Quasicrystals that project from nonisometric lattices: a generalization of a theorem by Hadwiger

1991 J. Phys. A: Math. Gen. 24 493

(http://iopscience.iop.org/0305-4470/24/2/021)

J. Phys. A: Math. Gen. 24 (1991) 493–500. Printed in the UK

Quasicrystals that project from non-isometric lattices: a generalization of a theorem by Hadwiger

A Gómez†, J L Aragón† and F Dávila‡

† Institutio de Fisíca, Universidad Nacional Autonoma de Mexico, PO Box 20-364 Mexico 01000 DF

‡ Departamento de Matemáticas, Escuela Superior de Fisíca y Matemáticas-IPN, UP Adolfo Lopez Mateos, edificio 9, Mexico 07738 DF

Received 10 July 1990

Abstract. In this work a theorem by Hadwiger that gives necessary and sufficient conditions for a vector star to be projected from an orthonormal basis in a higher-dimensional vector space is generalized. The generalized theorem is used to explore the lattices in higher-dimensional spaces from which (via 'cut' or 'cut and projection') non-periodic structures are obtained.

1. Introduction

Recently a new class of materials was discovered that are characterized by icosahedral long-range orientational order and quasiperiodic long-range translational order (Shechtman *et al* 1984). Shortly afterwards other quasiperiodic structures with decagonal orientational order were found (Bendersky 1985, Chattopadhyay *et al* 1985) and there are claims that octagonal and dodecagonal phases also exist (Wang *et al* 1987, Ishimas *et al* 1985). It was appreciated from the very beginning that a quasiperiodic structure (i.e. one having Bragg peaks indexing according to more than three rationally independent reciprocal vectors) can be regarded as a 'cut' through a periodic structure lying in a space of more than three dimensions (Bak 1985). At the same time other less general approaches were pursued leading to the so-called cut-projection scheme (Kalugin *et al* 1985, Elser 1985, Duneau and Katz 1985) and to the Grid methods (de Bruijn 1981, Kramer and Neri 1984, Socolar *et al* 1985, Socolar and Steinhardt 1986).

Since most of the theoretical work has dealt exclusively with the icosahedral phases, and since these phases can be regarded as cuts through cubic (isometric) lattices in six dimensions; very little attention has been paid to those cases in which the structures cannot be considered as cuts from a cubic hyperlattice. There are claims, for instance, that the decagonal phases require a hypertetragonal lattice in six dimensions (Mandal and Lele 1989), and it is possible that new phases, still undiscovered, will call for various non-isometric lattices.

The purpose of this paper is to explore the conditions under which a set of M vectors ('star') can be regarded as a projection of the M basic vectors that span a lattice in M-dimensional space. In order to achieve this, a generalization of a theorem

0305-4470/91/020493+08$03.50

due to Hadwiger (Hadwiger 1940, Coxeter 1973, Gancedo *et al* 1988, Torres *et al* 1989) is presented. In section 2 the cut method is briefly reviewed in order to set the stage for the generalization of the Hadwiger theorem. In section 3 the main theorems are proved. In section 4 some practical and computational aspects are discussed which are applied in section 5 to several cases of interest. In section 6 the results are discussed.

2. The cut method

The general quasiperiodic function can be regarded as a 'cut' of a periodic function in a higher-dimensional space (Bak 1985). This can be seen as follows. Let E be a Euclidean space which we will identify with the 'physical' space; consequently, $\dim(E)$ will be 3, though for illustrative purposes it will be taken sometimes as 2 or 1. Let $\{a_i\}_{i=1}^{M}$ be a subset of E such that (a) M is greater than $\dim(E)$, (b) $\{a_i\}$ spans E and (c) the set $\{a_i\}$ is rationally independent. Then we can see that a quasiperiodic function will have the form

$$f(r)=\sum A_{h_1h_2\dots h_M}\exp[2\pi\mathrm{i}(h_1a_1+h_2a_2+\dots+h_Ma_M)r] \tag{1}$$

where $h_i\in\mathbb{Z}$ and the sum is over all such integers. A quasiperiodic function is, then, a function having a spectrum that consists of 'Bragg' peaks at positions given by

