Crystals with their regular shape and pronounced faceting have fascinated humans for ages. About a century ago, the understanding of the internal structure increased considerably through the work of Max von Laue (Nobel prize in physics 1914) and William Henry Bragg and William Lawrence Bragg (father and son, joint Nobel prize in physics 1915). They developed X-ray crystallography and used it to show that a lattice-periodic array of atoms lies at the heart of the matter. This interpretation became the accepted model for solids with pure Bragg diffraction, which was later extended to allow for incommensurately modulated structures.

In 1982, the materials scientist Dan Shechtman discovered a perfectly diffractive solid with a non-crystallographic (icosahedral) symmetry [18]; see Figure 1 for a qualitatively similar experimental diffraction image. This discovery, for which he received the 2011 Nobel prize in chemistry, was initially met with disbelief and heavy criticism, although such structures could have been expected on the basis of Harald Bohr’s work on almost periodic functions. In fact, the situation is a classic case of a ‘missed opportunity’. Let us try to illustrate this a little further and thus explain some facets of what is now known as the theory of aperiodic order.

Let us consider a uniformly discrete point set $\Lambda$ in Euclidean space, where the points are viewed as idealizations of atomic positions (all assumed to be of one type for simplicity). Much of the terminology for such point sets was developed by Jeffrey C. Lagarias [9]. Placing unit point measures at each position in $\Lambda$ leads to the associated Dirac comb

$$\delta_\Lambda = \sum_{x \in \Lambda} \delta_x.$$  

A diffraction experiment measures the correlation between atomic locations. Mathematically, this is expressed through the diffraction measure, which is the
Fourier transform \( \hat{\gamma}_\Lambda \) of the autocorrelation

\[
\gamma_\Lambda = \lim_{R \to \infty} \frac{\delta_{\Lambda \cap B_R} * \delta_{-\Lambda \cap B_R}}{\text{vol}(B_R)},
\]

provided that this limit exists in the vague topology; see Hof’s contribution to [12] or [1] for details. Here, \( \hat{\gamma}_\Lambda \) describes the outcome of a (kinematic) diffraction experiment, such as the one sketched in Figure 2 with an optical bench, which should be available in most physics laboratories for experimentation.

For a lattice periodic point set, the diffraction measure is a pure point measure supported on the dual lattice. This implies that a tenfold symmetric diffraction diagram, such as the one of Figure 1, cannot be produced by a lattice periodic structure, as lattices in two or three dimensions can only have two-, three-, four- or sixfold rotational symmetry by the crystallographic restriction. This raises the question what types of point sets can generate such new kinds of diffraction measures, which are pure point and display non-crystallographic symmetries.

Let us begin with an example. Already in 1974, Roger Penrose constructed an aperiodic tiling of the entire plane, equivalent to the one shown in Figure 3. Taking this finite patch and considering the set of vertices as the point set \( \Lambda \), the diffraction measure is the one shown in Figure 4, which resembles what Alan L. Mackay observed when he performed an optical diffraction experiment with an assembly of small disks centered at the vertex points of a rhombic Penrose tiling, shortly before the discovery of quasicrystals [10]. For an infinite tiling, the diffraction measure is pure point and tenfold symmetric.

The Penrose tiling is a particularly prominent example of a large class of point sets, for which it has been shown that the diffraction measure exists and is pure point. Such sets, which were first introduced by Yves Meyer [11] and are nowadays called model sets, are constructed from a cut and project scheme (CPS)

\[
\begin{align*}
\mathbb{R}^d & \overset{\pi}{\leftarrow} \mathbb{R}^d \times H & \overset{\pi_{\text{int}}}{\longrightarrow} & H \\
\cup & \cup & \cup & \text{dense} \\
\pi (\mathcal{L}) & \overset{1-1}{\leftarrow} \mathcal{L} & \longrightarrow & \pi_{\text{int}} (\mathcal{L}) \\
\| & \| & \| \\
L & \overset{*}{\longrightarrow} & L^*
\end{align*}
\]

where \( \mathcal{L} \) is a lattice in \( \mathbb{R}^d \times H \) whose projection \( \pi_{\text{int}} (\mathcal{L}) \) to ‘internal space’ \( H \) is dense. The projection \( \pi \) to ‘physical space’ \( \mathbb{R}^d \) is required to be injective on \( \mathcal{L} \), so that \( \pi \) is...
a bijection between $L$ and $L = \pi(\mathcal{L})$. The CPS thus provides a well-defined mapping $\star : L \to H$ with $x \mapsto x^\star = \pi_{\text{int}}((\pi|_{\mathcal{L}})^{-1}(x))$. The internal space $H$ is often a Euclidean space, but the general theory works for locally compact Abelian groups. A model set is then obtained by choosing a ‘window’ $W \subset H$ and defining the point set

$$\Lambda = \{ x \in L | x^\star \in W \} \subset \mathbb{R}^d.$$ 

The Penrose point set arises in this framework with a two-dimensional Euclidean internal space and the root lattice $A_4$, while the generalisation to model sets with icosahedral symmetry was first discussed by Peter Kramer [8]. It was Robert V. Moody [13, 12] who recognized the connections to Meyer’s abstract concepts and championed their application in the theory of aperiodic order and their further development into the shape and form used today.

For a non-empty, compact window that is the closure of its interior and whose boundary has Haar measure 0, the resulting model set has a diffraction measure that is supported on the projection $\pi(\mathcal{L}^*)$ of the dual lattice, and hence is a pure point measure; see Schlottmann’s article in [3] for a proof. The diffraction intensities can be calculated explicitly in this setting.

