PHILOSOPHICAL MAGAZINE, 11 October 2003
VOL. 83, NO. 29, 3283–3307

Taylor & Francis
Taylor & Francis Group

Indexing schemes for quasilattices

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[*Received 20 July 1999 and accepted in revised form 25 July 2003*]

ABSTRACT

Various schemes have been proposed and employed, which extend the method of indexing lattice vectors and reciprocal-lattice vectors, so that it can be used in the context of quasicrystals. The concept of the *generalized inverse* of a matrix provides an elegant unified approach to the vectors and reciprocal vectors of quasilattices, and their associated zone laws and inflation rules. We present a survey, from the viewpoint provided by the concept of the Moore–Penrose inverse, of the indexing problem for quasicrystals.

§ 1. INTRODUCTION

The labelling of the vectors and reciprocal vectors of a Bravais lattice in E_3 by triplets of integers, satisfying a *zone law* $k_1x^1+k_2x^2+k_3x^3=0$, is straightforward and well known. The discovery of quasicrystals imposed a need to generalize this method of labelling. The non-crystallographic point symmetries of quasicrystals involve the necessity of employing more than three indices for the labelling of vectors and reciprocal vectors. The problem is complicated by the redundancy that arises when more than three numbers are employed to specify vectors in E_3. A survey of the literature reveals certain general geometrical and algebraic principles which have not, as far as we know, been explicitly stated or presented in one place as a unified theory. Our purpose is to present the general principles underlying indexing schemes for crystals and quasicrystals and to illustrate them with the aid of some well-known (and some less well-known) examples.

§ 2. THE MOORE–PENROSE INVERSE

Associated with any matrix $\mathbf{E}$, there is a unique matrix $\mathbf{E}^*$ that satisfies

$$\mathbf{E}\mathbf{E}^* = (\mathbf{E}\mathbf{E}^*)^{\mathrm{T}}, \quad \mathbf{E}^*\mathbf{E} = (\mathbf{E}^*\mathbf{E})^{\mathrm{T}}, \quad \mathbf{E}\mathbf{E}^*\mathbf{E} = \mathbf{E}, \quad \mathbf{E}^*\mathbf{E}\mathbf{E}^* = \mathbf{E}^*. \tag{1}$$

Several properties of $\mathbf{E}^*$ follow readily from these defining relations.

(i) If $\mathbf{E}$ is $n \times N$, of rank r, then $\mathbf{E}^*$ is $N \times n$, of rank r.
(ii) $(\mathbf{E}^*)^{\mathrm{T}} = (\mathbf{E}^{\mathrm{T}})^*$.
(iii) If $n = N = r$, then $\mathbf{E}^*$ is just the inverse $\mathbf{E}^{-1}$ of $\mathbf{E}$.

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Philosophical Magazine ISSN 1478–6435 print/ISSN 1478–6443 online © 2003 Taylor & Francis Ltd
http://www.tandf.co.uk/journals
DOI: 10.1080/14786430310001608729

$\mathbf{E}^*$ is the *Moore–Penrose* (*M–P*) *generalized inverse* of $\mathbf{E}$ (Ben-Israel and Greville 1977). The M–P inverse of $\mathbf{E}^*$ is $\mathbf{E}$. Mackay (1977) has discussed various applications of this concept, with special emphasis on crystallographic applications. In particular, the generalized inverse can be applied to obtain a set of reciprocal vectors from a redundant set of lattice translation vectors. (Essentially, if the columns of a matrix $\mathbf{E}$ are the components of a set of lattice translation vectors, referred to an orthonormal reference system, then the rows of $\mathbf{E}^*$ give the components of a set of reciprocal vectors.) This was demonstrated for the four vectors that generate a hexagonal lattice, in Weber's (1922) indexing scheme (Frank 1965), and for four tetrahedrally arranged vectors that generate the bcc lattice (Mackay 1977). The advantage of these schemes is that the point symmetry of the set of vectors given by $\pm\mathbf{E}$ is the point symmetry of the lattice. Mackay even discussed the set of reciprocal vectors associated with the six fivefold axes of an icosahedron, long before the discovery of quasicrystals. Of course, the four-index schemes for the hexagonal lattice and the bcc lattice have a certain elegance, but they are not compulsory. For quasicrystals, on the other hand, the redundancy of the set of generating vectors is the very essence of the structure, and the M–P inverse assumes more importance.

§3. Calculation of the Moore–Penrose inverse

There exist several algorithms that employ iterative schemes that converge on the M–P inverse of a given matrix (Ben-Israel and Greville 1977). They are sensitive to the choice of initial approximation. We give below a direct method that relies only on an algorithm for diagonalizing a symmetric matrix.

