WHAT IS...

Aperiodic Order?

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With their regular shape and pronounced faceting, crystals 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 became the accepted model for solids with pure point diffraction, which was later extended in various ways.

In 1982, the materials scientist Dan Shechtman discovered a perfectly diffractive solid with a noncrystallographic (icosahedral) symmetry; 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 Λ in Euclidean space, where the points are viewed as idealizations of atomic positions. Much of the terminology for such point sets was developed by Jeffrey C. Lagarias. Placing unit point measures at each position in Λ leads to the associated Dirac comb

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

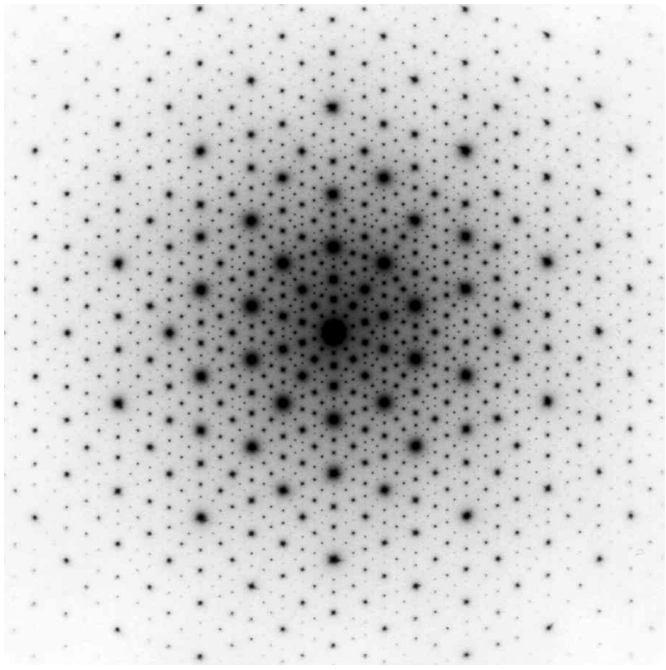

Image courtesy of Conradin Beeli.

Figure 1. Dan Shechtman received the 2011 Nobel Prize in Chemistry for his discovery of "impossible" symmetries, such as the tenfold symmetry in this electron diffraction image of an AlMnPd alloy (intensity inverted).

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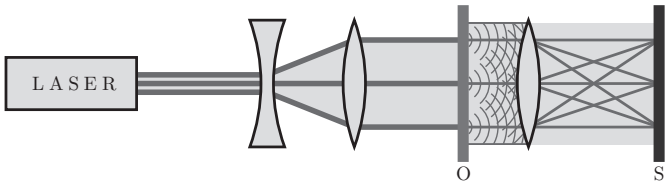

Figure 2. Schematic representation of an optical diffraction experiment. The object (O) is illuminated by a coherent light source, and the diffracted intensity is collected on a screen (S), with sharp intensity peaks arising from constructive interference of scattered waves.

A diffraction experiment measures the correlation between atomic locations. Mathematically, this is expressed through the diffraction measure, which is the Fourier transform $\widehat{\gamma_\Lambda}$ of the autocorrelation

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

provided this limit exists in the vague topology, in which a sequence of measures $\{\mu_n\}$ converges to μ if and only if $\mu_n(f) \to \mu(f)$ for all continuous functions f with compact support. This approach goes back to Hof (1995). Here, $\widehat{\gamma_\Lambda}$ describes the outcome of a (kinematic) diffraction experiment, such as that of Figure 2 with an optical bench, which should be available in most physics labs for experimentation.

For a lattice periodic point set, the diffraction measure is supported on a discrete point set, namely, 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 of what types of point sets can generate such new kinds of diffraction measures, which are pure point but display noncrystallographic 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 Λ, 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. 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 with pure point diffraction. Such sets, which were first introduced by Yves Meyer and are nowadays called model sets, are constructed from a