$$e=h_1a_1+h_2a_2+\dots+h_Ma_M. \tag{2}$$

Now it is always possible to embed E in a Euclidean space V, of dimension M, such that if $E^\perp$ is the orthogonal complement to E then $V=E+E^\perp$ and such that is has a basis $\{e_i\}_{i=1}^{M}$ that decomposes (projects) as $e_i=a_i+a_i^\perp$ for some $a_i^\perp\in E^\perp$. Consequently, the function defined in V by

$$F(R)=\sum A_{h_1h_2\dots h_M}\exp[2\pi\mathrm{i}(h_1e_1+h_2e_2+\dots+h_Me_M)R] \tag{3}$$

is periodic in V and has the property that, when restricted to E, $F(r)=f(r)$, so f can be said to be a 'cut' of the periodic function F. The cut (hyper)plane is the space E itself. The function F is periodic over the lattice spanned by the M vectors reciprocal to the set $\{e_i\}$. For this reason it is of practical and conceptual interest to find, given $\{a_i\}$ and E, the corresponding V and $\{e_i\}$.

When the lattice in V is hypercubic with lattice parameter equal to unity, the set $\{e_i\}$ satisfies $e_i\circ e_j=\delta_{ij}$ and the projected a_i are said to form a normalized eutactic star (Coxeter 1973). The conditions under which a given star $\{a_i\}$ is eutactic are given by a theorem due to Hadwiger (Hadwiger 1940, Coexter 1973, Gancedo *et al* 1988, Torres *et al* 1989), which is given below.

Hadwiger theorem. A star $\{a_i\}_{i=1}^{M}$ is normalized eutactic if and only if for any $P\in E$

$$P=T(P)$$

where T is defined by

$$T(P)=\sum_{i=1}^{M}(P\circ a_1)a_i. \tag{4}$$

It is the purpose of this paper to generalize the Hadwiger theorem to cover the case of non-isometric (cubic) lattices and to explore some other applications, e.g. to quasicrystalline structures such as the Penrose tiling in 2D and the T phases (decagonal quasicrystals).

3. Generalized Hadwiger theorem

As in the preceding section, we consider the M-dimensional Euclidean space $V=E+E^{\perp}$ equipped with the basis $\{e_i\}_{i=1}^{M}$. If $\{e_i^*\}_{i=1}^{M}$ is the basis of V reciprocal to $\{e_i\}_{i=1}^{M}$, and defined by $e_i^*\circ e_j=\delta_{ij}$ $(i, j=1\ldots M)$, then the relationship between real and reciprocal lattices is given by the linear transformation $e_i^*=\Sigma_{j=1}^{M} g_{ij}^* e_j$, where $g^{-1}=(g_{ij}^*)=(e_i^*\circ e_j^*)$ is the inverse of the metric tensor $g=(g_{ij})=(e_i\circ e_j)$.

Let $\Pi: V\to E$ be the orthogonal projector of V onto E; we say that a star $\{a_i\}\subset E$ is orthogonal projection of $\{e_i\}$ if $\Pi(e_i)=a_i\ \forall\ i=1,2\ldots M$.

Finally, given a star $\{a_i\}$ we define the linear vector transformation $T:E\to E$ as

$$T(P)=\sum_{i}^{M}\sum_{k}^{M} g_{ki}^*(a_i\circ P)a_k.$$

Theorem 3.1. If $\{a_i\}$ is the orthogonal projection of $\{e_i\}$ then $P=T(P)\ \forall\ P\in E$.

Proof. $\forall\ P\in V\ P=\Sigma_i^M (Pe_i^*)e_i$ where $\{e_i^*\}$ is the basis reciprocal to $\{e_i\}$. Since $P\in E$, $P=\Pi(P)$, so $P=\Sigma_i^M (P\circ e_i^*)a_i$ (since $\Pi(e_i)=a_i$), but $e_i^*=\Sigma_k^M g_{ki}^* e_k$ and

$$P=\sum_{i}^{M}\sum_{k}^{M} g_{ki}^*(P\circ e_k)a_i.$$

Finally, since $e_k=a_k+b_k$, with $b_k\in E^{\perp}$

$$P\circ e_k=P\circ(a_k+b_k)=P\circ a_k+P\circ b_k=P\circ a_k$$

we have

$$P=\sum_{i}^{M}\sum_{k}^{M} g_{ki}^*(P\circ a_k)a_i=T(P)$$

and this proves the theorem.

