

## Quasicrystals and almost periodic functions

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**Abstract.** We consider analogies between the “cut-and-project” method of constructing quasicrystals and the theory of almost periodic functions. In particular an analytic method of constructing almost periodic functions by means of convolution is presented. A geometric approach to critical points of such functions is also shown and illustrated with examples.

**1. Introduction.** In 1984 D. Shechtman and co-workers published selected electron diffraction patterns of an alloy of aluminium and manganese. What must have seemed rather striking to many physicists was the fact that the patterns showed sharp spots arrayed with icosahedral symmetry. Indeed, it is a long-proved theorem that only one-, two-, three-, four- or sixfold rotation axes are possible in a triply periodic crystal. Although a molecule may certainly have fivefold symmetry, its environment in the crystal cannot since the existence of such an axis is not compatible with the requirements of translational symmetry.

By that time structures with similar type of symmetry had already been known in mathematics. In 1978 R. Penrose published the paper [6], in which the famous plane tiling first appeared. In his approach the plane is entirely covered by rhombuses of two kinds (with angles  $108^\circ$  and  $72^\circ$ , and  $144^\circ$  and  $36^\circ$ , respectively). The Penrose tiling has a fivefold symmetry axis and therefore cannot be periodic, although it does behave “quasi-periodically”: roughly speaking, for any bounded portion we can find infinitely many translated copies of it scattered throughout the plane.

In 1981 de Bruijn [4] showed how the Penrose tiling could be obtained as a projection of a two-dimensional face of a polyhedral body that is the sum of suitably chosen unit cubes in  $\mathbb{R}^5$ . This “cut-and-project” method of constructing quasicrystals, later generalized by V. I. Arnold [1], will be briefly presented in Section 2.

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The connection between crystallography and the theory of periodic functions is quite natural and has long been recognized. There can be nothing surprising in the statement that every physical quantity that can be measured in a periodic crystal, viewed as a function of the space coordinates, must have the same periods as the crystal itself. Although the question whether the real quasicrystals bear actual resemblance to the structures mentioned above is still open, it seems natural to link quasicrystals with functions that are “not exactly periodic”. In Section 3 we shall give this vague notion a strict meaning.

In Section 4 we show another method leading to the construction of almost periodic functions, and we study how it is connected with quasicrystals as described in Section 2.

Finally in Section 5 we show a geometric way of finding critical points of quasiperiodic functions, which form an important subclass of almost periodic functions.

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**2. The projection method.** We fix a natural number  $n$  and choose an irrational subspace  $\mathbb{R}^k \subset \mathbb{R}^n$  (irrational here means containing no integer points besides the origin).

Let us divide the torus  $\mathbb{T}^n = \mathbb{R}^n / \mathbb{Z}^n$  into a finite number of prisms parallel to the given irrational subspace. Such partitions will be called *Penrose partitions*.

If we consider the traces of the Penrose partition on an affine  $k$ -dimensional subspace parallel to the given irrational subspace, then we can see that they are polyhedra, obtained from the bases of the prisms by translations. There are clearly only finitely many different polyhedra, because there are finitely many prisms. A *Penrose quasiperiodic tiling* of  $\mathbb{R}^k$  is now induced by a Penrose partition of a torus.

We do not intend to show here how Penrose’s original tiling can be obtained in this manner. Instead we shall consider a three-dimensional example.

EXAMPLE (following [1]). Consider the partition of  $\mathbb{R}^3$  into equal unit cubes with integer vertices. The cubes intersecting a given irrational plane  $P$  form an infinite polyhedral body bounded by two infinite polyhedral surfaces whose square faces are translations of three faces of a cube with a common vertex.

Project one of these surfaces onto the plane  $P$  along some straight line  $l$ . The projections of the faces form a quasiperiodic tiling of the plane by parallelograms of three kinds (translates of three parallelograms that are

visible when we are looking at a unit cube along  $l$ ). We shall show that it is a Penrose tiling of the plane.

Indeed, consider the set of points  $x \in \mathbb{R}^3$  such that the affine plane parallel to the given irrational plane  $P$  and passing through  $x$  is covered by the projection of a given face  $F$  of the polyhedral surface along the given direction  $l$ . We want to prove that this set is a prism with a base parallel to  $P$ . Note that the condition “ $F$  is a face of the polyhedral boundary of the union of cubes intersecting  $P$ ” is a condition on  $P$  only and that it describes a stratum between two planes parallel to  $P$ . If  $x$  is a point of a plane inside this stratum, it is covered by the projection of  $F$  along  $l$  if and only if it belongs to the union of the lines parallel to  $l$  which intersect  $F$ . Hence, the point  $x$  lies in the part of the product of  $F$  and  $l$  inside the stratum between two parallel planes. Such points form a prism with a base parallel to  $P$ . Moreover, every point  $x \in \mathbb{R}^3$  is covered by the projection of some face  $F$  of  $P$ .

