $\mathbb{R}^d$-action, one speaks of a system with *pure point dynamical spectrum*. Then, the set of eigenvalues forms a subgroup of $\mathbb{R}^d$, known as the *pure point spectrum*. We are thus not using the term 'spectrum' in the sense of the topological spectrum (which is closed), but in the sense of the set of eigenvalues (which need not be closed as a set). More generally, when the eigenfunctions are not total in $L^2(\mathbb{X}, \mu)$, the group of eigenvalues constitutes the pure point part of the dynamical spectrum, where the spectral measures attached to the eigenfunctions all are pure point measures. In particular, $(\mathbb{X}, \mathbb{R}^d, \mu)$ has pure point spectrum if and only if all spectral measures are pure point.

When ω is a pure point diffractive measure and μ is ergodic, the dynamical spectrum of $(\mathbb{X}, \mathbb{R}^d, \mu)$ is pure point and can be characterized as the smallest subgroup of $\mathbb{R}^d$ that contains the supporting set S_{FB} from equation (2). We shall say more about this later; see also the Appendix. More generally, the positive diffraction measure $\widehat{\gamma}$ has the unique decomposition

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

into its pure point, singular continuous and absolutely continuous components. Then, the Fourier–Bohr spectrum is the supporting set of $(\widehat{\gamma})_{\mathsf{pp}}$. As before, this set is a countable (and possibly dense) subset of $\mathbb{R}^d$. In this more general case, the dynamical spectrum is usually described via the spectral decomposition theorem for unitary operators, hence via a suitable collection of spectral measures of (preferably continuous) functions on $\mathbb{X}$, and with special emphasis on the spectral measure of maximal type; compare [**46**] for a

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concise summary. This is precisely the point of view we will be using below, in the sense that we will relate the spectral measures of $(\mathbb{X}, \mathbb{R}^d, \mu)$ with the diffraction measure $\widehat{\gamma}$ of the system and its factors of the same kind (to be made precise later). Further tools and methods will be introduced while we proceed.

3. *The case of symbolic dynamics*

Let us begin with the simpler case of symbolic dynamics; see [**38**] for background. Recall that the full shift space $\mathcal{A}^{\mathbb{Z}}$ over a finite alphabet $\mathcal{A}$ is compact in the usual product topology. The latter is also known as the *local topology*, because two elements $u, v \in \mathcal{A}^{\mathbb{Z}}$ are close when u and v agree on a large index range around 0 (this defines both a uniform structure and a metrizable topology). For $u \in \mathcal{A}^{\mathbb{Z}}$, we write $u = (u_n)_{n\in\mathbb{Z}}$ and use $u_{[m,n]} = u_m u_{m+1} \cdots u_n$, with $n \geq m$, for the finite subword ranging from m to n. In particular, $u_{[m,m]} = u_m$. The shift S acts on $\mathcal{A}^{\mathbb{Z}}$ via $(Su)_n := u_{n+1}$, which is continuous and invertible. In particular, S induces a group action by $\mathbb{Z}$, so that $(\mathcal{A}^{\mathbb{Z}}, \mathbb{Z})$ is a topological dynamical system.

Consider now a closed shift-invariant subset $\mathbb{X} \subset \mathcal{A}^{\mathbb{Z}}$, which is then compact and known as a subshift, with the additional property that $\mathbb{X}$ admits only one shift-invariant probability measure μ. In other words, we assume that $(\mathbb{X}, \mathbb{Z}, \mu)$ is a measure-theoretic dynamical system which is uniquely ergodic. If $\mathcal{A}_{\mathbb{X}}^*$ denotes the dictionary of $\mathbb{X}$, by which we mean the set of all finite words that occur as subwords of some element of $\mathbb{X}$, we know from Oxtoby's theorem [**44**, **46**] that unique ergodicity is equivalent to the uniform existence, in any element of $\mathbb{X}$, of all frequencies of the words from $\mathcal{A}_{\mathbb{X}}^*$. All such frequencies are strictly positive precisely when $\mathbb{X}$ is also minimal. The frequency ν_w of a non-empty word $w \in \mathcal{A}_{\mathbb{X}}^*$ defines the measure of any of the corresponding cylinder sets by setting $\mu(\{x \in \mathbb{X} \mid x_{[m,m+|w|-1]} = w\}) = \nu_w$, where $m \in \mathbb{Z}$ is arbitrary and $|w|$ is the length of w. More complicated word patterns are realized by suitable unions and intersections of (elementary) cylinder sets. By construction and standard arguments, this consistently defines a shift-invariant probability measure μ on $\mathbb{X}$; see [**38**].

With μ, one also has the Hilbert space $\mathcal{H} = L^2(\mathbb{X}, \mu)$, with scalar product

$$\langle g \mid h \rangle = \int_{\mathbb{X}} \overline{g(x)} h(x)\, d\mu(x),$$

written here in a way that is linear in the second argument. The shift S induces a unitary operator U on $\mathcal{H}$ via $Uf := f \circ S$, so that $(Uf)(x) = f(Sx)$ for all $x \in \mathbb{X}$. Since $\mathbb{X}$ is compact, the continuous functions $C(\mathbb{X})$ are dense in $L^2(\mathbb{X}, \mu)$ by standard arguments [**32**, Ch. VII.5]. The characteristic function specified by a finite word $w \in \mathcal{A}_{\mathbb{X}}^*$ together with an index $n \in \mathbb{Z}$ is defined by $1_{w,n}(x) = 1$ when $x_{[n,n+|w|-1]} = w$, and by $1_{w,n}(x) = 0$ otherwise. Any such function is continuous, and all of them together generate an algebra $\mathbb{A}(\mathbb{X})$ (under addition and multiplication) that is dense in $C(\mathbb{X})$ by the Stone–Weierstrass theorem [**32**, Theorem III.1.4]. It is not hard to see that

$$\mathbb{A}(\mathbb{X}) = \{f \in C(\mathbb{X}) \mid f \text{ takes only finitely many values}\}, \tag{3}$$

which provides an explicit characterization. Indeed, the inclusion $\subset$ is obvious; the reverse inclusion $\supset$ follows because any continuous function on $\mathbb{X}$ with finitely many values is determined by a finite 'window' around zero.

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Given an arbitrary function $f \in \mathcal{H}$, the map $n \mapsto \langle f \mid U^n f\rangle$ defines a complex-valued, positive-definite function on the discrete group $\mathbb{Z}$, so that, by the Herglotz–Bochner theorem [**48**, Theorem 1.4.3], there is a unique positive measure $\sigma = \sigma_f$ on the dual group $\mathbb{S}^1$ (which is identified with the 1-torus $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ here) such that

$$\langle f \mid U^n f\rangle = \int_0^1 e^{2\pi i n t}\, d\sigma_f(t).$$

This measure σ_f is known as the *spectral measure* of the function f.

Consider now an arbitrary, but fixed element $g \in \mathbb{A}(\mathbb{X})$ subject to the additional requirement that it takes values in $\{0, 1\}$ only. As $g \in \mathbb{A}(\mathbb{X})$, the value $g(x)$ is determined from a finite index range, the latter being independent of $x \in \mathbb{X}$. Define now the *sliding block map* $\varPhi_g : \mathbb{X} \longrightarrow \{0, 1\}^{\mathbb{Z}}$ via $(\varPhi_g(x))(n) = g(S^n x)$ for $x \in \mathbb{X}$ and $n \in \mathbb{Z}$; see [**38**] for background. Clearly, $\varPhi_g$ is a continuous map, wherefore $\mathbb{Y} := \varPhi_g(\mathbb{X}) \subset \{0, 1\}^{\mathbb{Z}}$ is compact. Since the diagram

$$\begin{array}{ccc} \mathbb{X} & \xrightarrow{\;S\;} & \mathbb{X} \\ {\scriptstyle \varPhi_g}\downarrow & & \downarrow{\scriptstyle \varPhi_g} \\ \mathbb{Y} & \xrightarrow{\;S\;} & \mathbb{Y} \end{array}$$

is commutative, $(\mathbb{Y}, \mathbb{Z})$ is a topological factor of $(\mathbb{X}, \mathbb{Z})$. Moreover, μ induces a shift-invariant measure $\mu_{\mathbb{Y}}$ on $\mathbb{Y}$ via $\mu_{\mathbb{Y}}(B) = \mu(\varPhi_g^{-1}(B))$ for arbitrary Borel sets $B \subset \mathbb{Y}$. By an application of [**20**, Proposition 3.11], we know that $(\mathbb{Y}, \mathbb{Z}, \mu_{\mathbb{Y}})$ is again uniquely ergodic.

Let $x \in \mathbb{X}$ be arbitrary but fixed, with $y = \varPhi_g(x) \in \mathbb{Y}$, and consider the corresponding Dirac comb $\omega = \sum_{n\in\mathbb{Z}} y_n \delta_n$, which is a translation bounded measure on $\mathbb{R}$. It possesses the autocorrelation measure $\gamma_\omega = \omega \circledast \widetilde{\omega} = \eta \delta_{\mathbb{Z}}$ with the coefficients

$$\eta(m) = \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} y_n \overline{y_{n-m}} = \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} \overline{y_n} y_{n+m}, \tag{4}$$

which are written in the general form that also applies to complex sequences (even though they are real here). All limits exist due to the unique ergodicity of $(\mathbb{Y}, \mathbb{Z}, \mu_{\mathbb{Y}})$, wherefore we can employ the stronger version of the ergodic theorem for the orbit average of a continuous function (for instance, that defined by $y \mapsto \overline{y_0 y_m}$), and γ_ω is a positive-definite measure. Its Fourier transform $\widehat{\gamma_\omega}$ thus exists, and is a positive measure of the form $\widehat{\gamma_\omega} = \varrho * \delta_{\mathbb{Z}}$, with $\varrho = \widehat{\gamma_\omega}|_{[0,1)}$. Equivalently, $\eta : \mathbb{Z} \longrightarrow \mathbb{R}$ is a positive-definite function on $\mathbb{Z}$, see [**10**, Lemma 8.4], with representation $\eta(m) = \int_0^1 e^{2\pi i m t}\, d\varrho(t)$, where ϱ is now interpreted as a positive measure on the 1-torus $\mathbb{T}$.

Observe next that $y_m = g(S^m x)$, wherefore the coefficient $\eta(m)$ can also be expressed as

$$\eta(m) = \lim_{N\to\infty} \frac{1}{2N+1} \sum_{n=-N}^{N} \overline{g(S^n x)} g(S^{n+m} x) = \int_{\mathbb{X}} \overline{g(x)} g(S^m x)\, d\mu(x) = \langle g \mid U^m g\rangle, \tag{5}$$

where the second equality is a consequence of unique ergodicity. This shows that $\varrho = \sigma_g$, with σ_g the spectral measure of g. In other words, the spectral measure of the function g

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occurs as the 'building block' of the diffraction measure of the factor that is defined via Φ_g. After this explicit, but somewhat informal, introduction we can now develop the more general structure.