As is easily verified by substitution into the equations (1),

$$\mathbf{E}^* = \mathbf{E}^{\mathrm{T}}\mathbf{S}^*, \quad \mathbf{S} = \mathbf{E}\mathbf{E}^{\mathrm{T}}.$$

At first sight, this may not seem very helpful; the problem of finding the M–P inverse of a given matrix $\mathbf{E}$ has been replaced by the problem of finding the M–P inverse of $\mathbf{S}$. However, since $\mathbf{S}$ is symmetric, it can be brought to diagonal form; there is a matrix $\mathbf{L}$ such that

$$\mathbf{D} = \mathbf{L}\mathbf{S}\mathbf{L}^{-1}$$

is a diagonal matrix (and there are well-known algorithms for finding a matrix $\mathbf{L}$). The M–P inverse of a diagonal matrix is, obviously, obtained simply by replacing its non-zero elements by their reciprocals. The M–P inverse of $\mathbf{S}$ is then

$$\mathbf{S}^* = \mathbf{L}\mathbf{D}^*\mathbf{L}^{-1}.$$

Note that, if $\mathbf{E}$ is $n \times N$, $\mathbf{S}$ is $n \times n$. We lose no generality by assuming that $n \leqslant N$ because if $n > N$ the procedure can be applied to $\mathbf{E}^{\mathrm{T}}$ instead of to $\mathbf{E}$. In many of the cases that we shall encounter, $\mathbf{S}$ is just a multiple of the unit matrix and the M–P inverse of $\mathbf{E}$ is just a multiple of $\mathbf{E}^{\mathrm{T}}$.

§4. Solutions of linear equations

Generalized inverses, in particular the M–P inverses, provide methods of obtaining solutions of sets of linear equations, in cases where the system is underdetermined or overdetermined. The following brief summary of the key formulae serves to establish our notation.

A set of n linear equations in N unknowns can be written as a matrix equation

$$\mathbf{x} = \mathsf{E}x.$$

The $n \times N$ matrix E and the n-component column $\mathbf{x}$ are given and the unknowns are the components of the N-component column x. The equations are consistent if and only if

$$\mathbf{px} = \mathbf{x} \,(\text{equivalently, } \mathbf{qx} = 0)$$

and the general solution is

$$x = \mathsf{E}^{*}\mathbf{x} + \mathbf{Qz}$$

where $\mathbf{z}$ is an *arbitrary* N-dimensional vector

$$\mathsf{q} = \mathsf{I} - \mathsf{p}, \quad \mathsf{p} = \mathsf{EE}^{*},$$

$$\mathsf{Q} = \mathsf{I} - \mathsf{P}, \quad \mathsf{P} = \mathsf{E}^{*}\mathsf{E}.$$

The symmetric $n \times n$ matrices p and q and the symmetric $N \times N$ matrices P and Q are *projection matrices*: they satisfy

$$\mathsf{q}^2 = \mathsf{q}, \quad \mathsf{p}^2 = \mathsf{p}, \quad \mathsf{pq} = \mathsf{qp},$$

$$\mathsf{Q}^2 = \mathsf{Q}, \quad \mathsf{P}^2 = \mathsf{P}, \quad \mathsf{PQ} = \mathsf{QP}.$$

§ 5. Z MODULES

Suppose that $\{\mathbf{e}_i\}$, $i = 1, \ldots, N$, is a set of N vectors in E_n. Then any set of N (real) numbers x^{i} determines a vector $\mathbf{x}$ in E_n and, conversely, a vector $\mathbf{k}$ determines a set of real numbers k_i:

$$\mathbf{x} = \mathbf{e}_i x^i, \tag{2}$$

$$k_i = \mathbf{k} \cdot \mathbf{e}_i. \tag{3}$$

Let E denote the $n \times N$ matrix whose columns are the components of the vectors $\{\mathbf{e}_i\}$ referred to an orthonormal basis. Then the above expressions can be written in matrix notation simply as

$$\mathbf{x} = \mathsf{E}x, \tag{4}$$

$$k = \mathbf{k}\mathsf{E}. \tag{5}$$

The set L of all points $\mathbf{x}$ for which the numbers x are *integers* is a *Z module*. In what follows we shall, for brevity, refer to Z modules simply as *modules*. A *lattice* is, of course, a particular instance of a module, and equations (4) and (5) generalize the concepts of lattice translations of reciprocal vectors. In general a module may consist of a dense set of points. The *projection method* is essentially the imposition of a selection rule that filters out a discrete point set (a 'quasilattice') from a module. This will be taken up in § 8, but in the main we do not need it; the underlying module suffices for an algebraic presentation of indexing schemes for quasicrystals.

