CHAPTER 1

Introduction

In April 1982, while on sabbatical at the National Bureau of Standards in Washington, DC, Dan Shechtman from the Technion at Haifa made a profound discovery, for which he was awarded the Wolf Prize in Physics in 1999 and the Nobel Prize in Chemistry in 2011. When inspecting various samples of a rapidly solidified Al Mn alloy with an electron microscope in diffraction mode, he noticed a phase that showed clear and sharp Bragg reflexes together with a rather perfect icosahedral symmetry, similar to the one shown in Figure 1.1. While a Bragg spectrum is a typical fingerprint of a crystal, fivefold or icosahedral symmetry is incompatible with the latter. He concluded that this phase must possess long-range order (to explain the Bragg reflexes) without being a perfect crystal (to be able to accommodate the unusual symmetry). It took Shechtman two years to convince colleagues until the result was finally published in [SBGC84]. Even after the paper appeared in print, prominent scientists (including Nobel Laureate Linus Pauling) expressed their scepticism, though they found themselves in a rapidly shrinking minority as other phases with similar properties were discovered.

In fact, Ishimasa, Nissen and Fukano [INF85] at the ETH Zürich found twelvefold (or dodecagonal) symmetry in a sample of a Ni Cr alloy before[1] they became aware of Shechtman's discovery, while Bendersky [Ben85] demonstrated the existence of another Al Mn phase with tenfold (or decagonal) symmetry soon after (at this stage, we do not distinguish between fivefold and tenfold symmetry). A little later, Kuo and his coworkers [WCK87] completed the list of presently known non-crystallographic symmetries with the discovery of V Ni Si and Cr Ni Si phases displaying eightfold (or octagonal) symmetry. Structures of this type are nowadays referred to as *quasicrystals*, a term that was coined by Levine and Steinhardt in [LS84]; see [SO87] for a compilation of early publications and [Jar88, JG89, Jan94, SSH02, Tre03] for initial accounts of the theory of quasicrystals.

While no further non-crystallographic symmetries have been observed so far in alloys, many different intermetallic phases with non-crystallographic (in

[1] They announced their result on a poster at the 'Workshop on Physics of Small Particles' in Gwatt (Switzerland) in October 1984.

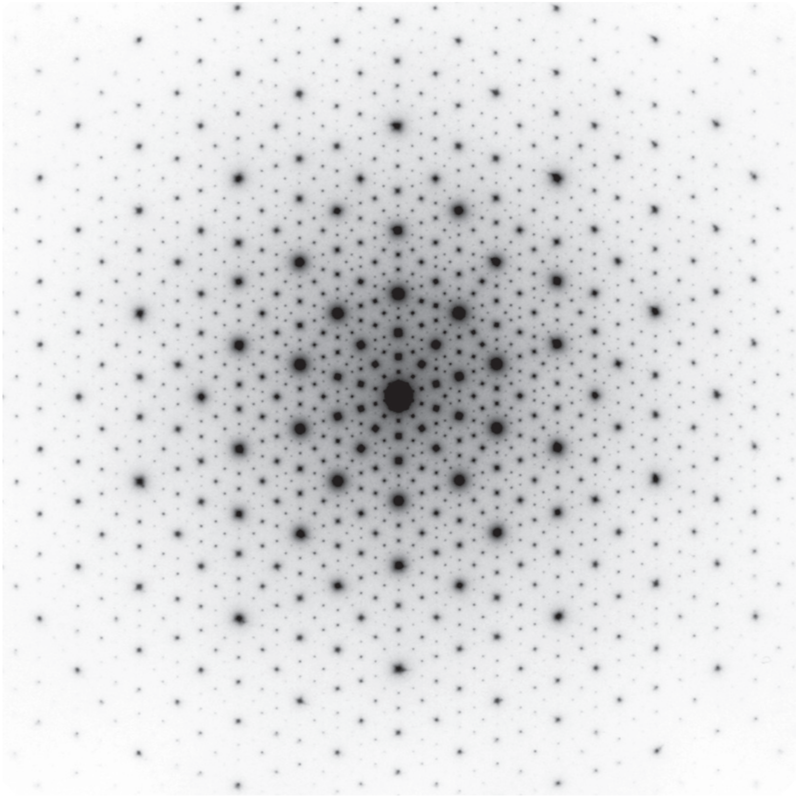


FIGURE 1.1. Electron diffraction pattern of a ternary Al Mn Pd alloy with icosahedral symmetry. Image © Conradin Beeli.

particular, icosahedral or decagonal) symmetry have been identified; for recent surveys, we refer to [Ste04, SD09]. Surprisingly, quasicrystalline phases are not restricted to solids, but can also occur in soft matter; see [LD07] and references therein. By now, various non-crystallographic symmetries (also beyond those mentioned above) have been exploited in engineered structures, such as phononic and photonic quasicrystals [SSW07]. Dodecagonal quasicrystalline phases also form in dense random tetrahedral packings [H-AE+09], which is one aspect of the fascinating question of how to pack tetrahedra [LZ12].