In order to prove the second part of the generalized Hadwiger theorem we first prove the following lemma which states that under an adequate change of basis we can get a eutactic star $\{\alpha_i\}$ from the star $\{a_i\}$.

Lemma 3.1. Let B be an $M\times M$ non-singular matrix such that for any $P\in E$

$$P=\sum_{i}^{M}\sum_{k}^{M}[B\circ B^T]_{ki}(P\circ a_k)a_i.$$

Then the set $\{\alpha_s\}_{s=1}^{M}\subset E$ defined by $\alpha_s=\Sigma_k^M B_{ks}a_k$ is a eutactic star.

Proof. Given $P\in E$, by hypothesis

$$\begin{aligned}P&=\sum_{i}^{M}\sum_{k}^{M}[B\circ B^T]_{ki}(P\circ a_k)a_i\\&=\sum_{i}^{M}\sum_{k}^{M}\sum_{s}^{M} B_{ks}B_{si}^T(P\circ a_k)a_i\\&=\sum_{s}^{M}\left(\sum_{k}^{M} B_{ks}a_k\right)\circ P\left(\sum_{i}^{M} B_{si}^T a_i\right)\\&=\sum_{s}^{M}(\alpha_s\circ P)(\alpha_s)\end{aligned}$$

then by the Hadwiger theorem $\{\alpha_s\}$ is a (normalized) eutactic star.

With this background we can state the converse of theorem 3.1.

Theorem 3.2. If $T(P)=\Sigma_k^M \Sigma_i^M g^*_{ki}(P\circ a_k)a_i$ is the identity in E then $\{a_i\}$ is the orthogonal projection of $\{e_i\}$.

Proof. Since g^{-1} is positive definite, a well known theorem of linear algebra assures that there exists a non-singular $M\times M$ matrix B such that $g^{-1}=BB^T$. From the previous lemma $\alpha_s=\Sigma_k^M B_{ks}a_k$ is a normalized eutactic star; consequently there is an orthonormal basis $\{C_i\}_{i=1}^M$ of V such that it decomposes (projects) uniquely as $C_s=\alpha_s+\alpha'_s\in E^\perp$. Consequently

$$\begin{aligned}\sum_s^M (B^{-1})_{sk}C_s &= \sum_s^M (B^{-1}_{sk})\alpha_s+\sum_s^M B^{-1}_{sk}\alpha'_s\\ &=\sum_s^M B^{-1}_{sk}\sum_{k'}^M B_{k's}a_{k'}+\sum_s^M B^{-1}_{sk}\alpha'_s\\ &=\sum_{k'}^M a_{k'}\sum_s^M B_{k's}B^{-1}_{sk}+\sum_s^M B^{-1}_{sk}\alpha'_s\\ &=a_k+\sum_s^M B^{-1}_{sk}\alpha'_s.\end{aligned}$$

Defining $e_i=\Sigma_s^M B^{-1}_{si}C_s$ we have a basis $\{e_i\}$ for V such that $e_i=a_i+\Sigma_s^M B^{-1}_{si}\alpha'_s$ with $\Sigma_s^M B^{-1}_{si}\alpha'_s\in E^\perp$.

Finally

$$\begin{aligned}e_i\circ e_j &= \sum_s\sum_t B^{-1}_{si}B^{-1}_{tj}C_s\circ C_t\\ &=\sum_s B^{-1}_{si}B^{-1}_{sj}=\sum_s (B^{-1^T})_{is}B^{-1}_{sj}=(B^{-1^T}\circ B^{-1})_{ij}\\ &=(B\circ B^T)^{-1}_{ij}=g_{ij}.\end{aligned}$$

4. Computational aspects and general strategy

Theorems 3.1 and 3.2 above give necessary and sufficient conditions for the existence of a higher-dimensional lattice that projects onto a given star. In practice it is easier to work with the expressions given in the following theorem.