If the rank of the matrix E is r, then all points of L will lie in an r-dimensional subspace of E_n. Any r given points in E_r that do not all lie in an $r-2$ space determine an $r-1$ space in which they all lie: a hyperplane. Let one of the r given points be chosen as the origin, and let X be the $n \times (r-1)$ matrix, of rank $r-1$, whose columns are the position vectors $\mathbf{x}$ for the remaining $r-1$ points. Then

$$\mathbf{k} \sim \mathbf{z}(\mathsf{I} - \mathsf{XX}^{*}) \tag{6}$$

is normal to the hyperplane of E_n whose intersection with the E_r is the hyperplane containing the r given points. ($\mathbf{z}$ is an arbitrary row vector and $\sim$ denotes equality up to an irrelevant scalar factor.) In particular, for $r=2$ this gives

$$\mathbf{k} \sim \mathbf{x}^{\mathrm{T}}\boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{7}$$

and for $r=3$, for the planes parallel to the two lines through $\mathbf{x}$ and $\mathbf{y}$, it gives

$$\mathbf{k} = \mathbf{x} \times \mathbf{y}. \tag{8}$$

The N-tuple k given by equation (5) provides a set of N indices for a family of hyperplanes. The index set k is not in general unique and, in general, a set of indices obtained in this way will not be rational, but the zone law remains valid in its usual form:

$$kx = k_i x^i = k_1 x^1 + k_2 x^2 + \cdots + k_N x^N = 0. \tag{9}$$

The ratios of the intercepts of the hyperplanes with the axes $\mathbf{e}_i$ are the ratios of the numbers $1/k_i$.

Instead of defining the indices for the hyperplanes through equation (5), one can define an alternative set of indices κ required to satisfy

$$\mathbf{k} = \kappa \mathsf{E}^*. \tag{10}$$

The *reciprocal vectors* $\{\mathbf{e}^i\}$ are then identified as those given (with reference to the orthogonal coordinate system) by the rows of E*. The relation between vectors and reciprocal vectors for a lattice ($\mathbf{e}^i \cdot \mathbf{e}_j = \delta^i_j$) is generalized to

$$\mathbf{e}^i \cdot \mathbf{e}_j = P^i_{j.} \tag{11}$$

In terms of the indices κ for the hyperplanes, the zone law is

$$\kappa \mathsf{P} x = 0. \tag{12}$$

A key question is then: for what kinds of r-dimensional module can the $(r-1)$-dimensional submodules be indexed by sets κ of *integers*?

§6. Inflation rules

If $\mathsf{P} \neq \mathsf{I}$, the equations $\mathsf{EP} = \mathsf{E}$ (equivalently, $\mathsf{EQ} = 0$) express the redundancy of the set of reference vectors $\{\mathbf{e}_i\}$. It follows from equations (3) and (6) that $k\mathsf{P} = \kappa\mathsf{P} = k$, which expresses the corresponding redundancy of the set of indices k. The components of k are not necessarily rational. Suppose, however, that they belong to some algebraic number field F, and that there is an *inflation rule* (Ostlund and Wright 1986) associated with an element λ of F. That is, for every point $\mathbf{x}$ of the module, $\lambda\mathbf{x}$ is also a point of the module. There is then a matrix T with integer elements, such that

$$\mathsf{ET} = \lambda \mathsf{E}.$$

Whenever a module possesses an inflation rule, integer indices can be assigned to the reciprocal vectors. Let $\{\lambda_\alpha\}$ be a basis for F, that is every element of F is a linear combination of the λ_α with *rational* coefficients, and write

$$\mathsf{ET}_\alpha = \lambda_\alpha \mathsf{E}.$$

If the components of the N-tuples k also belong to F, we can write $k = k^\alpha \lambda_\alpha$.

The components of the matrices $\mathbf{T}_\alpha$ and of the N-tuples k_α are rational. Then,

$$\kappa\mathbf{P} = k\mathbf{P} = k^\alpha \lambda_\alpha \mathbf{P} = k^\alpha (\mathbf{T}_\alpha)^{\mathrm{T}}\mathbf{P}.$$

Thus, for the hyperplanes specified by the index set k, a rational index set

$$\kappa = k^\alpha (\mathbf{T}_\alpha)^{\mathrm{T}} \tag{13}$$

(and hence an integer set) exists.

6.1. *Examples*

The module underlying the Penrose tiling patterns is generated by the matrix

$$\mathbf{E} = \begin{pmatrix} c_0 & c_1 & c_2 & c_3 & c_4 \\ s_0 & s_1 & s_2 & s_3 & s_4 \end{pmatrix} = \tfrac{1}{2}\begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau \end{pmatrix},$$

where $c_m = \cos(m\theta)$, $s_m = \sin(m\theta)$, $\theta = 2\pi/5$, $\tau = (1+5^{1/2})/2$, $\sigma = (1-5^{1/2})/2$ and $\beta = (3-\tau)^{1/2}$. The five vectors are position vectors of the vertices of a regular pentagon. They satisfy the inflation rule

$$\tau\mathbf{e}_1 = -\mathbf{e}_3 - \mathbf{e}_4 \quad \&\ \text{cycl.}$$

(& cycl. will be used to denote a set of equations obtained from a given equation by cyclic permutation of a set of labels, in this case (12345)). Thus, the module has the inflation rule

$$\tau\mathbf{E} = \mathbf{E}\mathbf{T}, \qquad \mathbf{T} = -\begin{pmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix} = \mathrm{cycl}\,(00\bar{1}\bar{1}0). \tag{14}$$