We have thus decomposed  $\mathbb{R}^3$  into prisms defined as above. This decomposition is periodic and hence defines a Penrose partition of  $\mathbb{T}^3$ . Its trace on  $P$  is the quasiperiodic tiling by parallelograms, the projection of the polyhedral boundary decomposition into faces. Hence, these parallelograms form a Penrose tiling.

The above reasoning holds in a more general situation. Consider an irrational  $k$ -dimensional subspace of an  $n$ -dimensional space. The cubes intersecting  $\mathbb{R}^k$  form a polyhedral body. Consider its  $k$ -dimensional faces. Their projections onto  $\mathbb{R}^k$  along some space  $l$  (of dimension  $n - k$ ) define a tiling of  $\mathbb{R}^k$  by polyhedra, which are intersections of parallelepipeds. Analysis similar to that in the previous case shows that the tiling defined above is a Penrose tiling.

Arnold has also introduced *Penrose functions* on  $\mathbb{T}^n$ , i.e. functions constant on every prism of a Penrose partition, and *Penrose quasiperiodic functions*, i.e. restrictions of Penrose functions on  $\mathbb{T}^n$  to irrational  $k$ -dimensional subspaces of  $\mathbb{R}^n$ . These definitions enabled him to observe that any quasiperiodic function, which by definition is the restriction of a function on  $\mathbb{T}^n$  to  $\mathbb{R}^k$ , admits arbitrarily close approximation by Penrose quasiperiodic functions.

**3. Almost periodic functions.** In 1923 H. Bohr introduced the following:

DEFINITION. A continuous function  $f : \mathbb{R} \rightarrow \mathbb{C}$  is called *almost periodic* if for every  $\varepsilon > 0$  there exists an  $l = l(\varepsilon) > 0$  such that every interval  $[a, b]$  of length  $b - a = l$  contains a number  $\tau = \tau(f, \varepsilon)$  for which

$$\forall x \in \mathbb{R} \quad |f(x + \tau) - f(x)| \leq \varepsilon.$$

We see that any metric space  $(X, \varrho)$  can be used instead of the set  $\mathbb{C}$  of complex numbers provided that the last inequality is replaced by

$$\forall x \in \mathbb{R} \quad \varrho(f(x + \tau), f(x)) \leq \varepsilon.$$

A number  $\tau$  for which this inequality holds is called an  $\varepsilon$ -*quasiperiod*.

The above definition is sufficient to prove several basic properties of almost periodic functions, e.g.

- If  $f$  is almost periodic then  $\overline{f(\mathbb{R})}$  is compact.
- Every almost periodic function is uniformly continuous.
- The limit of any uniformly convergent sequence of almost periodic functions is almost periodic.
- If  $f, g$  are complex-valued almost periodic functions then so are  $f + g$  and  $fg$ .

We shall not attempt to prove these facts here; the first three of them are straightforward and the reader is referred to [3] for the details. On the other hand, the direct proof that the class of almost periodic functions is closed under addition is considerably more tedious: given an  $\varepsilon > 0$  we try to find a  $\tau$  that is an  $\varepsilon$ -quasiperiod for *both*  $f$  and  $g$ .

For this purpose, however, another characterization of almost periodic functions, given by Bochner in [2], seems more useful.

First, note that we have the notion of a fundamental (or Cauchy) sequence of functions  $f_n : \mathbb{R} \rightarrow X$  where  $X$  is any metric space. To be precise,  $\{f_n\}$  is called *fundamental* if

$$(\forall \varepsilon > 0)(\exists N \in \mathbb{N})(\forall m, n > N)(\forall x \in X) \quad \varrho(f_m(x), f_n(x)) \leq \varepsilon.$$

Recall that a family  $H$  of functions  $f : \mathbb{R} \rightarrow X$  is called *conditionally compact* if any sequence  $f_n, n \in \mathbb{N}$ , of elements of  $H$  contains a fundamental subsequence.

We can now state Bochner's theorem.