Let $\mathbb{X} \subset \mathcal{A}^{\mathbb{Z}}$ be a subshift over the finite alphabet $\mathcal{A}$, and let $\mathcal{B}$ be a finite set (equipped with the discrete topology). Then, any continuous $g : \mathbb{X} \longrightarrow \mathcal{B}$ gives rise to a continuous map $\Phi_g : \mathbb{X} \longrightarrow \mathcal{B}^{\mathbb{Z}}$, defined by $(\Phi_g(x))(n) := g(S^n x)$, so that $\mathbb{Y} := \Phi_g(\mathbb{X})$ is a factor of $\mathbb{X}$. Moreover, any subshift factor of $\mathbb{X}$ over $\mathcal{B}$ arises in this manner. This is a variant of the Curtis–Lyndon–Hedlund theorem, compare [**38**, Theorem 6.2.9], which we formulate in our context as follows.

LEMMA 1. *Let $\mathbb{X}$ be a subshift over the finite alphabet $\mathcal{A}$ and let $\mathbb{Y}$ be a subshift over the finite set $\mathcal{B}$ that is a factor of $\mathbb{X}$, with factor map $\Phi : \mathbb{X} \longrightarrow \mathbb{Y}$. Then, $\Phi = \Phi_g$ for $g := \delta \circ \Phi$, where $\delta : \mathbb{Y} \longrightarrow \mathcal{B}$ is defined by $y \mapsto y(0)$ and where g is a continuous function that takes only finitely many values.*

Proof. Since $\Phi = \Phi_g$ is a factor map, we can calculate

$$(\Phi(x))(n) = g(S^n x) = (\Phi(S^n x))(0) = (S^n \Phi(x))(0) = (\Phi(x))(n),$$

which implies the first claim. Since g is continuous on $\mathbb{X}$ by construction, but takes only finitely many distinct values, $\Phi = \Phi_g$ is indeed a sliding block map. □

This shows that subshift factors over finite sets are in one-to-one correspondence with continuous functions that take finitely many values.

In view of the connection with diffraction, we now realize the alphabet as a finite subset of $\mathbb{C}$. Let $\mathbb{X}$ be a uniquely ergodic subshift over the finite set $\mathcal{A} \subset \mathbb{C}$. Then, $\mathbb{X}$ gives rise to a canonical autocorrelation $\gamma = \gamma_{\mathbb{X}}$ as follows. Consider the Dirac comb $\omega = \sum_n x_n \delta_n$ for an arbitrary $x \in \mathbb{X}$. Owing to unique ergodicity, the associated autocorrelation does not depend on x, hence effectively only on $\mathbb{X}$. It is this observation that will later pave the way to a more general (and abstract) approach. Note that $\gamma_{\mathbb{X}}$ is a positive-definite measure of the form $\gamma_{\mathbb{X}} = \eta_{\mathbb{X}} \delta_{\mathbb{Z}} := \sum_{m \in \mathbb{Z}} \eta_{\mathbb{X}}(m) \delta_m$, where positive-definiteness of $\gamma_{\mathbb{X}}$ as a measure on $\mathbb{R}$ is equivalent to that of the function $\eta_{\mathbb{X}} : \mathbb{Z} \longrightarrow \mathbb{C}$; see [**10**, Lemma 8.4]. The Fourier transform $\widehat{\gamma_{\mathbb{X}}}$ of $\gamma_{\mathbb{X}}$, which exists by general arguments [**15**], is a 1-periodic measure on $\mathbb{R}$, as follows from [**10**, Theorem 10.3]; see also [**2**]. This gives

$$\widehat{\gamma_{\mathbb{X}}} = \varrho_{\mathbb{X}} * \delta_{\mathbb{Z}},$$

with a finite positive measure $\varrho_{\mathbb{X}}$. The latter is not unique in the sense that different $\varrho_{\mathbb{X}}$ can lead to the same measure $\widehat{\gamma_{\mathbb{X}}}$. A canonical choice is $\varrho_{\mathbb{X}} = \widehat{\gamma_{\mathbb{X}}}|_{[0,1)}$, which is based on the natural fundamental domain $\mathbb{T} \simeq [0, 1)$ of a $\mathbb{Z}$-periodic structure. This particular choice permits the simultaneous interpretation of $\varrho_{\mathbb{X}}$ as a positive measure on $\mathbb{T}$, so that

$$\eta_{\mathbb{X}}(m) = \int_0^1 e^{2\pi i m t} \, d\varrho_{\mathbb{X}}(t), \tag{6}$$

in line with the Herglotz–Bochner theorem. We thus call $\varrho_{\mathbb{X}}$ the *fundamental diffraction* of the subshift $\mathbb{X}$.

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PROPOSITION 2. *Let $\mathbb{X}$ be a uniquely ergodic subshift over the finite alphabet $\mathcal{A}$. Let $\mathcal{B} \subset \mathbb{C}$ be finite and $g : \mathbb{X} \longrightarrow \mathcal{B}$ continuous, with spectral measure σ_g, and let $\mathbb{Y}$ denote the associated subshift factor. Then, the fundamental diffraction of $\mathbb{Y}$ satisfies $\varrho_{\mathbb{Y}} = \sigma_g$.*

Proof. This follows exactly as in our previous derivation around equations (4) and (5). □

Note that subsets of $\mathbb{C}$ are natural objects in the context of mathematical diffraction theory; see [**10**, Ch. 9] for background. Subsets of $\mathbb{R}$, $\mathbb{Q}$ or $\mathbb{Z}$ are special cases and also of interest. They are covered by Proposition 2 as well.

Let us now establish a link between the canonical shift-invariant measure μ of $\mathbb{X}$ (defined via its values on cylinder sets) and the diffraction measures of the subshift factors.

PROPOSITION 3. *Let $\mathbb{X}$ be a uniquely ergodic subshift over the finite alphabet $\mathcal{A}$. Let w be any finite word from $\mathcal{A}_{\mathbb{X}}^*$ and define $g := 1_{w,0}$ (so $g(x) = 1$ if w occurs in x starting at 0 and $g(x) = 0$ otherwise). Let $\mathbb{Y} \subset \{0, 1\}^{\mathbb{Z}}$ be the subshift factor associated to g. Then, the absolute frequency ν_w of $w \in \mathcal{A}_{\mathbb{X}}^*$ is determined by the spectral measure σ_g of g, via $\nu_w = \widehat{\sigma_g}(0) = \eta_{\mathbb{Y}}(0)$.*

Proof. The claim can be verified by a direct calculation,

$$\widehat{\sigma_g}(0) = \int_{\mathbb{T}} d\sigma_g = \langle g \mid g \rangle = \int_{\mathbb{X}} |g|^2 \, d\mu = \int_{\mathbb{X}} g \, d\mu = \nu_w.$$

Here, the penultimate step relies on g being a characteristic function, while the last step is an application of the ergodic theorem, as in equation (5). A comparison with Proposition 2 and equation (6) shows that one also has $\widehat{\sigma_g}(0) = \eta_{\mathbb{Y}}(0)$. □

Let now $(\mathbb{X}, \mathbb{Z})$ be a uniquely ergodic subshift. The cylinder sets defined by finite words $w \in \mathcal{A}_{\mathbb{X}}^*$ form a π-system of the Borel σ-algebra of $\mathbb{X}$. Consequently, the frequencies of the finite words uniquely and completely *determine* a shift invariant probability measure μ on $\mathbb{X}$. If $\mathbb{X}$ is minimal, then μ in turn determines $\mathbb{X}$ (as $\mathbb{X}$ is the support of μ). In this situation, we call the measure-theoretic, strictly ergodic subshift $(\mathbb{X}, \mathbb{Z}, \mu)$ *completely reconstructible* from a collection of measures on $\mathbb{T}$ if the frequency of any word can be determined from the Fourier coefficient at 0 of a suitable measure from the collection. Our findings so far can be summarized as follows.

THEOREM 4. *Let $\mathbb{X}$ be a uniquely ergodic subshift over the finite alphabet $\mathcal{A}$. Then, the following properties hold.*

(i) *The fundamental diffraction of any subshift factor of $\mathbb{X}$ over a finite $\mathbb{C}$-valued alphabet is a spectral measure of $\mathbb{X}$.*
(ii) *Any spectral measure of the form σ_g with g from the dense subspace $\mathbb{A}(\mathbb{X})$ of $L^2(\mathbb{X}, \mu)$ arises as the fundamental diffraction measure of a subshift factor over a finite $\mathbb{C}$-valued alphabet.*
(iii) *If $\mathbb{X}$ is also minimal, $(\mathbb{X}, \mathbb{Z}, \mu)$ is completely reconstructible from the fundamental diffraction measures of the collection of subshift factors with $\{0, 1\}$-valued alphabets (under the assumption that one knows the factor maps as well).*

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Proof. As shown in Lemma 1, any subshift factor over a finite set emerges from a function $g \in \mathbb{A}(\mathbb{X})$. Now, the first claim follows from Proposition 2.

To prove the second claim, we recall that $\mathbb{A}(\mathbb{X})$ is dense in $C(\mathbb{X})$ by the Stone–Weierstrass theorem, and hence also dense in $L^2(\mathbb{X}, \mu)$. Then, the remaining part of the claim follows from Proposition 2.

As already discussed just before the theorem, any strictly ergodic subshift is completely determined by the (positive) frequencies of its finite subwords. The corresponding shift invariant measure μ is given by its values on the π-system of cylinder sets defined by the finite subwords. Since we assume knowledge of the factor maps, any such frequency can be extracted as the Fourier coefficient $\widehat{\sigma_g}(0)$ with a $\{0, 1\}$-valued function g, as shown in Proposition 3. This proves the third claim. □

Remark 1. We distinguish $(\mathbb{X}, \mathbb{Z})$ and $(\mathbb{X}, \mathbb{Z}, \mu)$ at this point, in the sense that the knowledge of the former, even if it is known to be uniquely ergodic, does not provide the invariant measure *explicitly*. Of course, in the uniquely ergodic case, the measure μ is determined via the word frequencies, and the latter emerge from uniformly converging limits (averages). However, this does not provide their concrete values. Two notable exceptions have been studied in the literature, namely shift spaces that are defined via primitive substitutions (compare [**10**, **46**] and references therein), where the frequencies are available via Perron–Frobenius theory, and shift spaces that emerge from the projection method (see [**10**] for details), where the frequencies are given by certain integrals. The use of a suitable system of factors, as discussed above, contains both cases and extends them to a setting that is independent of substitutions or projections.