In E_2, the 'hyperplanes' are lines. A set of five integer indices x determines the two-component vector $\mathbf{x} = \mathbf{E}x$ and hence its normal $\mathbf{k} = \mathbf{x}^{\mathrm{T}}\boldsymbol{\varepsilon}$. The set of indices $k = \mathbf{k}\mathbf{E}$ is of the form $k = k(1) + \tau k(2)$ with rational sets $k(1)$ and $k(2)$. ($k(2)$ can be expressed in terms of $k(1)$). We have $\tau[k(1)+\tau k(2)] = [k(1)+\tau k(2)]\mathbf{T}$, from which it follows that $k(2) = k(1)\mathbf{T}$. In this example the algebraic field F is $Q(5^{1/2})$). The index set κ for the line through the origin and point $\mathbf{x}$ is then

$$\kappa = k(1) + k(2)\mathbf{T}.$$

Since $\mathbf{P} \sim \mathrm{cycl}(2-\sigma-\tau-\tau-\sigma)$, the zone law (12) splits, on equating coefficients of 1 and of τ, into the pair of rational zone laws

$$2(\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4 + \kappa_5 x^5) - (12) - (23) - (34) - (45) - (51) = 0,$$
$$(12) + (23) + (34) + (45) + (51) - (13) - (24) - (35) - (41) - (52) = 0,$$

where we have used an abridged notation: (12) for instance denotes $\kappa_1 x^2 + \kappa_2 x^1$.

A less simple example is the module in E_2 with sevenfold symmetry:

$$\mathbf{E} \sim \begin{pmatrix} c_0 & c_1 & c_2 & c_3 & c_4 & c_5 & c_6 \\ s_0 & s_1 & s_2 & s_3 & s_4 & s_5 & s_6 \end{pmatrix},$$

where $c_m = \cos(m\theta)$, $s_m = \sin(m\theta)$ and $\theta = 2\pi/7$. Although sevenfold symmetry has never been found to occur in quasicrystals, this case has some intrinsic interest arising from the fact that the inflation factor is a cubic rather than a quadratic irrational. The vectors $\mathbf{e}_i$, $i = 1, \ldots, 7$, given by the columns of E can be represented by the complex numbers ω^m, where ω is the seventh root of unity $\exp(i\theta)$, which satisfies $\omega^7 - 1 = 0$ and

$$1 + \omega^1 + \omega^2 + \omega^3 + \omega^4 + \omega^5 + \omega^6 = 0. \tag{15}$$

The geometry of the regular heptagon suggests three obvious inflation rules; the vectors $\mathbf{e}_i$ satisfy

$$\lambda_1 \mathbf{e}_1 = \mathbf{e}_2 + \mathbf{e}_7 \quad \text{\& cycl.},$$

$$\lambda_2 \mathbf{e}_1 = \mathbf{e}_3 + \mathbf{e}_6 \quad \text{\& cycl.},$$

$$\lambda_3 \mathbf{e}_1 = \mathbf{e}_4 + \mathbf{e}_5 \quad \text{\& cycl.},$$

where

$$\lambda_1 = 2c_1 = 2c_6, \qquad \lambda_2 = 2c_2 = 2c_5, \qquad \lambda_3 = 2c_3 = 2c_4.$$

It is obvious from the real part of equation (15) that the three inflation factors are not independent; they satisfy $1 + \lambda_1 + \lambda_2 + \lambda_3 = 0$. They are also the roots of the cubic equation

$$\lambda^3 + \lambda^2 - 2\lambda - 1 = 0$$

(verified by multiplying out the expression $(x - \omega - \omega^6)(x - \omega^2 - \omega^5)(x - \omega^3 - \omega^4)$). Writing $\lambda = \lambda_1$, well-known trigonometrical formulae give

$$\lambda_2 = \lambda^2 - 2, \qquad \lambda_3 = -\lambda^2 - \lambda - 1.$$

A 7-tuple x of integers determines the line of points of the module, through $\mathbf{x} \sim \mathsf{E}x$, normal to $\mathbf{k}$ and hence determines a $k \sim \mathbf{k}\mathsf{E}$, whose components are quadratics in λ with integer coefficients:

$$k \sim k(0) + k(1)\lambda + k(2)\lambda^2$$

(where $k(0)$, $k(1)$ and $k(2)$ are 7-tuples with integer components).