Let us return to the quasicrystals found in solids. The natural question of the atomic structure of these new alloys was disputed from various angles, displaying an entire spectrum of divided opinions. As early as 1982, and independently of the experimental discovery, Peter Kramer from Tübingen constructed a cell model with icosahedral symmetry [Kra82] based on ideas from group theory and projections from cells in higher dimensions. This

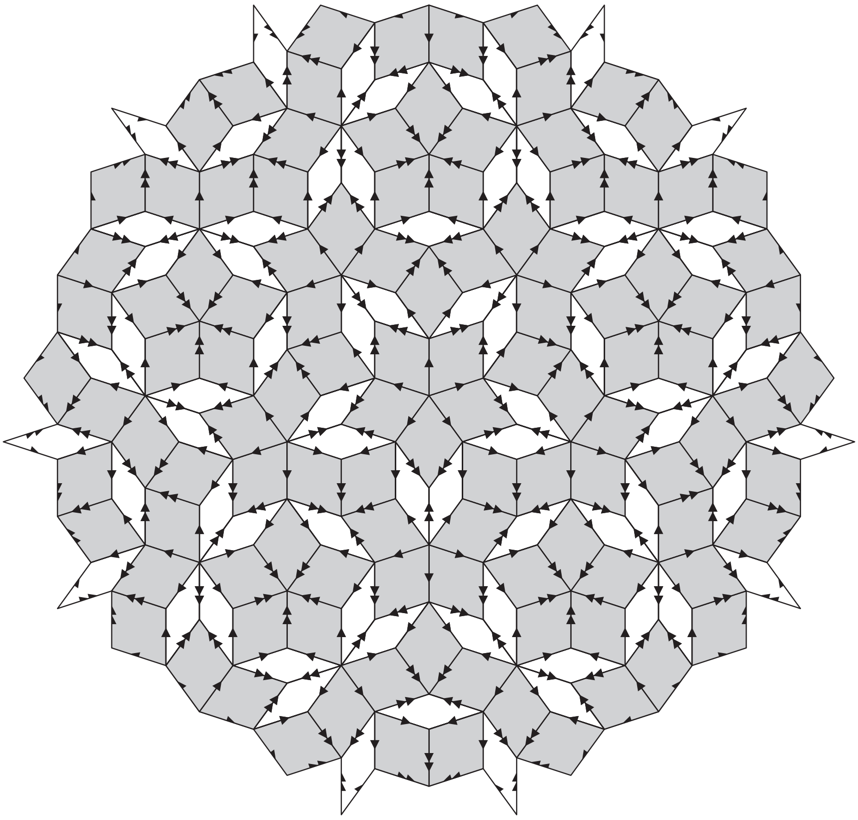


FIGURE 1.2. A fivefold symmetric patch of the rhombic Penrose tiling with edge matching rule decorations by two types of arrows.

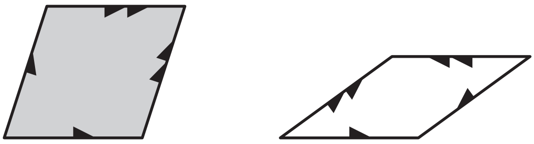
was followed by a projection model from 6-space in 1984, developed jointly with his student Roberto Neri [KN84]. Other groups favoured quasiperiodic density waves [Bak86], thus building on previous work on incommensurate phases [dWo74, JJ77], or random tilings [Els85] (see also [Hen99] and references therein) that explain the notion of order and symmetry in a probabilistic fashion. This situation led to interesting and long-lasting debates, in particular about specific models and tilings, and about the question how to find out what is 'typical'.

In mathematics, various predecessors existed that now found rather unexpected applications. Perhaps best known is the fivefold symmetric planar tiling due to Roger Penrose from Oxford [Pen74], which became popular and widely known through an article by Martin Gardner [Gar77]. Figure 1.2 shows its rhombic version and Figure 1.3 a realisation at Texas A&M University. The tiling is highly ordered, although it has no non-zero period at all.

It was later shown to be compatible with a projection from 5-space and to have a pure Bragg spectrum by de Bruijn [dBr81], thus substantiating an experimental observation made by Alan Mackay [Mac82]. Fivefold symmetry in the plane and icosahedral symmetry in 3-space are of particular importance, both theoretically and in practice. Mathematically, this can be seen as a continuation of the tradition founded by Felix Klein's famous monograph [Kle84]. Icosahedral structures of various kinds continue to attract scientific interest. Recent examples include quasicrystals, fullerenes (or 'buckyballs') and tensegrities; see [CT08] for a catalogue of the latter.