While a pure point diffraction detects order, it is not true that all ordered structures have pure point diffraction. A simple example can be generated by the Thue–Morse substitution $0 \mapsto 01, 1 \mapsto 10$, via taking a bi-infinite sequence that is invariant under the square of this rule

$$\ldots01101011000101100110010110\ldots$$

and taking only those $x \in \mathbb{Z}$ that correspond to the positions of 1s in the sequence. The diffraction measure of this one-dimensional point set is not pure point, as it contains a non-trivial singular continuous component.

There is a very useful connection between the diffraction measure and the spectral measures of an associated dynamical system. Starting from a point set $\Lambda \subset \mathbb{R}^d$ of finite local complexity (which means that, up to translations, there are only finitely many patches for any given size), we define its hull

$$X(\Lambda) = \{ x + \Lambda | x \in \mathbb{R}^d \}$$

where the closure is taken in the local topology (closeness forces coincidence on a large ball around the origin up to a small translation). $\mathbb{R}^d$ acts on $X(\Lambda)$ by translations. Assume that there is an invariant probability measure $\mu$. This induces an action of $\mathbb{R}^d$ on $L^2(X, \mu)$ via unitary operators. It is a fundamental result that the diffraction measure is pure point if and only if all spectral measures are pure point.

More generally, the spectral measures correspond to diffraction measures associated with elements of certain topological factors of the dynamical system $(X, \mathbb{R}^d, \mu)$ [2]. For example, the diffraction measure of the Thue–Morse point set consists of the pure point part $\delta_\mathbb{Z}$ and a non-trivial singular continuous component. The non-trivial point part of the dynamical spectrum, which is $\mathbb{Z}[\frac{1}{2}]$, is therefore not fully detected by the diffraction measure.
of the Thue–Morse point set, and only shows up in the
diffraction measure of a global 2-to-1 factor, which is a
model set, with $H = \mathbb{Z}_2$, the 2-adic numbers.

While the relation between dynamical and diffraction
spectra is by now well understood, it continues to be
an intriguing open problem to find the connection be-
tween these spectra and the spectra of Schrödinger oper-
ators associated with aperiodic structures. The interest
in the latter arises from quantum transport questions in
aperiodically ordered solids; see the article by Damanik,
Embree and Gorodetski in [8] for a survey. In particu-
lar, anomalous transport properties have for a long time
been expected (and are observed in experiments), and
could recently be rigorously confirmed in simple one-
dimensional models. Concretely, on the Hilbert space
$\ell_2(\mathbb{Z})$, let us consider the Fibonacci Hamiltonian

$$ (H\psi)_n = \psi_{n-1} + \psi_{n+1} + \lambda v_n \psi_n $$

with potential $v_n = \chi_{[1-\alpha,1)}(n\alpha \mod 1)$ (with constant
$\alpha = (\sqrt{5} - 1)/2$, the inverse of the golden ratio), which
alternatively could be generated by the Fibonacci sub-
stitution $0 \mapsto 1$, $1 \mapsto 10$. For $\lambda > 8$, quantum states
display anomalous transport in the sense that they do
not move ballistically or diffusively, nor do they remain
localized [6]. All spectral measures associated with $H$
are purely singular continuous, while diffraction and dy-
namical spectrum are pure point in this case.

Quantitative results about the local and global Haus-
dorff dimension of the spectrum and the density of states
measure are now available for all values of the coupling
constant $\lambda$. On the other hand, similar results are cur-
rently entirely out of reach for Schrödinger operators as-
associated with the Penrose tiling. However, there is re-
cent progress for higher-dimensional models obtained as
a Cartesian product of Fibonacci Hamiltonians; see Fig-
ure 5 for an illustration, in particular (of proven proper-
ties of the spectrum) for two dimensions, and [9] as well
as the article by Damanik, Embree and Gorodetski in [8]
for details and further references.

What we have sketched here is just one snapshot of
a field with many facets and new developments, as ev-

Figure 5: Numerical approximation of the spectrum of
the Fibonacci Hamiltonian (top) and the 2D model ob-
tained as the Cartesian product of two 1D Fibonacci
Hamiltonians (bottom). The $x$-axis corresponds to the
energy $E$, while the $y$-axis corresponds to the coupling
constant $\lambda$. The plots illustrate the instant opening of
a dense set of gaps for the 1D model as the potential is
turned on, whereas for the 2D model there are no gaps in
the spectrum for all sufficiently small $\lambda$. Images courtesy
of Mark Embree.

It is a somewhat surprising insight that the diffraction
measure, which is designed to reveal as much as possible
about the distributions of points and is thus clearly not
invariant under topological conjugacy, and the dynamical
spectrum, which is an important invariant under met-
cric conjugation of dynamical systems and thus blind to
details of the representative chosen, have such an import-
ant ‘overlap’. Consequently, one can translate various
results from either point of view to the other, and profit
from this connection.

While the relation between dynamical and diffraction
spectra is by now well understood, it continues to be
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What we have sketched here is just one snapshot of
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idenced by the contributions to \[12, 3, 15, 7\]. Connections exist with many branches of mathematics, including discrete geometry \[4\], topology \[17\] and ergodic theory \[16, 19\], to name but a few. Aperiodic order thus provides a versatile platform for cooperations and proves the point that mathematics is a unit, and not a collection of disjoint disciplines.

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