Hence, from equation (13), an integer set of indices for the 'reciprocal vector' k is

$$\kappa \sim k(0) + k(1)\mathsf{T}^1 + k(2)\mathsf{T}^2, \qquad \mathsf{T} = \mathrm{cycl}\,(010001).$$

$$\begin{aligned} \mathsf{P} &\sim \mathrm{cycl}\,(2\ \lambda_1\ \lambda_2\ \lambda_3\ \lambda_3\ \lambda_2\ \lambda_1) \\ &= \mathrm{cycl}\,(2\ 0\ {-2}\ 1\ 1\ {-2}\ 0) + \lambda\,\mathrm{cycl}\,(0\ 1\ 0\ {-1}\ {-1}\ 0\ 1) \\ &\quad + \lambda^2\,\mathrm{cycl}\,(0\ 0\ 1\ {-1}\ {-1}\ 1\ 0). \end{aligned}$$

On equating coefficients of 1, λ and λ^2, we obtain a set of three rational zone laws.

These results are generalizable to modules in E_2 with N-fold symmetry generated by N vectors directed to the vertices of a regular N-gon. The numbers $\lambda_m = 2\cos(m\theta)$, with $\theta = 2\pi/N$, are inflation factors. Now, $c_m = \cos(m\theta)$ can be expressed as a polynomial of order m in $c = c_1$, with integer coefficients, and $s_m = \sin(m\theta)$ can be expressed as $s\,(= s_1)$ times a polynomial of order $m - 1$ in c, with integer coefficients. This is most readily seen by separating the real and imaginary parts of the binomial expansion of

$$\exp(\mathrm{i}m\theta) = c_m + is_m = (c + is)^m.$$

This gives

$$c_m = \sum_{r=0}^{[mi2]} c^{m-2r}(-)^r(1-c^2)^r \binom{m}{2r},$$
$$s_m = s\sum_{r=0}^{[mj2]} c^{m-2r-1}(-)^r(1-c^2)^r \binom{m}{2r+1}.$$

$[mi2]$ denotes $m/2$ or $(m-1)/2$ accordingly as m is even or odd.

It follows that, for a given set of integer indices x, $\mathbf{x} = \mathbf{E}x$ has the form $[a, bs]$ where a and b are polynomials in λ with integer coefficients. The normal to $\mathbf{x}$ is indexed by an N-tuple

$$k \sim x^{\mathrm{T}}\mathbf{E}^{\mathrm{T}}\boldsymbol{\varepsilon}\mathbf{E}$$

with components that are polynomials in λ with integer coefficients. The *integer* index set κ is then given by equation (13).

We saw in the $N=7$ example that λ was in this case a root of a cubic equation. It was proved by Gauss that $\cos(2\pi/N)$ is a root of a quadratic if and only if the odd prime factors of N are all different and all of the form $2^{2^n}+1$. In these cases $\mathbf{E}^{\mathrm{T}}\boldsymbol{\varepsilon}\mathbf{E}$ is linear in λ and we have

$$\kappa = x^{\mathrm{T}}\mathbf{A}, \qquad \mathbf{A} = \mathbf{A}(0) + \mathbf{A}(1)\mathbf{T}, \qquad \mathbf{A}(0) + \mathbf{A}(1)\lambda = \mathbf{E}^{\mathrm{T}}\boldsymbol{\varepsilon}\mathbf{E},$$

where $\mathbf{A}(0)$ and $\mathbf{A}(1)$ are rational matrices. It is a curious fact that the smaller N values with this property, 3, 4, 5, 6, 8, 10, 12, are just those corresponding to the symmetries of crystals and quasicrystals.

The standard icosahedral module in $\mathbf{E}_3$ is generated by six base vectors directed along the six fivefold axes of an icosahedron. They can be taken to be the columns of

$$\mathbf{E} = \begin{pmatrix} 1 & 0 & \tau & 0 & \tau & -1 \\ \tau & 1 & 0 & -1 & 0 & \tau \\ 0 & \tau & 1 & \tau & -1 & 0 \end{pmatrix}. \qquad (16)$$

If we sum the position vectors of the five vertices of an icosahedron nearest to a vertex $\mathbf{e}$, we obtain $5^{1/2}\mathbf{e}$. This corresponds to the inflation rule

$$\mathbf{T} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & -\mathbf{A} \end{pmatrix}, \qquad \lambda = 5^{1/2},$$

where $\mathbf{A} = \mathrm{cycl}\,(0\ 1\ 1)$ and $\mathbf{B} = \mathrm{cycl}\,(-\ 1\ 1\ 1)$. The projection matrix $\mathbf{P}$ turns out to be

$$\mathbf{P} = \frac{1}{2\times 5^{1/2}}\left(\mathbf{T} + \mathbf{I}\,5^{1/2}\right).$$

Splitting the index sets x and κ into pairs of triplets $x = [x^1, x^2]$, $\kappa = (\kappa_1, \kappa_2)$, we obtain the pair of rational zone laws

$$\kappa x = \kappa_1 x^1 + \kappa_2 x^2 = 0,$$
$$\kappa_1\mathbf{A}x^1 - \kappa_2\mathbf{A}x^2 + \kappa_1\mathbf{B}x_2 + \kappa_2\mathbf{B}x^1 = 0.$$

Loreto *et al.* (1990) have proposed approximate indexing schemes for icosahedral quasicrystals, in which τ in the expression $k = a + \tau b$ is replaced by a Fibonacci approximant (ratio of two successive terms of the Fibonacci sequence) to obtain sets of three integer indices that give a close approximation to the irrational indices.