As so often, the Penrose tiling itself had various predecessors, such as the 'Aa' tiling of Johannes Kepler (which indirectly inspired Penrose to find his construction[2]) or old ornaments, particularly in Islamic art [Mak92]. The many attempts show that fivefold symmetry puzzled generations of scientists, yet there is no evidence that any of Penrose's predecessors (including Dürer and Kepler) had a proof for the extensibility of their constructions to infinite tilings of the plane with fivefold symmetry and a certain degree of homogeneity. For a brief historical summary, we refer to [Lüc00], while [Jar89, Sen95, AG95, Moo97, Pat98, BM00b] cover a decent part of the mathematical development.

Let us say a bit more about the rhombic Penrose tiling. A large patch is shown in Figure 6.44 on page 238, which highlights the hierarchy of meandering 'paths' built from thick rhombuses. Each of the two prototiles



occurs in ten distinct orientations. This version includes edge markers which, upon putting tiles together, are supposed to form complete single or double arrows. This condition constitutes a set of local rules with three remarkable properties. The first is that the rules are compatible with at least one (in fact, more than one) gapless, face to face tiling that covers the entire plane. Secondly, they guarantee that none of these tilings has any (non-zero) period. Finally, they also enforce that any two of these tilings are locally indistinguishable. They provide an example of what we will later call a set of perfect aperiodic local rules. There are many other fascinating aspects of the Penrose tiling (such as its self-similarity, which underlies the proof of the claims, and its description as a projection essentially from 4-space), some of which will be explained in this book.

[2]This was mentioned by Roger Penrose during his Kepler lecture at the University of Tübingen, Faculty of Physics, on June 11, 1997; compare the Foreword to this book.

FIGURE 1.3. Roger Penrose and his famous rhombus tiling in the foyer of the Mitchell Institute for Fundamental Physics and Astronomy at Texas A&M University. Photograph by user Solarflare100, available at `http://en.wikipedia.org/wiki/Penrose_tiling` under a Creative Commons Attribution 3.0 Unported License.

To appreciate the role of the symmetry in this matter, let us sketch a simple intuitive argument why a periodic point set in the plane, with minimal distance between distinct points, cannot have fivefold rotational symmetry. To see this, assume to the contrary that there is such a periodic point set with fivefold symmetry, where it is also assumed (for simplicity) that some points are rotation centres. Considering two rotation centres of minimal distance, one can rotate them around each other, as sketched in Figure 1.4. Unlike two-, three-, four- or sixfold symmetry, a fivefold rotation produces point

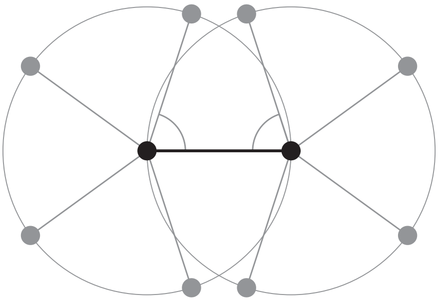


FIGURE 1.4. Sketch of the incompatibility between points of fivefold rotational symmetry at minimal distance (black) and lattice periodicity in the Euclidean plane.

pairs at a smaller distance, thus contradicting the starting assumption (this will be made more precise in Chapters 3 and 5). The same problem occurs for any rotation of order $n \geqslant 7$ in the plane.

Related tilings with other symmetries have also been constructed and studied intensively. Many early examples are due to Robert Ammann [Sen04], in particular examples with aperiodic local rules. A well-known tiling with eightfold symmetry is the octagonal or Ammann–Beenker tiling illustrated in Figure 1.5.

Another predecessor, which went largely unnoticed for a long time, is Yves Meyer's book [Mey72] on the connection between algebraic number theory and harmonic analysis. In fact, it essentially contains the abstract theory of the projection method, in the full generality of locally compact Abelian groups, though this was only systematically revealed by Jeffrey Lagarias [Lag96] and Robert Moody [Moo97a] much later. This can also be considered as an extension of the theory of almost periodic functions, which is largely due to Harald Bohr [Boh47], to the setting of point sets. Nevertheless, the original focus was a different one, and it is a remarkable fact that these abstractly investigated systems turn out to be precisely what is needed to describe the structure of perfect quasicrystals.

By the nature of the subject, a large variety of notions and concepts has been used during its development. Some of them appeared to be mutually incompatible, which resulted in long-lasting disputes between different schools. Thirty years after Shechtman's discovery, it has become apparent that one needs a unified framework to accommodate and reconcile these different viewpoints, and the mathematical theory of *measures* is able to provide just that. This is our main motivation to present an exposition that develops the subject in this direction and ultimately works with measures in a systematic manner.