Theorem 4.1. Let $\{C_i\}$ be an orthonormal basis for E. Then

$$\delta_{jh}=\sum_i^M\sum_k^M g^*_{ki}(C_j\circ a_k)(C_h\circ a_i) \tag{5}$$

if and only if $P=T(P)\ \forall\ P\in E$.

Proof. $\Leftarrow$) Since $C_h\in E$, we can write

$$C_h=\sum_i^M\sum_k^M g^*_{ki}(C_h\circ a_k)a_i$$

so

$$\delta_{jh} = C_j \circ C_h = \sum_{i}^{M} \sum_{k}^{M} g^*_{ki}(C_h \circ a_k)(C_j \circ a_i)$$

conversely $\Rightarrow$)

$$\begin{aligned} P = IP &= \sum_t \sum_s \delta_{st} P_t C_s \\ &= \sum_t \sum_s \sum_i \sum_k g^*_{ki}(C_t \circ a_k)(C_s \circ a_i) P_t C_s \\ &= \sum_i \sum_k g^*_{ki} \sum_t (C_t \circ a_k) P_t \sum_s (C_s \circ a_i) C_s \\ &= \sum_i \sum_k g^*_{ki} \sum_t (C_t \circ a_k) P_t a_i \\ &= \sum_i \sum_k g^*_{ki} \left(\left(\sum_t P_t C_t \right) \circ a_k \right) a_i \\ &= \sum_i \sum_k g^*_{ki} (P \circ a_k) a_i. \end{aligned}$$

This completes the proof of the theorem.

Consequently, a given star can be projected from a hyperlattice having a metric tensor g_{ij} if and only if the star satisfies equation (5). A practical procedure for analysing a given situation is as follows.

1. Start by asking if projection is possible from a cubic (isometric) lattice of lattice parameter equal to unity. This amounts to using $g_{ij} = \delta_{ij}$ in equation (5). The criterion reduces to the original theorem by Hadwiger.

2. If the star fails to satisfy the criterion in the original Hadwiger's theorem, try a cubic hyperlattice of parameter λ (so the star, though eutactic, is not normalized). Use in equation (5) $g_{ij} = \lambda\delta_{ij}$, so if equation (5) can be solved for λ (with $\lambda > 0$ to assure positive definiteness) then the projection is possible.

3. If the star cannot be projected from a cubic lattice, next try an orthohombic hyperlattice; set $g_{ij} = \lambda_i^2 \delta_{ij}$ and solve for λ_i (here λ_i is the lattice parameter in the ith direction). As explained elsewhere (Aragón *et al* 1990), the system of equations can be solved using the generalized inverse (Mackay 1977) or singular-value decomposition techniques. The system may have a solution, which may or may not be unique, or the system may fail to have a solution. A solution with all $\lambda_i > 0$ is required in order to get a matrix g that is positive definite.

4. If the above steps fail, try then a general (hyper)triclinic lattice. That there is always a solution to the problem can be seen as follows. Let $\{a_i\} \subset E$ be the given star. Assume (relabelling if necessary) that $a_1 \dots a_n$ is a basis for E. If $b_{n+1} \dots b_M$ is a basis for $E^\perp$, then $\alpha = \{a_1 \dots a_n, b_{n+1} \dots b_M\}$ is a basis for V. Define $\beta = \{a_1 \dots a_n, (a_{n+1} + b_{n+1}) \dots (a_M + b_M)\} = \{c_1 \dots c_M\}$. Then β can be shown to be a basis for V, and is already in the form $c_i = a_i + d_i$ where $d_i \in E^\perp$.

In the applications it is easier and clearer to write equation (5) in matrix form as

$$I = Ag^*A^T$$

where I is the $(N \times N)$ identity matrix (with $N = \dim(E)$) and the columns of A are the vectors $\{a_n\}_{n=1}^{M}$.

5. Some applications

5.1. *Pentagonal case*

The Penrose pattern in two dimensions can be obtained by cutting a 5D periodic icosahedral structure (Henley 1986) whose basis projects onto five vectors pointing to the vertices of a regular pentagon:

$$a_n = a(\cos 2\pi n/5, \sin 2\pi n/5) \qquad n = 0, 2, \ldots, 4.$$

This star is eutactic, so the lattice of the 5D periodic structure can be hypercubic.