Loreto *et al.* (1993) have also employed the zonal criterion extensively, in the context of icosahedral quasicrystals.

The standard indexing scheme for reciprocal vectors of icosahedral phases (Cahn *et al.* 1986) employs the six integers a_1, a_2, a_3, b_1, b_2 and b_3 in the expression $\mathbf{k} = \mathbf{a} + \tau\mathbf{b}$. They are conventionally written in the format

$$\left(\frac{a_1}{b_1}, \frac{a_2}{b_2}, \frac{a_3}{b_3}\right).$$

§ 7. Symmetry

The space group classification of periodic structures can be extended to aperiodic structures. The relevant space groups refer to spaces of higher dimension than the space in which the aperiodic structure resides (Janner and Janssen 1980a,b, Alexander 1986). (Janner and Janssen already employed higher dimensional methods in the context of incommensurate crystal phases, before the advent of quasicrystals.) Janssen (1986) explored the symmetry properties of quasicrystals and aperiodic tilings in terms of the theory of group representations (Boerner 1963, Burrow 1965). Here, we consider only the point-group symmetries of modules and demonstrate, by means of a few examples, how a module with a particular point-group symmetry can be generated (Duneau and Katz 1985, Katz and Duneau 1986).

The modules in E_2 discussed above may be called, for convenience, the C_N modules. The matrix $\mathbf{S} = \mathbf{E}\mathbf{E}^{\mathrm{T}}$ for all these cases is a multiple of the unit 2×2 matrix, so that $\mathbf{E}^*$ is, apart from a trivial factor, just the transpose of $\mathbf{E}$. The 'reciprocal vectors' $\mathbf{e}^i$ differ only in length from the module base vectors $\mathbf{e}_i$. This a very general feature of a set of vectors $\mathbf{e}^i$ 'generated by a point group'. If $\mathbf{e}_i$ are N vectors in E_n obtained from a single vector $\mathbf{v}$ by the action of a representation $\boldsymbol{\Gamma}$ of a point group G, we shall call the module a *G module*. The examples that we have used in previous sections are C_N modules. If $\mathbf{v}$ is 'special' in the sense that there is a non-trivial subgroup H that leaves $\mathbf{v}$ fixed, we shall call the resulting module a *G–H module*; the number of distinct base vectors

$$\mathbf{e}_i = \boldsymbol{\Gamma}(g_i)\mathbf{v}$$

is then $N = |G|/|H|$, one corresponding to each coset of the coset space G/H.

7.1. *Example 1*

The tetrahedral rotation group A_4. Its twelve elements are as follows:

$$\begin{aligned}
&e, \quad a_1 = (324), \quad a_2 = (134), \quad a_3 = (214), \quad a_4 = (123),\\
&a_1^2 = (234), \quad a_2^2 = (314), \quad a_3^2 = (124), \quad a_4^2 = (132),\\
&\gamma_1 = (14)(23), \quad \gamma_2 = (24)(31), \quad \gamma_3 = (34)(12).
\end{aligned}$$

The group is generated by $\boldsymbol{\gamma}_1$ and $\mathbf{a}_4$. The three-dimensional real representation arises when the abstract group is realized as the rotation group of the tetrahedron. We can choose

$$\gamma_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad \mathbf{a}_4 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

(i.e. twofold rotation about [100] and threefold rotation about [111]). If we choose $\mathbf{v} = [111]$, then H is C_3 and the four cosets are

$$\{e, a_4, a_4^2\}, \quad \{a_1, a_3^2, \gamma_2\}, \quad \{a_2, a_1^2, \gamma_3\}, \quad \{a_3, a_2^2, \gamma_1\}.$$

Four suitable coset representatives are

$$\mathbf{e} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}, \qquad \gamma_1 = \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix},$$

$$\gamma_2 = \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix}, \qquad \gamma_3 = \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}.$$

Operating on $\mathbf{v}$ with these four transformations we obtain the basis $\{\mathbf{e}_i\}$, $i = 1, \ldots, 4$, the columns of the matrix

$$\mathsf{E} = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

The rows are orthonormal if we introduce a normalization factor $\frac{1}{2}$. Suppose, alternatively, that we choose $\mathbf{v} = [100]$. Then $H = C_2$ and we have six cosets

$$\{e, \gamma_1\}, \quad \{a_1, a_3\}, \quad \{a_2, a_4\}, \quad \left\{a_1^2, a_2^2\right\}, \quad \left\{a_3^2, a_4^2\right\}, \quad \{\gamma_2, \gamma_3\}.$$

Operating on $\mathbf{v}$ with the six coset representatives, $\mathbf{e}$, $\mathbf{a}_1$, $\mathbf{a}_4$, $\mathbf{a}_1^2$, $\mathbf{a}_3^2$, γ_2, we obtain the basis $\{\mathbf{e}_i\}$, $i = 1, \ldots, 6$, given by the columns of the matrix

$$\mathsf{E} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

Introducing the normalization factor $1/2^{1/2}$, we again obtain a matrix E with orthonormal rows.