FIGURE 1.5. A 'real world' tessellation (in Greifswald, Germany) based on the eightfold Ammann–Beenker tiling. Photograph © Stan Sherer.

In order to keep the mathematical machinery adequately elementary, the book effectively consists of two parts. The first comprises Chapters 1–7 and covers the ground up to the cut and project method. We start with a general chapter on mathematical tools, with a focus on discrete geometry and algebraic methods. Chapter 3 covers some standard material from lattice theory, selected for our purpose and presented in a way to facilitate the entrance into the non-periodic world.

Here and below, we face the difficult task of selecting from the vast amount of material. It is thus inevitable that we have to refer to other sources for some of the proofs and further details, or that we sometimes only give a sketch of a proof. For this reason, we use the symbol □ to indicate 'end of proof' as well as 'absence of proof'. However, we have tried to cover some less common or unfamiliar results in a more complete fashion, in order to provide a reference for future work. While the core of the book is designed to be accessible, we sketch more advanced material in additional remarks, which usually include hints on the underlying arguments and further references.

Since one-dimensional structures are significantly easier to grasp, the chapter on lattices is followed by a detailed exposition of symbolic substitution sequences and the corresponding geometric inflation rules. Nevertheless, the reader should be aware that this only offers a glimpse at what is known collectively about such systems, to which we will refer via several standard monographs. Before we extend this to planar and higher-dimensional inflation tilings in Chapter 6, by way of important guiding examples, we develop appropriate and sufficiently general notions of discrete geometry in Chapter 5, which also contains a brief discussion of local rules (more on this topic will follow in the second volume of the book series). The treatment of systems with icosahedral symmetry focuses on the discussion of several important examples. In addition, we provide some useful material on the icosahedral group as an appendix. The geometric point of view is completed with the cut and project method in Chapter 7, which we develop step by step from a one-dimensional example. It is constructed in such a way that the generalisation to higher dimensions (and to the more algebraic setting of Meyer) is largely self-explanatory.

The second part of the book is mainly concerned with spectral properties of periodic and non-periodic systems, as accessible via mathematical diffraction theory. It starts with a selected review of methods from Fourier and harmonic analysis in Chapter 8, which includes a brief summary of quasiperiodic and almost periodic functions. The following substantial chapter on diffraction theory, which expands on two previous reviews [BG11, BG12], covers the general concepts, the treatment of crystallographic systems and that of cut and project sets. Once again, we develop the latter from a paradigmatic example, which reveals a natural path to the generalisations, where we restrict to pure point diffractive systems. Here, we also discuss the concept of homometry, which is important for the corresponding inverse problem.

In Chapter 10, we extend our analysis to (deterministic) systems with mixed spectra. In particular, we include complete treatments of the Thue–Morse and the Rudin–Shapiro system, which are (deterministic) paradigms for purely singular continuous and purely absolutely continuous diffraction. The theory of lattice subsets is then also developed, with a discussion of the set of visible lattice points. All this has an extension to the general setting of Meyer sets, which we briefly outline. As we go along, we keep mentioning the connections to dynamical systems and their spectra, for which we also provide an informal appendix.

Finally, Chapter 11 starts the corresponding development for systems with structural disorder, which means that we enter the territory of probability theory and stochastic processes. In comparison with the previous topics, the understanding of stochastic systems is much less developed, but has steadily been on the increase in recent years. At this stage, we selected systems and examples that mainly require classical tools of probability theory, such as the renewal process, Bernoulli and Markov systems, and employ the strong law of large numbers and some elementary results on Gibbs measures. This is perhaps the area with the largest gap between the physical intuition and results with mathematical rigour. In particular, some of the most obvious questions about random tiling ensembles are still open.

A quintessential summary of our tour through aperiodic order could be as follows. There is a good understanding of systems with perfect crystalline or quasicrystalline order, and a decent one of systems with sufficiently strong disorder. In between, however, we have only reached a limited understanding, although various examples with mixed spectrum have been worked out explicitly. In particular, it is unlikely that the known examples that are covered in this book suffice as a system of stepping stones to bridge this gap. Evidence for this claim is provided by systems such as the pinwheel tiling (which is deterministic, but still rather enigmatic; see Figure 6.58 on page 248 for a 'real world' example) or the non-crystallographic planar random tilings (which are understood heuristically but not rigorously). Further support for the underlying difficulties is given by dynamical systems of algebraic origin (such as Ledrappier's example or the $(\times 2, \times 3)$ system), or the huge class of Meyer sets with entropy, which is largely unexplored.

It is fair to say that a classification of a hierarchy of (aperiodic) order has not only not been achieved yet, but is actually not even in sight. We would be delighted if our mathematical invitation inspires some progress in this direction.