Another possibility arises from the fact that the vectors a_n $(n = 1, 2, \ldots, 5)$ are rationally dependent and it is sufficient to consider a four-dimensional periodic structure. Such a structure is obtained from the 5D icosahedral structure as a 4D section perpendicular to the body-diagonal [11111] direction; it is a dodecagonal one (Janssen 1986) and its basis projects onto vectors pointing to four vertices of a regular pentagon. This star is non-eutactic and it can also be seen (applying the criteria outlined in section 4 above) that this star must necessarily be generated as a projection of a four-dimensional basis which spans a triclinic lattice.

Following the path outlined in section 4 above, and by taking $c_n = \cos 2\pi n/5$, $s_n = \sin 2\pi n/5$ and $a = 1$, we find that a possible basis in R^4 that projects onto the star is given by

$$e_1 = (1, 0, 0, 0)$$

$$e_2 = (c_1, s_1, 0, 0)$$

$$e_3 = (c_2, s_2, 1, 0)$$

$$e_4 = (c_3, s_3, 0, 1)$$

giving rise to a metric tensor:

$$g = \begin{bmatrix} 1 & c_1 & c_2 & c_2 \\ c_1 & 1 & c_1 & c_2 \\ c_2 & c_1 & 2 & c_1 \\ c_2 & c_2 & c_1 & 2 \end{bmatrix}.$$

5.2. *Decagonal phase*

In reciprocal space, the decagonal phase can be specified by the following set of vectors:

$$z_0 = 2\cos\alpha\hat{z} \qquad a_n = \cos\alpha\hat{z} + \sin\alpha R^n\hat{x} \qquad n = 0, \ldots, 4$$

where R is a rotation about the $\hat{z}$ axis by $2\pi/5$. The vectors $\{z_0 a_n\}$ and $\{z_0 - a_n\}$ are the lower and upper edges of a pentagonal bipyramid (Ho 1986). This star is non-eutactic but step 3 in section 4 shows that it can be obtained as a projection of a basis which generates an orthorhombic (reciprocal) lattice, as is well known (Mandal and Lele 1989, Aragón *et al* 1990).

An interesting exercise consists in discarding the z_0 vector (which can be obtained as a rational combination of the five vectors a_n), and obtaining a star a_n, $n = 0, \ldots, 4$, which, according to our criteria, cannot be projected either from a cubic or an orthorhombic basis.

As in the previous example, one can easily find a basis for the lattice in R^5 as

$$\begin{aligned} e_1 &= (s_\alpha, 0, c_\alpha, 0, 0) \\ e_2 &= (-c_1 s_\alpha, s_1 s_\alpha, c_\alpha, 0, 0) \\ e_3 &= (c_2 s_\alpha, -s_2 s_\alpha, c_\alpha, 0, 0) \\ e_4 &= (-c_3 s_\alpha, s_3 s_\alpha, c_\alpha, 1, 0) \\ e_5 &= (c_4 s_\alpha, -s_4 s_\alpha, c_\alpha, 0, 1) \end{aligned}$$

where $c_n = \cos 2\pi n/5$, $s_n = \sin 2\pi n/5$ ($n = 0, \ldots, 4$ or α). The associated metric tensor is

$$g = \begin{bmatrix} 1 & -c_1 s_\alpha^2 + c_\alpha^2 & c_2 s_\alpha^2 + c_\alpha^2 & -c_3 s_\alpha^2 + c_\alpha^2 & c_4 s_\alpha^2 + c_\alpha^2 \\ & 1 & -s_\alpha^2(c_1 c_2 + s_1 s_2) + c_\alpha^2 & s_\alpha^2(c_1 c_3 + s_1 s_3) + c_\alpha^2 & -c_\alpha^2(c_1 c_4 + s_1 s_4) + c_\alpha^2 \\ & & 1 & -s_\alpha^2(c_2 c_3 + s_2 s_3) + c_\alpha^2 & c_\alpha^2(c_2 c_4 + s_2 s_4) + c_\alpha^2 \\ & \text{symmetrical} & & 2 & -s_\alpha^2(c_3 c_4 + s_3 s_4) + c_\alpha^2 \\ & & & & 2 \end{bmatrix}.$$

It should be remarked that the procedure used in these examples provides a solution but it is not necessarily the 'best' nor the one that displays the symmetry of the lattice in V (Janssen 1986).