7.2. *Example 2*

The icosahedral rotation group, of order 60, is generated by

$$\boldsymbol{\beta} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\gamma} = \tfrac{1}{2}\begin{pmatrix} -\tau & 1 & -\sigma \\ 1 & -\sigma & \tau \\ -\sigma & \tau & -1 \end{pmatrix} \tag{17}$$

(i.e. a threefold rotation about [111] and a twofold rotation about $[-\sigma\ \tau\ 1]$; $\alpha = \beta\gamma$ is a fivefold rotation about $[1\ \tau\ 0]$). If $\mathbf{v}$ is a general vector, we obtain 60 vectors $\mathbf{e}_i$. By choosing $\mathbf{v}$ to be at a vertex, or at a face centre, or at the midpoint of an edge of the icosahedron, we have $H = C_5$ giving 12 vectors, $H = C_3$ giving 20 vectors, or $H = C_2$ giving 30 vectors, respectively. In each of these three cases the vectors occur in pairs $\pm\mathbf{e}_i$; so we obtain three kinds of icosahedral module, corresponding to generating matrices $\mathbf{E}$ that are 3×6, 3×10 or 3×15, respectively. The 3×6 matrix is given by equation (16). It generates the module underlying the standard icosahedral quasilattice: the tiling of E_3 by two rhombohedral units (Kramer and Neri 1984, Duneau and Katz 1985, Levine and Steinhardt 1985, Katz and Duneau 1986, Socolar and Steinhardt 1986).

The important relation $\mathbf{EE}^{\mathrm{T}}=\mathbf{I}$ that we noted for the C_N modules is valid for any G module for which the representation $\boldsymbol{\Gamma}$ of G that generates its set of base vectors is irreducible. This follows from the property

$$\sum_{g\in G}\Gamma^{\beta}_{\alpha}(g)\,\Gamma^{\delta}_{\gamma}(g^{-1})=\frac{|G|}{n}\delta^{\delta}_{\alpha}\,\delta^{\beta}_{\gamma} \tag{18}$$

of an n-dimensional irreducible representation $\boldsymbol{\Gamma}$ of a finite group G (Boerner 1963, Burrow 1965). The M–P inverse of $\mathbf{E}$ is then just the transpose of $\mathbf{E}$. The 'reciprocal module' associated with the G–H module L is then L itself (apart from a possible scaling factor).

§8. Projection

The concept of a 'quasilattice' has played a prominent role in the theoretical understanding of quasicrystal structure. A quasilattice is essentially a discrete set of points filtered out from a Z module through the imposition of a selection rule. In the standard projection method (Kramer and Neri 1984, Elser 1985, Katz and Duneau 1986) a hypercubic lattice in E_n is projected to two orthogonal subspaces $E_{\parallel}$ and $E_{\perp}$, giving a module in each. The selection is imposed by choosing a 'window' region in $E_{\perp}$ (Cahn and Gratias 1986). The quasilattice consists of the projected images in $E_{\parallel}$ of the selected points.

$\mathbf{EE}^{\mathrm{T}}=\mathbf{I}$ means that the rows of $\mathbf{E}$ are orthonormal. $N-n$ additional rows can be introduced, so that $\mathbf{E}$ is extended to an orthogonal $N\times N$ matrix

$$\mathbf{R}=\begin{pmatrix}\mathbf{E}\\ \mathbf{F}\end{pmatrix},\quad \mathbf{RR}^{\mathrm{T}}=\mathbf{I}, \tag{19}$$

that generates a primitive hypercubic lattice in E_N. Therefore, whenever $\mathbf{EE}^{\mathrm{T}}\sim\mathbf{I}$, the module generated by $\mathbf{E}$ is the image, under an orthogonal projection, of a hypercubic lattice in E_N on to an n-dimensional subspace $E_{\parallel}$. The $(N-n)$-dimensional subspace $E_{\perp}$ orthogonal to it contains a module generated by $\mathbf{F}$. This observation gives rise to the projection method for generating quasilattices.

There are an infinite number of matrices $\mathbf{F}$ that will extend $\mathbf{E}$ to an orthogonal matrix $\mathbf{R}$. They are related to each other by rotations in $E_{\perp}$.

In this prescription the projection matrices that project E_N to $E_{\parallel}$ and $E_{\perp}$ are, obviously, of the form $\left(\begin{smallmatrix}\mathbf{I}&\mathbf{0}\\ \mathbf{0}&\mathbf{0}\end{smallmatrix}\right)$ and $\left(\begin{smallmatrix}\mathbf{0}&\mathbf{0}\\ \mathbf{0}&\mathbf{I}\end{smallmatrix}\right)$. The hypercubic lattice is tilted, by the rotation $\mathbf{R}$, relative to the coordinate axes in E_N.