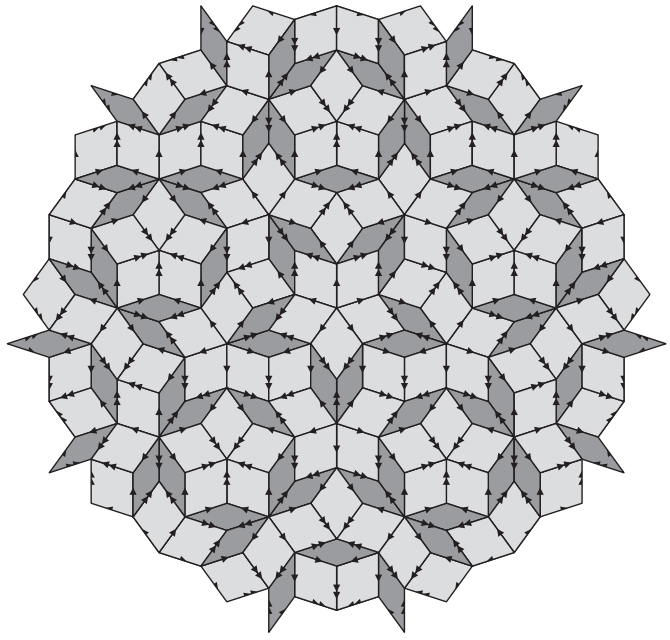

Figure 3. Fivefold symmetric patch of the rhombic Penrose tiling, which is equivalent to many other versions. The arrow markings represent local rules that enforce aperiodicity.

cut and project scheme (CPS)

$$\begin{array}{ccccc}
\mathbb{R}^d & \xleftarrow{\ \pi\ } & \mathbb{R}^d \times H & \xrightarrow{\ \pi_{\mathrm{int}}\ } & H \\
\cup & & \cup & & \cup \ \text{dense} \\
\pi(\mathcal{L}) & \xleftarrow{\ 1-1\ } & \mathcal{L} & \longrightarrow & \pi_{\mathrm{int}}(\mathcal{L}) \\
\| & & & & \| \\
L & & \xrightarrow{\qquad\star\qquad} & & L^\star
\end{array}$$

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

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

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 in 1984. It was Robert V. Moody who recognized the connections to Meyer's abstract concepts and championed their application in the theory of aperiodic order and their further development.

For a nonempty, 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

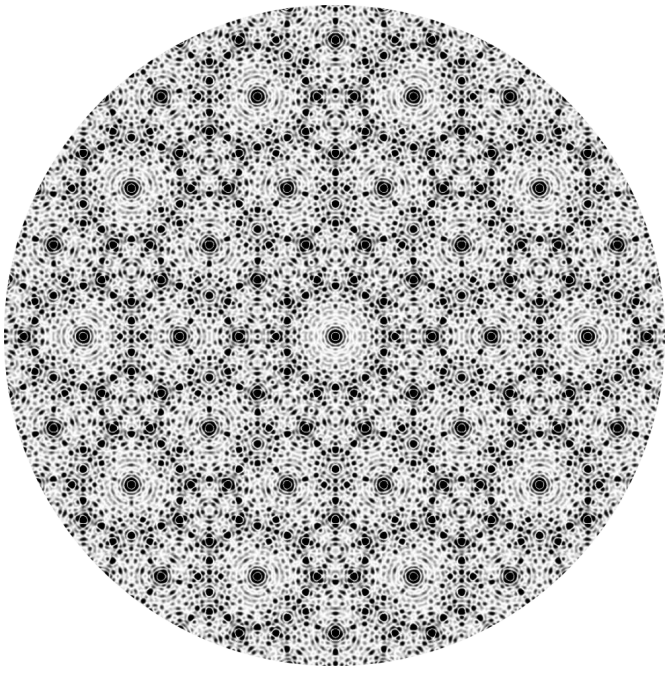

Figure 4. Central part of the (intensity inverted) diffraction image of the patch of Figure 3, with point measures placed on all vertex points of the rhombic tiling.

hence is a pure point measure. 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. As an example, consider the bi-infinite sequence

$$\dots 01101001100101\,10|01101001100101\,10\dots$$

and notice that it is invariant under the square of the Thue–Morse substitution $0 \mapsto 01$, $1 \mapsto 10$. Now, take only those $x \in \mathbb{Z}$ that correspond to the positions of 1s in this sequence. The diffraction measure of this one-dimensional point set is not pure point, as it contains a nontrivial 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 $\varLambda \subset \mathbb{R}^d$ of finite local complexity (which means that, up to translations, there are only finitely many patches for any given size), we define its hull

$$\mathbb{X}(\varLambda) \;=\; \overline{\{x+\varLambda \mid x \in \mathbb{R}^d\}}$$

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 $\mathbb{X}(\varLambda)$ by translations. Select an invariant probability measure μ, which is always possible. Then, one gets an action of $\mathbb{R}^d$ on $L^2(\mathbb{X},\mu)$ 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 $(\mathbb{X},\mathbb{R}^d,\mu)$.

For example, the diffraction measure of the Thue–Morse point set consists of the pure point part $\delta_{\mathbb{Z}}$ and a nontrivial singular continuous component. The nontrivial 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 shows up only 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.