Remark 2. A spectral measure σ is called *maximal* if any other spectral measure of the same dynamical system is absolutely continuous with respect to σ. In general, it is not true (compare [**29**] and Remark 4) that the maximal spectral measure of a subshift can be realized as the fundamental diffraction of a subshift factor. However, the theorem opens up the possibility to construct a measure equivalent to a maximal spectral measure via diffractions of factors. To do so, one chooses a countable subset $\mathcal{D}$ of $\mathbb{A}(\mathbb{X})$, which is dense in $C(\mathbb{X})$ and hence in $L^2(\mathbb{X}, \mu)$. Now, Theorem 4(ii) implies that, for any $f \in \mathcal{D}$, the fundamental diffraction ϱ_f of the subshift factor associated to f is just the spectral measure σ_f. If $\{f_n \mid n \in \mathbb{N}\}$ is an enumeration of the elements of $\mathcal{D}$, the measure

$$\varrho := \sum_{n=1}^{\infty} \frac{1}{2^n(1 + \varrho_{f_n}(\mathbb{T}))} \varrho_{f_n}$$

is equivalent to the maximal spectral measure, meaning that it has the same null sets. Indeed, ϱ is absolutely continuous with respect to any maximal spectral measure as any ϱ_f is a spectral measure. Conversely, for any $h \in L^2(\mathbb{X}, \mu)$, we can find a sequence $(h_n)_{n\in\mathbb{N}}$ in $\mathcal{D}$ that converges to h (due to the denseness of $\mathcal{D}$). Then, $\varrho_{h_n} = \sigma_{h_n}$ converges to σ_h in the sense that $\varrho_{h_n}(A) \xrightarrow{n\to\infty} \sigma_h(A)$ for any measurable $A \subset \mathbb{T}$. Consequently, σ_h must be absolutely continuous with respect to ϱ.

Remark 3. It is not hard to see that arbitrarily close to any $g \in \mathbb{A}(\mathbb{X})$ one can find a function g' such that the factor associated to g' is actually a *conjugacy*. This means that one can

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construct a spectral measure out of the diffractions of topological conjugacies along the lines indicated in Remark 2. In particular, the collection of diffractions of all topologically conjugate subshifts is then equivalent to the dynamical spectrum of the original system. This ties in well with the fact that the dynamical spectrum is an invariant under conjugacy, whereas the diffraction measure is not. More specifically, this corroborates that the 'obvious' invariant created from diffraction by collecting the diffraction measures of all conjugate systems is indeed equivalent to the dynamical spectrum of the initial system.

Remark 4. Some classic subshifts were mentioned in the introduction, including the Thue–Morse chain and its generalizations; compare [**5**, **7**] and references therein. Other cases include random dimers [**4**] or the Rudin–Shapiro chain [**10**]. The unifying property of these examples is that one needs just *one* specific factor to complete the picture. However, it was recently shown in [**29**] that this is not always the case, in the sense that there are examples where one really needs to consider infinitely many (sliding block) factors, each of them being periodic, to cover the entire pure point part of the dynamical spectrum. Only all of them together thus replace the knowledge obtainable from Fraczek's factor.

Our exposition of the case of symbolic dynamics has an obvious extension to block substitutions (or lattice substitutions) in higher dimensions, where one deals with (uniquely ergodic) dynamical systems $(\mathbb{X}, \mathbb{Z}^d, \mu)$ in an analogous way; compare [**9**, **26**, **47**] and references therein. Since this extension is straightforward, we leave the explicit formulation to the reader. For recent examples, we refer to [**6**, **9**].

More complex is the situation for Delone dynamical systems, which we need to describe in a geometric setting. In particular, we now have to deal with the continuous translation action of the group $\mathbb{R}^d$ (rather than $\mathbb{Z}^d$).

4. *Delone dynamical systems*

Let $\varLambda \subset \mathbb{R}^d$ be a point set of FLC. By Schlottmann's characterization [**50**, §2], the latter property means that $\varLambda - \varLambda = \{x - y \mid x, y \in \varLambda\}$ is a locally finite set. For FLC sets, the (continuous) hull is defined as

$$\mathbb{X}(\varLambda) := \overline{\{t + \varLambda \mid t \in \mathbb{R}^d\}}, \tag{7}$$

where the closure is taken in the local topology. Here, two FLC sets are ε-close (for small ε say) when they agree on a centred ball of radius $1/\varepsilon$, possibly after shifting one set by an element $t \in B_\varepsilon(0)$. Note that the hull from equation (7) is compact as a result of the FLC property [**11**, **50**]. An important subset is given by

$$\mathbb{X}_0(\varLambda) := \{\varLambda' \in \mathbb{X}(\varLambda) \mid 0 \in \varLambda'\},$$

which is also known as the *discrete* (or punctured) hull or transversal. We now assume that $\varLambda$ is Delone, hence certainly not a finite set, and that the topological dynamical system $(\mathbb{X}(\varLambda), \mathbb{R}^d)$ is uniquely ergodic, with invariant probability measure μ. This, in turn, induces a unique probability measure μ_0 on $\mathbb{X}_0(\varLambda)$, which (again by Oxtoby's theorem [**44**], see [**40**] and [**27**] for a general formulation in the context of Delone sets) is given via the relative patch frequencies as the measures of the corresponding cylinder sets. Here, the

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term 'relative' refers to the definition of the frequency per point of $\varLambda$, not per unit volume of $\mathbb{R}^d$. The system is strictly ergodic (meaning uniquely ergodic and minimal) if and only if the frequencies of all legal patches exist uniformly and are strictly positive.

Below, we first approach the factors in a way that is suggested by the situation in the symbolic case, hence by identifying certain patches and working with their locator (or repetition) sets. To establish the connection with diffraction, we will then need some smoothing (via the convolution with a continuous function of small support), because we are now working with the translation action of $\mathbb{R}^d$. Viewing point sets as 'equivalent' to measures (via their Dirac comb), we will be led to a more general (and perhaps also more natural) approach via measures.

If $K \subset \mathbb{R}^d$ is a compact neighbourhood of $0 \in \mathbb{R}^d$, we call the finite sets of the form $P = (\varLambda - x) \cap K$, with $x \in \varLambda$, the *K-clusters* of $\varLambda$. As they are defined, K-clusters are non-empty, and always contain the point 0 (as its reference point, say). This definition avoids certain trivial pathologies that emerge when the empty cluster is included.

Let P be a K-cluster of $\varLambda$. For any $\varLambda' \in \mathbb{X}(\varLambda)$, the set of K-clusters of $\varLambda'$ is a subset of the K-clusters of $\varLambda$, as a consequence of the construction of the hull $\mathbb{X}(\varLambda)$. We may thus define the *locator set*

$$T_{K,P}(\varLambda') := \{t \in \mathbb{R}^d \mid (\varLambda' - t) \cap K = P\} = \{t \in \varLambda' \mid (\varLambda' - t) \cap K = P\} \subset \varLambda',$$

which contains the cluster reference points of all occurrences of P in $\varLambda'$. Note that the second equality follows from our definition of a cluster. Clearly, $T_{K,P}(\varLambda') \subset \varLambda'$ inherits the FLC property, although it need not be a Delone set (the Delone property is guaranteed if $\mathbb{X}(\varLambda)$ is minimal). If we now set

$$\mathbb{Y} = \mathbb{Y}_{K,P} := \{T_{K,P}(\varLambda') \mid \varLambda' \in \mathbb{X}(\varLambda)\}, \tag{8}$$

we obtain a topological factor of $\mathbb{X}(\varLambda)$. This follows from the observation that the mapping $\varLambda' \mapsto T_{K,P}(\varLambda')$ is continuous in the local topology and commutes with the translation action of $\mathbb{R}^d$, since $T_{K,P}(t + \varLambda') = t + T_{K,P}(\varLambda')$. We call any factor of this type a *derived factor* of $(\mathbb{X}, \mathbb{R}^d, \mu)$, and the collection of all of them the *set of derived factors*. Note that, in our case at hand, μ induces a unique invariant probability measure $\mu_{\mathbb{Y}}$ on $\mathbb{Y}$, so that $(\mathbb{Y}, \mathbb{R}^d, \mu_{\mathbb{Y}})$ is also uniquely ergodic, again by an application of [**20**, Proposition 3.11]; see also Proposition 10 below. This setting will later be generalized beyond (unique) ergodicity in §5.

In view of this situation, we may employ $\varLambda$ itself, together with its image in $\mathbb{Y}$, to analyse the factor and its properties. To this end, consider the Dirac comb $\omega = \delta_{T_{K,P}(\varLambda)}$, which is a translation bounded measure by construction. Its autocorrelation measure γ_ω exists, due to (unique) ergodicity, and reads $\gamma_\omega = \omega \circledast \widetilde{\omega} = \sum_{z \in \varLambda - \varLambda} \eta_{K,P}(z)\delta_z$, with

$$\eta_{K,P}(z) = \lim_{R \to \infty} \frac{1}{\mathrm{vol}(B_R(0))} \mathrm{card}((T_{K,P}(\varLambda) \cap B_R(0)) \cap (z + T_{K,P}(\varLambda))). \tag{9}$$

Note that we have used [**50**, Lemma 1.2] for the derivation of this expression. In particular, γ_ω is a pure point measure with support in $\varLambda - \varLambda$, which is a locally finite subset of $\mathbb{R}^d$. Moreover, the coefficient $\eta(0)$ is the density of the set $T_{K,P}(\varLambda)$, which equals the absolute frequency of the K-cluster P in $\varLambda$ by construction. Consequently, $\eta_{K,P}(0)/\mathrm{dens}(\varLambda)$ is

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the relative frequency of the cluster P within $\varLambda$. Recall that the diffraction measure $\widehat{\gamma_\omega}$ contains a point (or Dirac) measure at 0, whose intensity $I(0)$ satisfies $I(0) = (\eta_{K,P}(0))^2$; see [**10**, Corollary 9.1]. This gives access to the relative frequency of P.

The situation is thus as follows. Knowing the diffraction measures of all derived factors of $(\mathbb{X}, \mathbb{R}^d, \mu)$ means knowing their autocorrelations. If one also knows the corresponding pairs (K, P), one can then extract all cluster frequencies, and hence the measure μ_0 on $\mathbb{X}_0(\varLambda)$. The measure μ on $\mathbb{X}(\varLambda)$ is uniquely determined from μ_0 by standard methods, compare [**10**] and references therein (in some cases, and for $d = 1$ in particular, this can be seen via the suspension as a special flow, compare [**16**, **23**]). The family of these factors thus permits a reconstruction of the measure-theoretic dynamical system $(\mathbb{X}(\varLambda), \mathbb{R}^d, \mu)$, and hence its dynamical spectrum, at least in an abstract sense. In fact, viewing $\varLambda$ as an example of an (r, R)-set with packing radius r and covering radius R, the factor maps select the list of possible clusters in $\varLambda$, and the diffraction of a factor then gives the corresponding cluster frequency. We have thus shown the following result.