**THEOREM 1.** *Let  $f : \mathbb{R} \rightarrow X$  be a continuous function. Then  $f$  is almost periodic if and only if the family  $H = \{x \mapsto f(x+h) : h \in \mathbb{R}\}$  is conditionally compact.*

**PROOF.** Let  $f$  be almost periodic and let  $\{f^{h_n}\} = \{f(\cdot + h_n)\}$  be any sequence of functions from  $H$ . Since  $\overline{f(\mathbb{R})}$  is compact, for every fixed  $r \in \mathbb{R}$  we can choose a subsequence  $\{h_{k_n}\}$  of  $\{h_n\}$  such that  $\{f(r + h_{k_n})\}$  is a Cauchy sequence in  $X$ . Applying the diagonal process we can find a subsequence of  $\{h_n\}$  (call it again  $\{h_n\}$  to simplify notation) such that  $\{f(r + h_n)\}$  is Cauchy for all rational numbers  $r$  (we use the fact that the rationals form a countable set). The assertion now follows easily by the uniform continuity of  $f$ . The proof of the converse is easier and will be omitted.

J. von Neumann observed that the above criterion can be used to extend the theory to arbitrary groups. For example, we shall sometimes consider functions  $f : \mathbb{R}^n \rightarrow X$  in the sequel.

**4. Generalized quasicrystal constructions.** In this section we establish some links between the “cut-and-project” method and the theory of almost periodic functions.

**THEOREM 2.** *If  $f : \mathbb{R}^n \rightarrow X$  is an almost periodic function and  $\mathbb{R}^k \subset \mathbb{R}^n$  is a subspace (rational or not) then  $f|_{\mathbb{R}^k}$  is also almost periodic.*

**PROOF.** First, note the obvious fact that if a sequence of functions  $f_i : \mathbb{R}^n \rightarrow X$  is fundamental then a fortiori so is the sequence  $f_i|_{\mathbb{R}^k}$ . Application of the Bochner criterion is now sufficient to complete the proof.

**EXAMPLE.** Let  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  be a periodic function, e.g.  $f(x, y) = \sin x + \sin y$ , and let a one-dimensional subspace be defined by the equation  $y = \sqrt{2}x$ . Since all periodic functions are almost periodic we can apply the preceding theorem to see that the restricted function  $f|_{\mathbb{R}}(x) = \sin x + \sin \sqrt{2}x$  is almost periodic.

The same argument proves that any function  $f(x) = \sum_{i=1}^k a_i \sin(\lambda_i x + \varphi_i)$  is almost periodic (it is periodic iff all the quotients  $\lambda_i/\lambda_j$  are rational). In fact, according to Bohr’s approximation theorem, the functions of this type form a dense subset in the set of all almost periodic functions equipped with the uniform convergence metric.

**THEOREM 3.** *If  $f : \mathbb{R}^n \rightarrow \mathbb{C}$  is an almost periodic function and  $g : \mathbb{R}^n \rightarrow \mathbb{C}$  is integrable (say  $\int |g(u)| du = I < \infty$ ) then the function  $F(x) = \int f(x - u)g(u) du$  is also almost periodic.*

**PROOF.** Observe that

$$|F(x + \tau) - F(x)| = \left| \int (f(x + \tau - u) - f(u))g(u) du \right| \leq I \sup |f(x + \tau - u) - f(u)|.$$

Hence every  $\varepsilon$ -quasiperiod of  $f$  becomes an  $I\varepsilon$ -quasiperiod of  $F$  and the conclusion follows by definition.

**EXAMPLE.** For practical reasons we have to choose the integrable function  $g$  in such a way that the integral  $\int f(x - u)g(u) du$  can be explicitly computed at least for  $f(x) = \sin(\lambda_i x + \varphi_i)$ . In the one-dimensional case this is possible for instance if  $g(u) = e^{-u^2}$ ,  $g(u) = e^{-|u|}$  or  $g(u) = 1/(u^2 + 1)$ . Put  $g(u) = e^{-u^2}/\sqrt{\pi}$ . If

$$f(x) = \sum_{i=1}^k a_i \sin(\lambda_i x + \varphi_i)$$

then we can directly calculate that

$$F(x) = \sum_{i=1}^k b_i \sin(\lambda_i x + \varphi_i),$$

where  $b_i = e^{-\lambda_i^2/4} a_i$ . We see that  $F$  has exactly the same frequencies  $\lambda_i$  as  $f$  but the corresponding amplitudes have changed considerably. The exact formula for the new coefficients  $b_i$  depends on the choice of  $g$ , e.g. in the case described above oscillations with high frequencies are almost completely eliminated.