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 metric conjugation of dynamical systems and thus blind to details of the representative chosen, have such an important

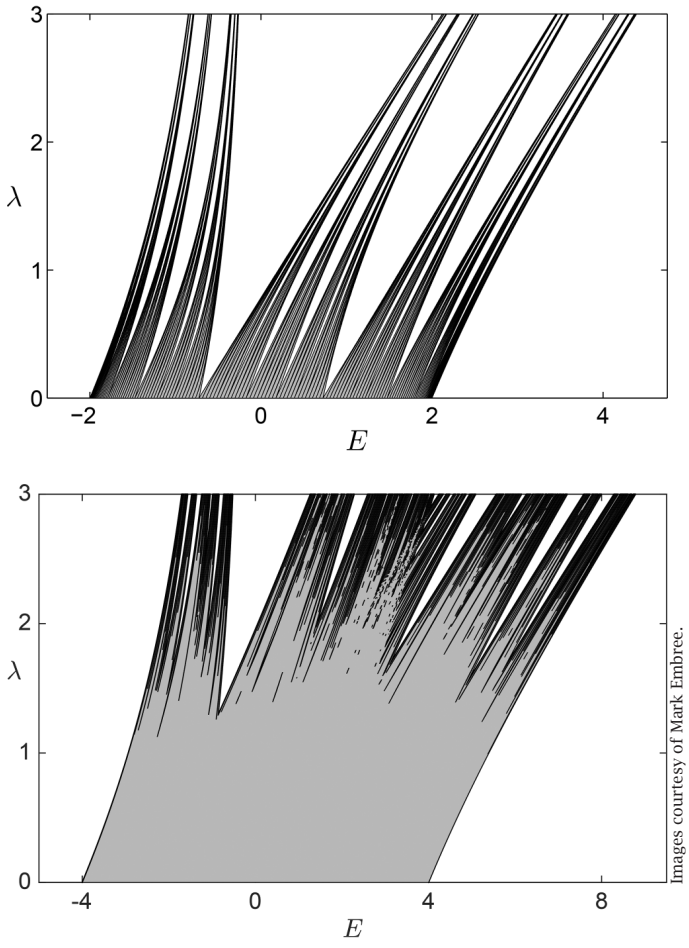

Figure 5. Numerical approximation of the spectrum of the 1D Fibonacci Hamiltonian (top) and of the Cartesian product of two of them (bottom). The x-axis corresponds to the energy E, and the y-axis to λ. The plots illustrate the instant opening of a dense set of gaps for the 1D model as λ is turned on, whereas for the 2D model there are no gaps in the spectrum for all sufficiently small λ.

"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 an intriguing open problem to find the connection between these spectra and the spectra of Schrödinger operators associated with aperiodic structures. The interest in the latter arises from quantum transport questions in aperiodically ordered solids. In particular, 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 $\ell^2(\mathbb{Z})$, let us consider the bounded self-adjoint operator, known as the Fibonacci Hamiltonian,

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

with potential $v_n = \chi_{[1-\alpha,1)}(n\alpha \bmod 1)$ (with constant $\alpha = (\sqrt{5}-1)/2$), which alternatively could be generated by the Fibonacci substitution $0 \mapsto 1$, $1 \mapsto 10$. For $\lambda > 8$, quantum states display anomalous transport in the sense that they do not move ballistically or diffusively, nor do they remain localized.

The spectrum of H, which is

$$\sigma(H) = \{E \mid (H - E\cdot\mathbb{1}) \text{ is not invertible}\},$$

has a dense set of gaps; see Figure 5. All spectral measures associated with H by the spectral theorem are purely singular continuous, while diffraction and dynamical spectrum are pure point in this case. For all values of the coupling constant λ, there are now quantitative results on the local and global Hausdorff dimension of the spectrum and on the density of states measure. On the other hand, similar results are currently entirely out of reach for Schrödinger operators associated with the Penrose tiling. However, there is recent progress for higher-dimensional models obtained as a Cartesian product of Fibonacci Hamiltonians; see Figure 5 for an illustration (of proven properties of the spectrum).

Our above sketch is just one snapshot of a field with many facets and new developments. Connections exist with many branches of mathematics, including discrete geometry, topology, and ergodic theory, to name but a few. Aperiodic order thus provides a versatile platform for cooperation and proves the point that mathematics is a unified whole, not a collection of disjoint subjects.

Further Reading

[1] M. Baake and U. Grimm, *Aperiodic Order. Volume 1: A Mathematical Invitation*, Cambridge University Press, Cambridge, 2013. MR3136260

[2] J. Kellendonk, D. Lenz, and J. Savinien (eds.), *Mathematics of Aperiodic Order*, Birkhäuser, Basel, 2015. MR3380566

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Michael Baake's research interests include aperiodic order, harmonic analysis, dynamical systems and mathematical biology. He likes analogue electronics, photography and cycling, with an active role in building his own gear.

Photo courtesy of The Open University.

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Photo by Antje Damanik.

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