PROPOSITION 5. *Let $\varLambda$ be an FLC Delone set such that its hull $\mathbb{X} = \mathbb{X}(\varLambda)$ defines a uniquely ergodic dynamical system under the translation action of $\mathbb{R}^d$. Then, the cluster frequencies can directly be computed from the diffraction measures of all locator sets of finite clusters within $\varLambda$. Any explicit knowledge of a generating set of clusters, together with their frequencies as extracted from the diffraction measure of the corresponding factors, explicitly specifies the invariant measure and thus the measure-theoretic dynamical system* $(\mathbb{X}, \mathbb{R}^d, \mu)$.

Let us pause to comment on the term 'generating' in the above formulation. It is clear that the set of all clusters suffices, but that is more than one really needs. A collection of clusters (or patches, if one restricts to closed balls as compact sets) is called an *atlas* if it defines the hull $\mathbb{X}(\varLambda)$ via the rule that the latter contains all Delone sets which comply with the atlas (in the sense that no patch of an element of $\mathbb{X}(\varLambda)$ is in violation of the atlas; see [**10**] for more on this notion). Under certain circumstances, such an atlas can be finite, in which case $\varLambda$ is said to possess *local rules*. The vertex set of the classic Penrose tiling in the Euclidean plane is a famous aperiodic example of this situation.

To expand on the connection between the hull $\mathbb{X}(\varLambda)$ and its factors, we need a refinement of our arguments in §3, as the characteristic function of a cluster is not continuous on $\mathbb{X}(\varLambda)$, wherefore it does not lead to a complete analogue of a sliding block map as used in §3, in the sense that the continuous factor map from $\mathbb{X}$ to a derived factor is not a 'sliding cluster map' built from a continuous function on the hull that is defined locally. Moreover, there is no immediate connection between the spectral measures of $(\mathbb{X}, \mathbb{R}^d, \mu)$ and the diffraction measures of derived factors. To establish a connection, we need some 'smoothing' or 'regularizing' operation, as we will now describe; compare [**30**, **35**] for related ideas.

Let $K \subset \mathbb{R}^d$ be compact, P a K-cluster of $\varLambda$, and choose a (real-valued) function $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$ with $\mathrm{supp}(\varphi) \subset B_{r_{\mathsf{p}}}(0)$, where r_{p} is the *packing radius* of $\varLambda$,

$$r_{\mathsf{p}} = \sup\{r > 0 \mid B_r(x) \cap B_r(y) = \varnothing \text{ for all distinct } x, y \in \varLambda\}.$$

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For instance, $\varphi_\varepsilon(t) = 1 - |t|/\varepsilon$ for $t \in B_\varepsilon(0)$ and $\varphi_\varepsilon(t) = 0$ otherwise is a possible choice, with $\varepsilon < r_{\mathsf{p}}$. Now, define a function $\chi^{(\varphi)}_{K,P} : \mathbb{X}(\varLambda) \longrightarrow \mathbb{R}$ by

$$\chi^{(\varphi)}_{K,P}(\varLambda') = \begin{cases} \varphi(-t) & \text{if } (\varLambda' - t) \cap K = P \text{ for some } t \in B_\varepsilon(0), \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

Owing to the condition on the support of φ, there is at most one possible translation $t \in B_\varepsilon(0)$ for the occurrence of P, wherefore $\chi^{(\varphi)}_{K,P}$ is indeed well-defined. Moreover, it is a continuous function on $\mathbb{X}(\varLambda)$ by construction. Note that $\chi^{(\varphi)}_{K,P}(\varLambda')$ can be rewritten as

$$\chi^{(\varphi)}_{K,P}(\varLambda') = \sum_{x \in T_{K,P}(\varLambda')} \varphi(-x) = (\varphi * \delta_{T_{K,P}(\varLambda')})(0).$$

This, in turn, can be used to define $\chi^{(\varphi)}_{K,P} : \mathbb{X}(\varLambda) \longrightarrow \mathbb{C}$ for an *arbitrary* $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$. The relevance of this class of functions emerges from the following completeness result [**50**].

PROPOSITION 6. *The linear span of all functions of the form $\chi^{(\varphi)}_{K,P}$, with $K \subset \mathbb{R}^d$ compact, P a K-clusters of $\varLambda$ and $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$, is a subalgebra of $C(\mathbb{X})$ which is dense with respect to the supremum norm.*

Proof. For $\varLambda' \in \mathbb{X}$, we set $\chi^{(\varphi)}_{K,P}(\varLambda') = \sum_{x \in T_{K,P}(\varLambda')} \varphi(-x)$, as motivated above. The statement about the denseness is then an immediate consequence of [**50**, Proposition 2.5]. Note that there is no need to deal with the empty set in our situation, as our original set $\varLambda$ is Delone. The proof of Proposition 2.5 in [**50**] (which uses the Stone–Weierstrass theorem) also shows that the linear span is an algebra, which completes the proof. □

The induced mapping $\alpha^{(\varphi)}_{K,P} : \mathbb{R}^d \times \mathbb{X}(\varLambda) \longrightarrow \mathbb{R}$ defined by

$$(t, X) \longmapsto \alpha^{(\varphi)}_{K,P}(t, X) = \chi^{(\varphi)}_{K,P}(X - t)$$

is continuous. One can check that

$$\alpha^{(\varphi)}_{K,P}(t, X) = (\varphi * \delta_{T_{K,P}(X)})(t) = \sum_{x \in T_{K,P}(X)} \varphi(t - x).$$

The function φ acts as a 'regularization', and gives rise to a 'smoothed sliding cluster map' on $\mathbb{X}(\varLambda)$ via $X \mapsto \varphi * \delta_{T_{K,P}(X)}$, the latter now interpreted as a regular, translation bounded measure. This mapping is continuous and commutes with the translation action of $\mathbb{R}^d$, so that we obtain a factor system $(\mathbb{Y}, \mathbb{R}^d, \mu_{\mathbb{Y}})$ that is again uniquely ergodic. Note that the elements of $\mathbb{Y}$, which approximate derived factors without being derived themselves, may both be considered as (absolutely continuous) translation bounded measures and as continuous functions on $\mathbb{R}^d$. The latter point of view allows us to take (pointwise) products, which will become useful shortly.

Consider the regular measure $\omega_\varphi = \varphi * \delta_{T_{K,P}(\varLambda)}$ as representative, and observe the relation

$$\gamma_{\omega_\varphi} = (\varphi * \widetilde{\varphi}) * (\omega \circledast \widetilde{\omega}) = (\varphi * \widetilde{\varphi}) * \gamma_\omega \tag{11}$$

with the measure $\omega = \delta_{T_{K,P}(\varLambda)}$ from above. Note that γ_{ω_φ} is absolutely continuous as a measure (relative to Lebesgue measure), with a Radon–Nikodym density that is continuous

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as a function on $\mathbb{R}^d$. Moreover, γ_{ω_φ} clearly is a (Fourier) transformable measure, in the sense that the Fourier transform exists and is again a measure; compare [**10**, **15**] for background. Here, one obtains

$$\widehat{\gamma_{\omega_\varphi}} = |\widehat{\varphi}|^2 \widehat{\gamma_\omega} \tag{12}$$

by an application of the convolution theorem [**15**].

When we use the tent-shaped function $\varphi = \varphi_\varepsilon$ from above, $\widehat{\varphi_\varepsilon}(0) = (2\pi^{n/2}\varepsilon^n)/\Gamma(n/2)$, where Γ denotes the gamma function, is the volume of the cone defined by the graph of the function φ_ε over $\mathbb{R}^d$, so that the value of $\widehat{\gamma_\omega}(\{0\})$, and thus the density of the set $T_{K,P}(\Lambda)$, can be calculated from $\widehat{\gamma_{\omega_\varphi}}(\{0\})$.

Recall $\omega_\varphi = \varphi * \delta_{T_{K,P}(\Lambda)}$ and observe that

$$\begin{aligned} \gamma_{\omega_\varphi}(t) &= \lim_{r\to\infty} \frac{1}{\mathrm{vol}(B_r(0))} \int_{B_r(0)} \overline{\omega_\varphi(s)}\omega_\varphi(s+t)\, ds = \int_{\mathbb{Y}} \overline{Y(0)}Y(t)\, d\mu_{\mathbb{Y}}(Y) \\ &= \int_{\mathbb{X}} \overline{\chi^{(\varphi)}_{K,P}(X)} U_t \chi^{(\varphi)}_{K,P}(X)\, d\mu(X) = \langle \chi^{(\varphi)}_{K,P} \mid U_t \chi^{(\varphi)}_{K,P} \rangle, \end{aligned} \tag{13}$$

which essentially is an application of Dworkin's argument [**19**, **22**, **50**] to this situation. The new twist (or interpretation) is that it appears by linking the original system with a factor. Note that, under the second integral, the element $Y \in \mathbb{Y}$ is interpreted as a continuous function on $\mathbb{R}^d$, so that its evaluation at a point is well defined, as mentioned earlier.

Since the (continuous) function $\gamma_{\omega_\varphi}(t)$ is positive-definite, Bochner's theorem links it to a unique positive measure on the dual group via Fourier transform. In our case, this gives

$$\gamma_{\omega_\varphi}(t) = \int_{\mathbb{R}^d} e^{2\pi i t x}\, d\widehat{\gamma_{\omega_\varphi}}(x) = \int_{\mathbb{R}^d} e^{2\pi i t x} |\widehat{\varphi}(x)|^2\, d\widehat{\gamma_\omega}(x), \tag{14}$$

which is the desired connection between the spectral measure of $\chi^{(\varphi)}_{K,P}$ and the diffraction measures of ω_φ and ω, via a comparison with equation (13).

As we already saw, the connection between the spectral measure of a function and the diffraction of a factor is not restricted to functions φ with small support. The latter were chosen above to establish the connection with the locator sets of clusters and to highlight the relation to our treatment of the symbolic case in §3. Independently, for any given $\mathbb{X} = \mathbb{X}(\Lambda)$ with an FLC point set Λ and for any $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$, one may directly define the mapping $\chi_\varphi : \mathbb{X}(\Lambda) \longrightarrow \mathbb{C}$ by $X \mapsto \chi_\varphi(X) = (\varphi * \delta_X)(0)$. Our previous reasoning around equations (13) and (14) can now be repeated, which leads to the following result.

PROPOSITION 7. *Let $\Lambda \subset \mathbb{R}^d$ be an FLC point set such that its hull $\mathbb{X} = \mathbb{X}(\Lambda)$ defines a uniquely ergodic dynamical system $(\mathbb{X}, \mathbb{R}^d)$ under the action of $\mathbb{R}^d$. For $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$, consider the continuous function $g_\varphi : \mathbb{X} \longrightarrow \mathbb{C}$ defined by $X \mapsto g_\varphi(X) := \varphi * \widetilde{\varphi} * \gamma_X$, where γ_X is the autocorrelation of δ_X. Then, one has*

$$g_\varphi(t) = \langle \chi_\varphi \mid U_t \chi_\varphi \rangle = \int_{\mathbb{R}^d} e^{2\pi i t s}\, d\sigma(s)$$

with the spectral measure $\sigma = |\widehat{\varphi}|^2 \widehat{\gamma_X}$.