It is evident that the preceding theorem remains valid in the case where  $g$  is replaced by a suitable distribution (the simplest case could be Dirac's  $\delta$ —but then  $F(x) = f(x)$ ).

Combining Theorems 2 and 3 we obtain a new method of transforming a periodic (or even almost periodic) function  $f : \mathbb{R}^n \rightarrow X$  into a new function  $F$  on  $\mathbb{R}^k$ , which can be proved to be almost periodic as well.

This procedure seems to be slightly more natural from the physical point of view because it replaces the rather unusual choice of the nearest element with integration over the whole domain, which we are more likely to encounter if we apply physical methods to explain why atoms sometimes form a quasicrystal rather than a periodic crystal.

Note also that the formula for  $F$  in the last theorem resembles the definition of convolution, which is widely used in the theory of integral transformations. It is worth pointing out that what can be measured in experiments is usually a diffraction pattern, i.e. a particular Fourier transform. This connection can also be investigated further.

**5. Singularities of almost periodic functions.** We now investigate the behaviour of critical points of almost periodic functions. Let us start with a simple example of a straightforward computation.

EXAMPLE. Consider the function  $f(x) = \sqrt{2} \sin x - \sin \sqrt{2} x$ . From the Taylor formula it is obvious that  $x = 0$  is a degenerate critical point of this function, since its expansion begins with  $-(\sqrt{2}/3)x^3$ . In order to find other critical points of  $f$  we compute the derivative

$$f'(x) = \sqrt{2}(\cos x - \cos \sqrt{2}x) = 2\sqrt{2} \sin \frac{\sqrt{2}+1}{2}x \sin \frac{\sqrt{2}-1}{2}x.$$

We can easily see that

$$f'(x) = 0 \Leftrightarrow x = 2(\sqrt{2}-1)n\pi \text{ or } x = 2(\sqrt{2}+1)n\pi \text{ for some } n \in \mathbb{Z},$$

i.e. we obtain two infinite sequences of critical points. It is worth pointing out that the only common point of these sequences is  $x = 0$ .

We can also check whether any of these critical points is degenerate. Having in mind that

$$f''(x) = -\sqrt{2}\sin x + 2\sin\sqrt{2}x$$

we see that  $x$  would be a degenerate critical point if and only if  $\cos x = \cos\sqrt{2}x$  and  $\sin x = \sqrt{2}\sin\sqrt{2}x$ . These equalities imply immediately

$$1 = \cos^2 x + \sin^2 x = \cos^2\sqrt{2}x + 2\sin^2\sqrt{2}x = 1 + \sin^2\sqrt{2}x.$$

This gives  $\sin x = \sin\sqrt{2}x = 0$ , and consequently  $x = 0$ .

Let us write down some properties of the critical points of  $f$ .

- $f$  has infinitely many nondegenerate critical points, which form two arithmetic sequences. We can say that the pattern of these points is a (1-dimensional) quasicrystal.

- There is no critical point of type  $x^3$  except  $x = 0$ .

- Although the equality  $2(\sqrt{2} - 1)m\pi = 2(\sqrt{2} + 1)n\pi$  cannot hold for any integers  $m, n$ , its sides may differ by an arbitrarily small number. For example the difference between  $x_1 = 70(\sqrt{2} - 1)\pi$  and  $x_2 = 12(\sqrt{2} + 1)\pi$  is less than  $1/13$  (we have taken  $35/6$  as a rational approximation of  $(\sqrt{2} + 1)/(\sqrt{2} - 1)$ ). Note that  $x_1 \approx x_2 \approx 29\pi$  and  $\sqrt{2}x_1 \approx \sqrt{2}x_2 \approx 41\pi$ , which means that  $f(x - x_1)$  is approximately equal to  $-f(x)$ . Analogously  $f(x - 2x_1) \approx f(x)$ .

This can be heuristically interpreted in the following way: there is no degenerate critical point except  $x = 0$ , but in the whole domain there are some pairs of close nondegenerate critical points—exactly in the same way as the function  $x^3$  after deformation becomes equivalent to  $x^3 + \varepsilon x$  rather than to  $x^3$ .

We restrict ourselves to a narrower class of functions in order to explain this kind of phenomena more systematically.