6. Discussion

A very general result in the theory of quasiperiodic structures states that a quasiperiodic function can be seen as a cut through a periodic function in a higher-dimensional space (Bak 1985). There are indications in the experimental literature in the sense that this approach must be used for a full description of the materials (de Boissieu *et al* 1990) rather than simply using less general approaches, such as cut and projection, grid methods or straight decoration of Penrose tiles.

On the other hand there are quasiperiodic structures that, unlike the icosahedral quasicrystals, cannot be seen as cuts from hypercubic lattices (although, strictly speaking, one can always arrange things so as to use only isometric lattices; see Bak and Goldman 1988). It is having such cases in mind that the Hadwiger theorem concerning the projectability of lattices onto given stars was generalized. Presumably new phases that call for various non-isometric lattices will be discovered in the near future and the results obtained here might be useful for their characterization in the 'cut' scheme.

Finally we would like to point out that although this work was done having in mind quasiperiodic functions, it might be useful in other contexts. For instance Elser (1989) has shown that the random quasicrystals can be thought of as packings of clusters of atoms (with suitable symmetry) whose centres are the projections of a subset of a lattice in the higher-dimensional space V. In this case the formalism presented here retains is usefulness since many of the properties of the quasicrystals (mostly their diffraction properties) depend on the behaviour of the subset of the lattice (the hypersurface).

Acknowledgments

The authors are indebted to David Romeu for useful discusssions and comments. Support by CONACYT and DGAPA (UNAM), through grants P228CCOX-891641 and IN-014989 respectively, is gratefully acknowledged.

References

Aragón J L, Romeu D, Gómez A and Dávila F 1990 *Scripta Met.* **24** 719

Bak P 1985 *Phys. Rev. Lett.* **54** 1517

Bak P and Goldman A I 1988 Quasicrystallography *Introduction to Quasicrystals* ed M V Jarič (New York: Academic)

Bendersky L 1985 *Phys. Rev. Lett.* **55** 1461

Coxeter H S M 1973 *Regular Polytopes* (New York: Dover)

Chattopadhyay K, Lele S, Ranganathan S, Subbnna G N and Thangaraj N 1985 *Current Sci* **54** 895

de Boissieu M, Janot C and Dubois J M 1990 *J. Phys. C: Condens. Matter* 2 2499

de Bruijn N 1981 *Ned. Akad. Weten. Proc. Ser.* A **45** 39

Duneau M and Katz A 1985 *Phys. Rev. Lett.* **54** 2688

Elser V 1985 *Phys. Rev.* B **32** 4892

—— 1989 *The Growth of the Icosahedral Phase in Extended Icosahedral Structures* ed M V Jarič (New York: Academic)

Gancedo E, Pastor G, Ferreiro A and Torres M 1988 *Int. J. Math. Educ. Sci. Technol.* **19** 489

Hadwiger H 1940 *Comentarii Mathematici Helvetici* **13** 90

Henley C L 1986 *Phys. Rev.* B **34** 797

Ho T L 1986 *Phys. Rev. Lett.* **56** 468

Ishimasa T, Nissen H U and Fukano Y 1985 *Phys. Rev. Lett.* **55** 511

Janssen T 1986 *Acta Cryst.* A **42** 261

Kalugin P A, Kitaev A Y and Levitov L C 1985 *JETP Lett.* **41** 145

Kramer P and Neri R 1984 *Acta. Cryst.* A **40** 580

Mackay A L 1977 *Acta Cryst.* A **33** 212

Mandal R K and Lele S 1989 *Phys. Rev. Lett.* **62** 2695

Schechtman D, Blech I Gratias D and Cahn J W 1984 *Phys. Rev. Lett.* **53** 1951

Socolar J E S and Steinhardt P J 1986 *Phys. Rev.* B **34** 617

Socolar J E S, Steinhardt P J and Levine D 1985 *Phys. Rev.* B **32** 5547

Torres M, Pastor G, Jiménez I and Fayos I 1989 *Phys. Status Solidi* b **154** 439

Wang N, Chen H and Kuo K H 1987 *Phys. Rev. Lett.* **59** 1010