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When $\operatorname{supp}(\varphi) \subset B_{r_{\mathsf{p}}}(0)$, this result is a special case of our previous situation, with P the (trivial) singleton cluster and $K = \overline{B_{\varepsilon}(0)}$ for some $\varepsilon < r_{\mathsf{p}}$. The findings of this section can now be summarized as follows.

THEOREM 8. *Let $\varLambda$ be an FLC point set with hull $\mathbb{X} = \mathbb{X}(\varLambda)$ such that $(\mathbb{X}, \mathbb{R}^d)$ is a uniquely ergodic dynamical system, with invariant measure μ. Let $K \subset \mathbb{R}^d$ be compact and P a K-cluster of $\varLambda$. Then, the following properties hold.*

(i) *The absolute frequency of P in $\varLambda$ is $\eta_{K,P}(0)$, where $\eta_{K,P}$ is the autocorrelation coefficient from equation (9). Moreover, when γ_ω is the autocorrelation measure of the translation bounded measure $\omega = \delta_{T_{K,P}(\varLambda)}$, one has $\widehat{\gamma_\omega}(\{0\}) = (\eta_{K,P}(0))^2$.*

(ii) *If $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$, the regularization $\omega_\varphi = \varphi * \omega = \varphi * \delta_{T_{K,P}(\varLambda)}$ possesses the autocorrelation measure $\gamma_{\omega_\varphi} = \varphi * \widetilde{\varphi} * \gamma_\omega$ and the positive diffraction measure $\widehat{\gamma_{\omega_\varphi}} = |\widehat{\varphi}|^2 \widehat{\gamma_\omega}$. The latter is the spectral measure of the continuous function $\chi^{(\varphi)}_{K,P} : \mathbb{X} \longrightarrow \mathbb{C}$ defined by $X \mapsto \chi^{(\varphi)}_{K,P}(X) = \sum_{x \in T_{K,P}(X)} \varphi(-x)$, and one has $\widehat{\gamma_{\omega_\varphi}}(\{0\}) = |\widehat{\varphi}(0)|^2 \cdot (\eta_{K,P}(0))^2$.*

(iii) *Every spectral measure of $(\mathbb{X}, \mathbb{R}^d, \mu)$ can be approximated arbitrarily well by a finite linear combination of diffraction measures of factors that are obtained by smoothed sliding cluster maps based on functions of type $\chi^{(\varphi)}_{K,P}$. In this sense, the diffraction spectra of such factors explore the entire dynamical spectrum of $(\mathbb{X}, \mathbb{R}^d, \mu)$.*

Proof. The first claim derives from equation (9) and the arguments given there, while the connection between $\widehat{\gamma_\omega}(\{0\})$ and $\eta_{K,P}(0)$ is standard; compare [**10**, Corollary 9.1].

The first part of the second claim is a consequence of equation (11), which follows from an elementary calculation, and equation (12), which results from an application of the convolution theorem to this situation; compare [**10**, Theorem 8.5]. The second part is the combination of equations (13) and (14); see also Proposition 7, applied to $\varLambda' = T_{K,P}(\varLambda)$.

The third claim follows from Proposition 6 and the observation that the closeness of two continuous functions on $\mathbb{X}$ in the norm topology implies that the corresponding spectral measures are close in the vague topology. □

Let us finish this section by formulating a variant of Theorem 8. Let $\varLambda \subset \mathbb{R}^d$ be an FLC Delone set, and $(\mathbb{X}, \mathbb{R}^d)$ the associated topological dynamical system. Recall that any K-cluster P of $\varLambda$ comes with a factor

$$\mathbb{Y}_{K,P} := \{T_{K,P}(\varLambda') \mid \varLambda' \in \mathbb{X}(\varLambda)\},$$

which is derived from $\mathbb{X}$ via (K, P). If the original system is uniquely ergodic, then so are all of its factor systems, and all derived factors in particular. Our previous calculations then show that the autocorrelation measure of the factor $\mathbb{X}_{K,P}$ is given as

$$\gamma_{K,P} = \gamma_\omega = \omega \circledast \widetilde{\omega} = \sum_{z \in \varLambda - \varLambda} \eta_{K,P}(z) \delta_z, \tag{15}$$

with the coefficients $\eta_{K,P}$ from equation (9). We can now turn Theorem 8 into the following analogue of Theorem 4 from §3.

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COROLLARY 9. *Let $\Lambda \subset \mathbb{R}^d$ be an FLC Delone set, and assume that the associated dynamical system $(\mathbb{X}, \mathbb{R}^d)$ is uniquely ergodic, with invariant measure μ. Then, the following properties hold.*

(i) *Whenever $\widehat{\gamma}$ is the diffraction measure of a derived factor of $(\mathbb{X}, \mathbb{R}^d, \mu)$, the measure $|\widehat{\varphi}|^2\widehat{\gamma}$, with $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$ arbitrary, is a spectral measure of $(\mathbb{X}, \mathbb{R}^d, \mu)$.*

(ii) *There is a dense set $\mathcal{D} \subset C(\mathbb{X})$, hence also dense in $L^2(\mathbb{X}, \mu)$, such that the spectral measure σ_g of any $g \in \mathcal{D}$ has the form $|\widehat{\varphi}|^2\widehat{\gamma}$, for some $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$ and with $\widehat{\gamma}$ being the diffraction measure of a derived factor of $(\mathbb{X}, \mathbb{R}^d, \mu)$.*

Note that, in contrast to Theorem 4, a derived factor in this setting in general does not emerge from a factor map of sliding block or cluster type. Let us also emphasize that, similarly to equation (3), the subspace $\mathcal{D} \subset C(\mathbb{X})$ is again completely explicit, as formulated in Proposition 6.

Remark 5. In view of these findings, it is suggestive to take a closer look at systems with finitely many (non-periodic) factors, up to topological conjugacy or up to metric isomorphism. Examples of the former type include linearly repetitive FLC systems [**17**, **21**], while Bernoulli shifts provide the paradigm of the latter [**43**]; see also [**49**, Ch. 7] for further connections. It is a challenge in this context to understand how the diffraction spectra of equivalent systems are related. So far, the study of examples (compare also our Appendix) suggests that further progress via the diffraction approach is indeed possible for systems with finitely many factors (up to equivalence).

Let us now embark on an abstract reformulation in the more general setting of LCAGs. For convenience, we will give a self-contained exposition, so that the generalization of our previous notions becomes transparent.

5. *An abstract approach*

Our considerations will primarily be set in the framework of topological dynamical systems. We are dealing with σ-compact locally compact topological groups and compact spaces. All topological spaces are assumed to be Hausdorff. The general approach to diffraction via measure dynamical systems discussed below is largely taken from [**11**]; see [**12**, **34**, **37**] as well.

When $\mathcal{X}$ is a σ-compact locally compact space, we denote the space of continuous functions on $\mathcal{X}$ by $C(\mathcal{X})$, and the subspace of continuous functions with compact support by $C_{\mathsf{c}}(\mathcal{X})$. The space $C_{\mathsf{c}}(\mathcal{X})$ is equipped with the locally convex limit topology induced by the canonical embeddings $C_K(\mathcal{X}) \hookrightarrow C_{\mathsf{c}}(\mathcal{X})$, where $C_K(\mathcal{X})$ is the space of complex continuous functions with support in a given compact set $K \subset \mathcal{X}$. Here, each $C_K(\mathcal{X})$ is equipped with the topology induced by the standard supremum norm.

As $\mathcal{X}$ is a topological space, it carries a natural σ-algebra, namely the Borel σ-algebra generated by all closed subsets of X. The set $\mathcal{M}(\mathcal{X})$ of all complex regular Borel measures on G can then be identified with the space $C_{\mathsf{c}}(\mathcal{X})^*$ of complex-valued, continuous linear functionals on $C_{\mathsf{c}}(\mathcal{X})$. This is justified by the Riesz–Markov representation theorem; compare [**45**, Ch. 6.5] for details. In particular, we can write $\int_{\mathcal{X}} f \, d\mu = \mu(f)$ for $f \in C_{\mathsf{c}}(\mathcal{X})$ and simplify the notation this way. The space $\mathcal{M}(\mathcal{X})$ carries the vague

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topology, which is the weakest topology that makes all functionals $\mu \mapsto \mu(\varphi)$ on $\varphi \in C_{\mathsf{c}}(\mathcal{X})$ continuous. The total variation of a measure $\mu \in \mathcal{M}(\mathcal{X})$ is denoted by $|\mu|$. Note that, unless $\mathcal{X}$ is compact, an element $\mu \in \mathcal{M}(\mathcal{X})$ need not be bounded.

Let G now be a fixed σ-compact LCAG. The dual group of G is denoted by $\widehat{G}$, and the pairing between a character $\widehat{s} \in \widehat{G}$ and $t \in G$ is written as $(\widehat{s}, t)$. Whenever G acts on the compact Hausdorff space $\mathbb{X}$ by a continuous action

$$\alpha : G \times \mathbb{X} \longrightarrow \mathbb{X}, \quad (t, \omega) \mapsto \alpha_t(\omega),$$

where $G \times \mathbb{X}$ carries the product topology, the pair $(\mathbb{X}, \alpha)$ is called a *topological dynamical system* over G. We shall often write $\alpha_t\omega$ for $\alpha_t(\omega)$, and think of this as a translation action. If $\omega \in \mathbb{X}$ satisfies $\alpha_t\omega = \omega$, the element $t \in G$ is called a *period* of ω. If all $t \in G$ are periods, ω is called G-invariant, or α-*invariant* to refer to the action involved.

The set of all Borel probability measures on $\mathbb{X}$ is denoted by $\mathcal{P}(\mathbb{X})$, and the subset of α-invariant probability measures by $\mathcal{P}_G(\mathbb{X})$. An α-invariant probability measure is called *ergodic* if every (measurable) α-invariant subset of $\mathbb{X}$ has either measure zero or measure one. The ergodic measures are exactly the extremal points of the convex set $\mathcal{P}_G(\mathbb{X})$. The dynamical system $(\mathbb{X}, \alpha)$ is called *uniquely ergodic* if $\mathcal{P}_G(\mathbb{X})$ is a singleton set (which means that it consists of exactly one element). As usual, $(\mathbb{X}, \alpha)$ is called *minimal* if, for all $\omega \in \mathbb{X}$, the G-orbit $\{\alpha_t\omega \mid t \in G\}$ is dense in $\mathbb{X}$. If $(\mathbb{X}, \alpha)$ is both uniquely ergodic and minimal, it is called *strictly ergodic*.