DEFINITION (see [5]). A function  $U : \mathbb{R}^k \rightarrow \mathbb{R}$  is called *quasiperiodic* if it has a decomposition  $U = f \circ \varrho$ , where  $\varrho : \mathbb{R}^k \rightarrow \mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$ ,  $k < n$ , is a linear mapping such that the image  $\varrho(\mathbb{R}^k)$  is dense in the torus  $\mathbb{T}^n$ , and  $f : \mathbb{T}^n \rightarrow \mathbb{R}$  belongs to the category we want to consider, for instance is analytic or smooth.

EXAMPLE. Let  $n = 2$  and take  $F(x, y) = a \sin 2\pi x + b \sin 2\pi y$ . This function is periodic in both variables and therefore induces a well defined function  $f$  on a two-dimensional torus. Further we assume that  $k = 1$  and define a linear mapping  $\varrho : \mathbb{R} \rightarrow \mathbb{T}^2$  by  $\varrho(t) = (\frac{t}{2\pi} \bmod 1, \alpha \frac{t}{2\pi} \bmod 1)$  where  $\alpha$  is any irrational number. The irrationality of  $\alpha$  guarantees that  $\varrho$  is one-to-one and its image is dense in the torus. The composition  $U = f \circ \varrho$  is now equal to  $U(t) = \sin t + \sin \alpha t$ .

To find critical points of the quasiperiodic function  $U$  it is necessary to investigate its differential. Since  $\varrho$  is linear we see easily that the critical points of  $U$  are exactly those points at which the restriction of the differential  $df$  to the image of  $\mathbb{R}^k$  on the torus is the zero functional. This condition is in fact a system of linear equations connecting the partial derivatives of  $f$ .

DEFINITION. For every differentiable function  $f : \mathbb{T}^n \rightarrow \mathbb{R}$  we denote by  $M(f)$  the set of  $x \in \mathbb{T}^n$  at which the restriction of  $df$  to  $\varrho(\mathbb{R}^k) \subset T_x\mathbb{T}^n$  is zero.

EXAMPLE. Let us return to the previous example where  $f(x, y) = a \sin 2\pi x + b \sin 2\pi y$  and  $\varrho(t) = (\frac{t}{2\pi} \bmod 1, \alpha \frac{t}{2\pi} \bmod 1)$ , taking for instance  $\alpha = \sqrt{2}$ . The set  $M$  is clearly defined by the equation  $a \cos 2\pi x + b\sqrt{2} \cos 2\pi y = 0$ . In order to obtain  $U(x) = \sqrt{2} \sin x - \sin \sqrt{2}x$  we must put  $a = \sqrt{2}$  and  $b = -1$ . The condition defining  $M$  now becomes  $\cos 2\pi x = \cos 2\pi y$ , i.e.  $y = x$  or  $y = 1 - x$ . In fact for any  $a, b$  the set  $M$  is an analytic manifold with possible exception of a finite number of points on the torus (in this case  $(0, 0)$  and  $(1/2, 1/2)$ ).

PROPOSITION. *The point  $x \in \mathbb{R}^k$  is a critical point of  $U = f \circ \varrho$  if and only if  $\varrho(x) \in M(f)$ . It is nondegenerate if  $\varrho(x)$  is a point where  $\varrho(\mathbb{R}^k)$  and  $M(f)$  intersect transversally.*

The reader can find similar results in [5] where the density of critical points is also considered.

Returning to our example (where  $\varrho(t) = (\frac{t}{2\pi} \bmod 1, \frac{\sqrt{2}t}{2\pi} \bmod 1)$ ) we see that  $\varrho(x) = (0, 0) \Leftrightarrow x = 0$  and  $(1/2, 1/2) \notin \varrho(\mathbb{R})$ . This explains both the fact that the function  $\sqrt{2} \sin x - \sin \sqrt{2}x$  has only one degenerate critical point at  $x = 0$  and the occurrence of pairs of arbitrarily close nondegenerate critical points when the straight line  $\varrho(\mathbb{R})$  passes close to one of the singular points  $(0, 0)$  and  $(1/2, 1/2)$ , for instance  $\varrho(70(\sqrt{2} - 1)\pi) \approx (0.4975, 0.5025)$  and  $\varrho(12(\sqrt{2} + 1)\pi) \approx (0.4853, 0.4853)$ .

REMARK. It seems important to point out that the validity of the above result relies strongly on properties of  $f$ . The analyticity condition implies namely that  $M(f)$  is an analytic manifold except for finitely many points. This need not hold true for smooth functions since according to a well known fact every closed subset of  $\mathbb{R}^n$  is the zero set of an appropriate  $C^\infty$  function.

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