Given a $\mu \in \mathcal{P}_G(\mathbb{X})$, we can form the Hilbert space $L^2(\mathbb{X}, \mu)$ of square integrable measurable functions on $\mathbb{X}$. This space is equipped with the inner product

$$\langle f \mid g \rangle = \langle f \mid g \rangle_{\mathbb{X}} := \int_{\mathbb{X}} \overline{f(\omega)} g(\omega)\, d\mu(\omega).$$

The action α gives rise to a unitary representation $T = T^{\mathbb{X}} := T^{(\mathbb{X},\alpha,\mu)}$ of G on $L^2(\mathbb{X}, \mu)$ by

$$T_t : L^2(\mathbb{X}, \mu) \longrightarrow L^2(\mathbb{X}, \mu), \quad (T_t f)(\omega) := f(\alpha_{-t}\omega),$$

for every $f \in L^2(\mathbb{X}, \mu)$ and arbitrary $t \in G$.

By Stone's theorem, compare [**39**, §36D], there exists a projection-valued measure

$$E_T : \{\text{Borel sets of } \widehat{G}\} \longrightarrow \{\text{projections on } L^2(\mathbb{X}, \mu)\}$$

with

$$\langle f \mid T_t f \rangle = \int_{\widehat{G}} (\widehat{s}, t)\, d\langle f \mid E_T(\cdot) f \rangle(\widehat{s}) := \int_{\widehat{G}} (\widehat{s}, t)\, d\sigma_f(\widehat{s}),$$

where $\sigma_f = \sigma_f^{\mathbb{X}} := \sigma_f^{(\mathbb{X},\alpha,\mu)}$ is the (positive) measure on $\widehat{G}$ defined by setting $\sigma_f(B) := \langle f \mid E_T(B) f \rangle$. In fact, by Bochner's theorem [**48**], σ_f is the unique measure on $\widehat{G}$ with $\langle f \mid T_t f \rangle = \int_{\widehat{G}} (\widehat{s}, t)\, d\sigma_f(\widehat{s})$ for every $t \in G$. The measure σ_f is called the *spectral measure* of f.

The projection-valued measure E_T contains the entire spectral information on the dynamical system. It is desirable to encode this spectral information in terms of measures on $\widehat{G}$. One way of doing so is via the family of spectral measures. More generally, we introduce the following definition.

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Definition 1. Let $T = T^{(\mathbb{X},\alpha,\mu)}$ be the unitary representation associated to the invariant probability measure μ on the dynamical system $(\mathbb{X}, \alpha)$, and let E_T be the corresponding projection-valued measure. A family $\{\sigma_\iota\}$ of measures on $\widehat{G}$ (with ι in some index set J) is called a *complete spectral invariant* when $E_T(A) = 0$ holds for a Borel set $A \subset \widehat{G}$ if and only if $\sigma_\iota(A) = 0$ holds for all $\iota \in J$.

Let us now turn to factors. Here, we essentially follow the presentation given in [**12**], to which we refer for further details and proofs. Let two topological dynamical systems $(\mathbb{X}, \alpha)$ and $(\mathbb{Y}, \beta)$ under the action of G and a mapping $\Phi : \mathbb{X} \longrightarrow \mathbb{Y}$ be given. Then, $(\mathbb{Y}, \beta)$ is called a *factor* of $(\mathbb{X}, \alpha)$, with factor map Φ, if Φ is a continuous surjection with $\Phi(\alpha_t(\omega)) = \beta_t(\Phi(\omega))$ for all $\omega \in \mathbb{X}$ and $t \in G$.

In this situation, $(\mathbb{Y}, \beta)$ inherits many features from $(\mathbb{X}, \alpha)$. For example, $U \subset \mathbb{Y}$ is open if and only if $\Phi^{-1}(U)$ is open in $\mathbb{X}$. Also, Φ induces a map $\Phi_* : \mathcal{M}(\mathbb{X}) \longrightarrow \mathcal{M}(\mathbb{Y})$, $\rho \mapsto \Phi_*(\rho)$, via $(\Phi_*(\rho))(g) := \rho(g \circ \Phi)$ for all $g \in C(\mathbb{Y})$. If μ is a probability measure on $\mathbb{X}$, its image $\nu := \Phi_*(\mu)$ is a probability measure on $\mathbb{Y}$. Moreover, if Φ is a factor map, invariance under the group action is preserved. In fact, Φ_* is a continuous surjection from the set $\mathcal{P}_G(\mathbb{X})$ of invariant measures on $\mathbb{X}$ onto the set $\mathcal{P}_G(\mathbb{Y})$ of invariant measures on $\mathbb{Y}$. Based on the results of [**20**], some important properties can be summarized as follows; see [**12**] as well.

PROPOSITION 10. *Let $(\mathbb{Y}, \beta)$ be a factor of $(\mathbb{X}, \alpha)$, with factor map $\Phi : \mathbb{X} \longrightarrow \mathbb{Y}$. If the system $(\mathbb{X}, \alpha)$ is ergodic, uniquely ergodic, minimal, or strictly ergodic, the analogous property holds for $(\mathbb{Y}, \beta)$ as well.*

Now, let $(\mathbb{Y}, \beta)$ be a factor of $(\mathbb{X}, \alpha)$ with factor map $\Phi : \mathbb{X} \longrightarrow \mathbb{Y}$, and let $\mu \in \mathcal{P}_G(\mathbb{X})$ be fixed. Denote the induced measure on $\mathbb{Y}$ by $\nu = \Phi_*(\mu)$. Consider the mapping

$$i^\Phi : L^2(\mathbb{Y}, \nu) \longrightarrow L^2(\mathbb{X}, \mu), \quad f \mapsto f \circ \Phi, \tag{16}$$

and let $p_\Phi : L^2(\mathbb{X}, \mu) \longrightarrow L^2(\mathbb{Y}, \nu)$ be the adjoint of i^Φ. Then, the maps i^Φ and p_Φ are partial isometries, and i^Φ is an isometric embedding with

$$p_\Phi \circ i^\Phi = \mathrm{id}_{L^2(\mathbb{Y},\nu)} \quad \text{and} \quad i^\Phi \circ p_\Phi = P_{i^\Phi(L^2(\mathbb{Y},\nu))},$$

where $\mathrm{id}_{L^2(\mathbb{Y},\nu)}$ is the identity on $L^2(\mathbb{Y}, \nu)$ and $P_{i^\Phi(L^2(\mathbb{Y},\nu))}$ is the orthogonal projection of $L^2(\mathbb{X}, \mu)$ onto $\mathcal{V} := i^\Phi(L^2(\mathbb{Y}, \nu))$.

Given these maps, we can now summarize the relation between the spectral theory of $T^{\mathbb{X}}$ and that of $T^{\mathbb{Y}}$ as follows; compare [**12**, Theorem 1].

THEOREM 11. *Fix some $\mu \in \mathcal{P}_G(\mathbb{X})$ and let $L^2(\mathbb{X}, \mu)$ and $L^2(\mathbb{Y}, \nu)$ be the canonical Hilbert spaces attached to the dynamical systems $(\mathbb{X}, \alpha)$ and $(\mathbb{Y}, \beta)$, with factor map Φ and $\nu = \Phi_*(\mu)$. Then, the partial isometries i^Φ and p_Φ are compatible with the unitary representations $T^{\mathbb{X}}$ and $T^{\mathbb{Y}}$ of G on $L^2(\mathbb{X}, \mu)$ and $L^2(\mathbb{Y}, \nu)$, in the sense that*

$$i^\Phi \circ T_t^{\mathbb{Y}} = T_t^{\mathbb{X}} \circ i^\Phi \quad \text{and} \quad T_t^{\mathbb{Y}} \circ p_\Phi = p_\Phi \circ T_t^{\mathbb{X}}$$

hold for all $t \in G$. Similarly, the spectral families $E_{T^{\mathbb{Y}}}$ and $E_{T^{\mathbb{X}}}$ satisfy

$$i^\Phi \circ E_{T^{\mathbb{Y}}}(\cdot) = E_{T^{\mathbb{X}}}(\cdot) \circ i^\Phi \quad \text{and} \quad E_{T^{\mathbb{Y}}}(\cdot) \circ p_\Phi = p_\Phi \circ E_{T^{\mathbb{X}}}(\cdot).$$

The corresponding spectral measures satisfy $\sigma_g^{\mathbb{Y}} = \sigma_{i^\Phi(g)}^{\mathbb{X}}$ for every $g \in L^2(\mathbb{Y}, \nu)$.

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Let us now specify the dynamical systems we are dealing with and discuss the necessary background from diffraction theory. The material is directly taken from [**11**], where the proofs and further details as well as references to related literature can be found.

Let $C > 0$ and a relatively compact open set $V \subset G$ be given. A measure $\omega \in \mathcal{M}(G)$ is called (C, V)-*translation bounded* if $\sup_{t\in G} |\omega|(t + V) \leq C$. It is called *translation bounded* if there exists a pair C, V so that ω is (C, V)-translation bounded. The set of all (C, V)-translation bounded measures is denoted by $\mathcal{M}_{C,V}(G)$, the set of all translation bounded measures by $\mathcal{M}^\infty(G)$. In the vague topology, the set $\mathcal{M}_{C,V}(G)$ is a compact Hausdorff space. There is an obvious action of G on $\mathcal{M}^\infty(G)$, again denoted by α, given by

$$\alpha : G \times \mathcal{M}^\infty(G) \longrightarrow \mathcal{M}^\infty(G), \quad (t, \omega) \mapsto \alpha_t\omega := \delta_t * \omega.$$

Restricted to $\mathcal{M}_{C,V}(G)$, this action is continuous. Here, the convolution of two convolvable measures ρ, σ is defined by

$$(\rho * \sigma)(\varphi) = \int_G \varphi(r + s)\, d\rho(r)\, d\sigma(s)$$

for test functions $\varphi \in C_{\mathsf{c}}(G)$.

Definition 2. We call $(\mathbb{X}, \alpha)$ a dynamical system of translation bounded measures on G (*TMDS* for short) if there exist a constant $C > 0$ and a relatively compact open set $V \subset G$ such that $\mathbb{X}$ is a closed α-invariant subset of $\mathcal{M}_{C,V}(G)$.

Having introduced our systems, we can now discuss the necessary pieces of diffraction theory. Let $(\mathbb{X}, \alpha)$ be a TMDS, equipped with an α-invariant measure $\mu \in \mathcal{P}_G(\mathbb{X})$. We will profit from the introduction of the mapping $N = N^{\mathbb{X}} : C_{\mathsf{c}}(G) \longrightarrow C(\mathbb{X})$ defined by $\varphi \mapsto N_\varphi$ with

$$N_\varphi(\omega) := \int_G \varphi(-s)\, d\omega(s) = (\varphi * \omega)(0).$$

The mapping N provides a natural way to consider $C_{\mathsf{c}}(G)$ as a subspace of $L^2(\mathbb{X}, \mu)$ for the given dynamical system, which is important for our approach. In particular, we will need the subspace

$$\mathcal{U}^{\mathbb{X}} := \text{Closure of the linear span of } N_\varphi, \text{ with } \varphi \in C_{\mathsf{c}}(G), \text{ in } L^2(\mathbb{X}, \mu).$$

There exists a unique measure $\gamma = \gamma_\mu$ on G, called the *autocorrelation measure*, or autocorrelation for short, of the TMDS, with

$$\gamma(\overline{\varphi} * \psi_{\tilde{}}) = \langle N_\varphi \mid N_\psi \rangle$$

for all φ, $\psi \in C_{\mathsf{c}}(G)$, where $\psi_{\tilde{}}(s) := \psi(-s)$. As usual, the convolution $\varphi * \psi$ is defined by $(\varphi * \psi)(t) = \int_G \varphi(t - s)\psi(s)\, ds$.

There is an explicit formula for γ as follows. Choose an arbitrary non-negative function $\psi \in C_{\mathsf{c}}(G)$ with $\int_G \psi(t)\, dt = 1$. Then, we have

$$\gamma(\varphi) = \int_{\mathbb{X}} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \varphi(t + s)\psi(t)\, d\widetilde{\omega}(s)\, d\omega(t)\, d\mu(\omega), \tag{17}$$

for every $\varphi \in C_{\mathsf{c}}(G)$, with $\widetilde{\omega}$ as defined in §2. The measure γ is positive definite, and does *not* depend on the choice of ψ; see [**11**] for details. Therefore, its Fourier transform $\widehat{\gamma}$ exists and is a positive measure; compare [**10**, Proposition 8.6]. It is called the *diffraction measure* of the TMDS.

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Remark 6. Let us emphasize that this concept of an autocorrelation does not rely on a local averaging procedure. Instead, it uses an averaging along the measure on the dynamical system, also known as an *ensemble average*. This has the advantage that we can deal with rather general situations. In fact, not even ergodicity of the measure on the dynamical system is needed. However, one then loses the connection to the notion of an autocorrelation of an individual member of the hull, which may become relevant for applications.

The crucial connection between the spectral theory of the dynamical system and the diffraction theory can be expressed in the following way, as has been discussed in various places.

PROPOSITION 12. *Let $(\mathbb{X}, \alpha)$ be a TMDS over G with invariant probability measure μ, and let $\widehat{\gamma}$ be the associated TMDS diffraction measure. Then, for every $\varphi \in C_{\mathsf{c}}(G)$, the spectral measure of the function N_φ is given by*

$$\sigma_{N_\varphi} = |\widehat{\varphi}|^2 \widehat{\gamma}.$$

This spectral measure is the diffraction measure of the factor TMDS defined by $\omega \mapsto \varphi * \omega$.

Proof. In the form stated here, the first claim can be found explicitly in [**11**]; compare [**19**, **22**, **34**, **36**, **37**] for related and partly even more general versions.

The second claim follows from the explicit calculations that we have used above in the setting of Delone sets, which readily generalizes to the setting of LCAGs. □

Remark 7. Let us expand on the meaning of Proposition 12 for $G = \mathbb{R}^d$. In general, the diffraction measure $\widehat{\gamma}$ does not assign finite mass to $\mathbb{R}^d$, and thus cannot be a spectral measure of $(\mathbb{X}, \mathbb{R}^d, \mu)$. However, Proposition 12 shows that replacing $\widehat{\gamma}$ by $|\widehat{\varphi}^2|\widehat{\gamma}$, which reflects a smoothing by convolution on the level of the autocorrelation, yields a spectral measure for any $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$. In fact, it is possible to extend the result to show that, for any non-negative $h \in L^1(\widehat{\mathbb{R}^d}, \widehat{\gamma})$, the measure $h\widehat{\gamma}$ is a spectral measure.

The argument for this extension can be sketched as follows. The proposition allows one to show that there is a unique isometric linear map

$$\Theta : L^2(\widehat{\mathbb{R}^d}, \widehat{\gamma}) \longrightarrow L^2(\mathbb{X}, \mu),$$

mapping $\widehat{\varphi}$ to N_φ for any $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$; compare [**19**, **35**, **36**]. This map is not only isometric, but also intertwines the translation action by $t \in \mathbb{R}^d$ with the multiplication by $e^{it(\cdot)}$ (as can easily be seen for $\varphi \in C_{\mathsf{c}}(\mathbb{R}^d)$ and then follows by approximation in the general case). Consider now $g := \Theta(\sqrt{h})$, where $\sqrt{h}$ is an L^2-function, and the associated spectral measure σ_g. Its (inverse) Fourier transform is then given as $t \mapsto \langle g \mid T_t g\rangle$. Now, a short calculation invoking the properties of Θ shows that

$$\langle g \mid T_t g\rangle = \langle \Theta(\sqrt{h}) \mid \Theta(e^{it(\cdot)}\sqrt{h})\rangle = \int_{\widehat{\mathbb{R}^d}} e^{itk} h(k)\, d\widehat{\gamma}(k).$$

Consequently, the (inverse) Fourier transform of σ_g equals that of $h\widehat{\gamma}$, and the desired statement follows.

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Returning to the general setting, we can describe the *main idea* behind our subsequent reasoning as follows. Proposition 12 implies that the diffraction controls the dynamical spectral theory of the subspace $\mathcal{U}^{\mathbb{X}}$. Whenever $(\mathbb{Y}, \beta)$ is a TMDS factor of $(\mathbb{X}, \alpha)$ (by which we mean a factor which is also a TMDS), the diffraction of $\mathbb{Y}$ will control the dynamical spectral theory of the subspace $\mathcal{U}^{\mathbb{Y}}$ of the factor. Via the factor map, this means that the diffraction of $\mathbb{Y}$ actually controls the dynamical spectral theory of the subspace $i^{\Phi}(\mathcal{U}^{\mathbb{Y}})$ of the original dynamical system. If there are sufficiently many factors, their diffraction will control the complete dynamical spectral theory. Here, the concept of 'control the dynamical spectrum' is made precise in the above definition of a complete spectral invariant. The concept of 'sufficiently many' factors is given a precise meaning as follows.

Definition 3. Let $(\mathbb{X}, \alpha)$ be a TMDS with invariant probability measure μ. Let $(\mathbb{Y}_\iota, \beta_\iota)$ with $\iota \in J$ be a family of TMDS factors with factor maps Φ_ι and induced probability measures $\nu_\iota := (\Phi_\iota)_*(\mu)$. Then, this family is said to be *total* if the linear hull of the spaces $i^{\Phi_\iota}(\mathcal{U}^{\mathbb{Y}_\iota})$, with $\iota \in J$, is dense in $L^2(\mathbb{X}, \mu)$.

The main result of this section now reads as follows.

THEOREM 13. *Let $(\mathbb{X}, \alpha)$ be a TMDS over G with invariant probability measure μ and corresponding unitary representation T. Let $(\mathbb{Y}_\iota, \alpha)$, with $\iota \in J$, be a total family of TMDS factors equipped with the induced measures $\nu_\iota := (\Phi_\iota)_*(\mu)$ and associated diffraction measures $\widehat{\gamma}_\iota$. Then, the measures $\widehat{\gamma}_\iota$, with $\iota \in J$, constitute a complete spectral invariant of T.*

Proof. We have to show that $E_T(A) = 0$ holds for a Borel set $A \subset \widehat{G}$ if and only if $\widehat{\gamma}_\iota(A) = 0$ holds for all $\iota \in J$. For a Borel set $A \subset \widehat{G}$ and a function $\varphi \in C_{\mathsf{c}}(G)$, a short calculation gives

$$\int_{\widehat{G}} |\widehat{\varphi}|^2 1_A \, d\widehat{\gamma}_\iota = \int_{\widehat{G}} 1_A \, d\sigma^{\mathbb{Y}_\iota}_{N_\varphi^{\mathbb{Y}_\iota}} = \int_{\widehat{G}} 1_A \, d\sigma^{\mathbb{X}}_{i^{\Phi_\iota}(N_\varphi^{\mathbb{Y}_\iota})} = \langle i^{\Phi_\iota}(N_\varphi^{\mathbb{Y}_\iota}) \mid E_T(A) i^{\Phi_\iota}(N_\varphi^{\mathbb{Y}_\iota}) \rangle .$$

Here, 1_A denotes the characteristic function of A. The first equality is a consequence of Proposition 12, applied to the TMDS $(\mathbb{Y}_\iota, \alpha)$. The second follows from Theorem 11, and the last from the definition of the spectral measure.

Now, by standard reasoning, $\widehat{\gamma}_\iota(A) = 0$ if and only if $\int_{\widehat{G}} |\widehat{\varphi}|^2 1_A \, d\widehat{\gamma} = 0$ for all $\varphi \in C_{\mathsf{c}}(G)$. Also, by our assumption of totality, $E_T(A) = 0$ holds if and only if $\langle i^{\Phi_\iota}(N_\varphi^{\mathbb{Y}_\iota}) \mid E_T(A) i^{\Phi_\iota}(N_\varphi^{\mathbb{Y}_\iota}) \rangle = 0$ for all $\varphi \in C_{\mathsf{c}}(G)$ and $\iota \in J$. This easily gives the desired equivalence. □

We finish this section by briefly indicating how the discussion of Delone dynamical systems from §4 fits into the present context (and is, in fact, contained in it). For simplicity, and as this is the case in the previous section, we restrict our attention to $G = \mathbb{R}^d$ (even though all considerations work in the general case as well). First of all, let us note that via the map

$$\delta : \{\text{FLC sets in } G\} \longrightarrow \{\text{translation bounded measure on } G\}, \quad \varLambda \mapsto \delta_\varLambda = \sum_{x \in \varLambda} \delta_x ,$$

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any FLC set can actually be considered as a translation bounded measure. In particular, any Delone dynamical system can be considered as a TMDS, and the theory developed in this section applies.

Let $\varLambda$ now be an FLC Delone set and $(\mathbb{X}, \alpha)$ the associated dynamical system. Then, any K-cluster P of $\varLambda$ gives rise to a factor

$$\mathbb{Y} = \mathbb{Y}_{K,P} := \{T_{K,P}(\varLambda') \mid \varLambda' \in \mathbb{X}(\varLambda)\},$$

compare equation (8), with the factor map

$$\varPhi = \varPhi_{K,P} : \mathbb{X} \longrightarrow \mathbb{Y}, \quad X \mapsto T_{K,P}(X).$$

This factor will be called the factor *derived from* $(\mathbb{X}, \alpha)$ *via the* K*-cluster* P *of* $\varLambda$. In the uniquely ergodic case, the autocorrelation $\gamma_{K,P}$ and the diffraction $\widehat{\gamma_{K,P}}$ of the factor $\mathbb{Y}_{K,P}$ have been calculated in §4, see equation (15), under the name of γ_ω and $\widehat{\gamma_\omega}$, respectively.

The N-function associated to this factor is given by

$$N = N^{K,P} : C_{\mathsf{c}}(G) \longrightarrow C(\mathbb{Y}), \quad N_\varphi(\varGamma) = \sum_{x \in \varGamma} \varphi(-x).$$

Thus, the function $N^{K,P} \circ \varPhi_{K,P}$ is given by the formula

$$N^{K,P} \circ \varPhi_{K,P}(X) = \sum_{x \in T_{K,P}(X)} \varphi(-x)$$

Note that $N^{K,P} \circ \varPhi_{K,P} = \chi^{(\varphi)}_{K,P}$ with $\chi^{(\varphi)}_{K,P}$ as considered above in equation (10). Proposition 6 then gives the following result, where we need not assume ergodicity.

PROPOSITION 14. *Let* $\varLambda \subset \mathbb{R}^d$ *be an FLC Delone set and* $(\mathbb{X}, \alpha)$ *the associated dynamical system, with* $\alpha_t X = t + X$*, and assume that an invariant measure* μ *is given. Let* J *be the set of all pairs* (K, P) *so that* K *is compact and* P *is a* K*-cluster of* $\varLambda$*. Then, for any* $\iota \in J$*, the factor* $(\mathbb{Y}_\iota, \alpha)$ *inherits a canonical measure* μ_ι *that is induced by* μ*, and the family of all such factors is total for* $(\mathbb{X}, \alpha, \mu)$.

Note that the result depends on the correct choice of the measures μ_ι on the factors, which enter the autocorrelations via the formula from equation (17). As a consequence of Proposition 14 and Theorem 13, we can now generalize the main result of §4 as follows.

THEOREM 15. *Let* $\varLambda \subset \mathbb{R}^d$ *be an FLC Delone set and* $(\mathbb{X}, \alpha)$ *the associated dynamical system, equipped with an invariant probability measure* μ*. Let* J *be the set of all pairs* (K, P) *such that* $K \subset \mathbb{R}^d$ *is compact and* P *is a* K*-cluster of* $\varLambda$*. Then, for any* $\iota \in J$*, the derived factor* $(\mathbb{Y}_\iota, \alpha)$ *inherits a canonical probability measure* μ_ι *that is induced by* μ*, and the family of diffraction measures* $\widehat{\gamma_\iota}$*, with* $\iota \in J$*, is a complete spectral invariant for* $(\mathbb{X}, \alpha)$.

If the original system in Theorem 15 is uniquely ergodic, then so are its factors. Thus, any of the factors carries a canonical invariant probability measure that gives rise to an autocorrelation and hence to a diffraction measure. Thus, we obtain the following corollary, which recovers the main result of §4.

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COROLLARY 16. *Let $\Lambda \subset \mathbb{R}^d$ be an FLC Delone set and $(\mathbb{X}, \alpha)$ the associated dynamical system, which we assume to be uniquely ergodic. Let J be the set of all pairs (K, P) such that K is compact and P is a K-cluster of Λ. Then, the family of diffraction measures $\widehat{\gamma_\iota}$, with $\iota \in J$, is a complete spectral invariant for $(\mathbb{X}, \alpha)$.*

In the situation of Corollary 16, it does not matter whether one uses the diffraction measure of an element of $\mathbb{X}$ (as we did in §4) or that of the dynamical system (which is our main focus in this section).

It is also possible to embed the situation of §3 into the abstract setting. Indeed, any symbolic sequence gives rise to a weighted Dirac comb on $\mathbb{Z}$, where the weights are chosen according to the corresponding symbol in the sequence. The analogous comment applies to subshifts under the action of $\mathbb{Z}^d$. Since the connection between the spectral and the diffraction measures is more concrete in this case, the approach described in §3 is ultimately more useful here.

Remark 8. In the situation of Theorem 15, we can actually choose a countable index set for J. More precisely, it suffices to consider compact sets which are balls around the origin whose radius is an integer number. For each such ball, there are then only finitely many clusters, due to the FLC assumption. In some favourable cases, the set J can be reduced even further, as briefly discussed in §4.

Remark 9. In the case of symbolic dynamics, compare Remark 3, one can actually restrict oneself to considering topological conjugacies rather than (more general) factors. At this point, we do not know whether one can also derive such a stronger statement in more general FLC situations. Moreover, even in the case of symbolic dynamics, examples show that these conjugacies can be more complicated than the factors needed to obtain the full dynamical spectrum. Therefore, in practice, our theorems about the collection of factors being sufficient to obtain the full dynamical spectrum may be the more viable way to proceed.

While the main thrust of our work is certainly the situation where the diffraction is not pure point, some new insights may also be gained from our considerations in the pure point situation. This is briefly discussed in the Appendix.

In many explicitly treated examples, it turned out that very few factors (often just one, in fact) were needed to explore the maximal spectral measure, which is then an interesting alternative to Fraczek's theorem from [**25**]. It is thus an obvious question to search for good sufficient criteria to assess the totality of a family of factors.

Our general result of Theorem 15 neither depends on ergodicity nor on the FLC property. Nevertheless, it remains to be analysed how it can concretely be used in the further understanding of such more general dynamical systems.

A. *Appendix. A brief look at pure point diffraction in the light of factors*

As is well known (compare our discussion in the introduction), pure point diffraction is equivalent to pure point dynamical spectrum. One key result of [**11**] gives the following precise formulation for the case $G = \mathbb{R}^d$ as follows.

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PROPOSITION A1. *Let* $(\mathbb{X}, \mathbb{R}^d, \mu)$ *be a TMDS with diffraction measure* $\widehat{\gamma}$. *Then,* $\widehat{\gamma}$ *is a pure point measure if and only if* $(\mathbb{X}, \mathbb{R}^d, \mu)$ *has pure point dynamical spectrum. In this case, the group of eigenvalues of* $(\mathbb{X}, \mathbb{R}^d, \mu)$ *is the subgroup of* $\mathbb{R}^d$ *that is generated by the Fourier–Bohr spectrum of the autocorrelation, as defined in equation (2).*

This result shows that the spectrum of the dynamical system is completely determined by the set of pure points or 'atoms' of the diffraction (the Fourier–Bohr spectrum) if one has pure point diffraction. This does not mean, however, that the diffraction measure is a complete spectral invariant. More precisely, it can happen that there are eigenvalues of the system which do not appear in the Fourier–Bohr spectrum (although our results show that they must appear in the Fourier–Bohr spectrum of suitable factors). Such points are known as *extinctions*; compare [**10**, **35**]. However, even in the presence of extinctions, it is still possible to construct a spectral invariant out of the diffraction $\widehat{\gamma}$ as follows. Choose a strictly positive Schwartz function h on $\mathbb{R}^d$ such that

$$\nu_h := h\widehat{\gamma}$$

is a probability measure on $\mathbb{R}^d$. Such a choice is always possible, as $\widehat{\gamma}$ is a translation bounded measure by general principles [**10**, **15**]. We note in passing that ν_h is a spectral measure of $(\mathbb{X}, \mathbb{R}^d, \mu)$ by Remark 7. Consider now the n-fold convolution

$$\nu_h^{*n} := \nu_h * \cdots * \nu_h$$

of ν_h with itself for any natural number n, where $\nu_h^{*1} = \nu_h$. Then, Theorem 15 together with some basic facts on convolutions shows that the family $\{\nu_h^{*n}\}_{n\in\mathbb{N}}$ is a complete spectral invariant.

In some cases, it is known that there exists a natural number N such that any eigenvalue can be expressed as a sum of no more than N elements of the Fourier–Bohr spectrum; see [**35**] for a detailed discussion of this phenomenon. In this case, when 0 is an element of the Fourier–Bohr spectrum (which is always true for the autocorrelation of the standard Dirac comb of a Delone set), ν_h^{*N} alone forms a complete spectral invariant.

For a TMDS that is based on an FLC Delone set, one can obtain further information on the extinctions. Our above results, and Theorem 15 in particular, show that the diffraction measures of all derived factors (all being FLC point sets here) form a complete spectral invariant. We may conclude that, for any extinction point of the original system, there is an FLC point set factor which covers this extinction via its Fourier–Bohr spectrum. This is interesting for pure point diffractive Delone sets that are known to possess no non-trivial Delone factors (up to topological conjugacy), except (possibly) periodic ones [**17**]. In such a situation, all extinctions are related to periodic factors (if any exists at all) or to topologically conjugate point sets. Here, one has to bear in mind that the Fourier–Bohr spectrum is *not* an invariant of topological conjugacy, while the dynamical spectrum clearly is.

An interesting example is provided by the silver mean point set Λ in its formulation as a regular model set; compare [**12**] as well as [**10**, §9.3]. It gives rise to a uniquely ergodic dynamical system. When the elementary distances are 1 (short) and $\lambda = 1 + \sqrt{2}$ (long), the diffraction measure of the canonical Dirac comb with point masses of weight one on

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every point of $\varLambda$ reads

$$\widehat{\gamma_{\varLambda}} = \sum_{k \in L^{\circledast}} I_{\varLambda}(k)\delta_k,$$

where the Fourier module $L^{\circledast} = \frac{\sqrt{2}}{4}\mathbb{Z}[\sqrt{2}]$ coincides with the dynamical spectrum (which is pure point in this case), while the extinction set is

$$S_{\mathrm{ext}} = \{k \in L^{\circledast} \mid I_{\varLambda}(k) = 0\} = \{k \in L^{\circledast} \mid k^{\star} = m/\sqrt{2} \text{ for some } 0 \neq k \in \mathbb{Z}\}, \tag{A1}$$

see [**10**, Remark 9.10] for the details. Clearly, the Fourier module satisfies $\lambda L^{\circledast} = L^{\circledast}$.

Now, keeping all points from $\varLambda$ at the beginning of a long interval (and deleting the others) defines a derived factor, as this map works for the continuous hulls and commutes with translation. The resulting point sets are silver mean chains on a larger scale, obtained from the original one by multiplication with λ, which simply reflects the local inflation symmetry of this aperiodic example. Consequently, the factor is actually locally equivalent (MLD; see [**10**] for details) and thus topologically conjugate. Interestingly, since we have

$$I_{\lambda\varLambda}(k) = I_{\varLambda}(\lambda k),$$

the new intensities are non-zero on all points of the original set S_{ext} from equation (A1), while the extinctions are now located at the set S_{ext}/λ, which had no extinctions for the original diffraction measure. So, the two diffraction measures constitute a complete spectral invariant in this case.

Alternatively, one may view the previous example as a weighted model set, with different weights for points at the beginning of short or long intervals. A generic choice of these weights will lead to a diffraction measure without any extinctions on $L^{\circledast}$, which is then a complete spectral invariant.

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