In an alternative but equivalent projection method (Conway and Knowles 1986) the hypercubic lattice is aligned with the coordinate axes, but the pair of subspaces $E_{\parallel}$ and $E_{\perp}$ are tilted. Observe that $\mathbf{EE}^{\mathrm{T}}=\mathbf{I}$ implies that $\mathbf{P}=\mathbf{E}^{\mathrm{T}}\mathbf{E}$, so that the vectors $\mathbf{p}_i$ in E_N given by the columns of $\mathbf{P}$ have the same lengths and angle relationships as the E_n vectors $\mathbf{e}_i$. That is,

$$\mathbf{P}^{\mathrm{T}}\mathbf{P}=\mathbf{E}^{\mathrm{T}}\mathbf{E},$$

or $\mathbf{p}_i \cdot \mathbf{p}_j = \mathbf{e}_i \cdot \mathbf{e}_j$. We can therefore identify the E_n spanned by the vectors $\mathbf{p}_i$ with $E_\parallel$. The space $E_\perp$ is then similarly spanned by the columns of $\mathbf{Q}$. The orthogonality of these two subspaces is a consequence of $\mathbf{PQ} = 0$ (i.e. $\mathbf{p}_i \cdot \mathbf{q}_j = 0$). In this approach the projection of the hypercubic lattice (generated by $\mathbf{I}$) is effected by the projection matrices $\mathbf{P}$ and $\mathbf{Q}$.

The problem of constructing a matrix $\mathbf{F}$ that extends $\mathbf{E}$ to a square orthogonal matrix $\mathbf{R}$ is usually solved by resorting to the theory of group representations (Jannsen 1986, Boerner 1963, Burrow 1965). Suppose that $\mathbf{e}$ is a general vector, so that $N = |G|$. An N-dimensional matrix representation of G is the regular representation, in which each element g is represented by the permutation matrix obtained by permuting the set of all elements of G by multiplying them by g.

The number of inequivalent irreducible representations of a finite group G is equal to the number k of equivalence classes of G (two elements g_1 and g_2 are 'equivalent' if there is an element g such that $gg_1g^{-1} = g_2$). The regular representation is equivalent to a direct sum of irreducible representations and contains each n_1-dimensional irreducible representation just n_1 times. Correspondingly,

$$n_1 + n_2 + \cdots + n_k = |G|. \tag{20}$$

8.1. *Example 1*

The irreducible representations of the icosahedral rotation group A_5 are two inequivalent three-dimensional representations, a four-dimensional representation, a five-dimensional representation and the trivial one-dimensional representation. Equation (20) becomes

$$1^2 + 3^2 + 3^2 + 4^2 + 5^2 = 60.$$

The two three-dimensional representations are related to each other by the interchange of τ and σ in their matrices ($5^{1/2} \to -5^{1/2}$). Taking $\mathbf{e} = [1\ \tau\ 0]$, $H = C_5$ and the three-dimensional representation given by equation (17), we obtain the matrix (16). Introducing a normalization factor to give the rows unit length, we have

$$\mathbf{E} = (\tau\beta 2^{1/2})^{-1} \begin{pmatrix} 1 & 0 & \tau & 0 & \tau & -1 \\ \tau & 1 & 0 & -1 & 0 & \tau \\ 0 & \tau & 1 & \tau & -1 & 0 \end{pmatrix}.$$

For the other three-dimensional representation we can take $\mathbf{e} = [1\ \sigma\ 0]$, which gives us

$$\mathbf{F} = (\beta 2^{1/2})^{-1} \begin{pmatrix} 1 & 0 & \sigma & 0 & \sigma & -1 \\ \sigma & 1 & 0 & -1 & 0 & \sigma \\ 0 & \sigma & 1 & \sigma & -1 & 0 \end{pmatrix}$$

$$= (\tau\beta 2^{1/2}) \begin{pmatrix} \tau & 0 & -1 & 0 & -1 & -\tau \\ -1 & \tau & 0 & -\tau & 0 & -1 \\ 0 & -1 & \tau & -1 & -\tau & 0 \end{pmatrix}.$$

Observe that the rows of $\mathbf{F}$ are orthogonal to those of $\mathbf{E}$. The hypercubic lattice from which the standard icosahedral quasilattice can be projected is thus generated by the resulting orthogonal matrix

$$\mathbf{R} = \begin{pmatrix} \mathbf{E} \\ \mathbf{F} \end{pmatrix} = (\tau\beta 2^{1/2})^{-1} \begin{pmatrix} 1 & 0 & \tau & 0 & \tau & -1 \\ \tau & 1 & 0 & -1 & 0 & \tau \\ 0 & \tau & 1 & \tau & -1 & 0 \\ \tau & 0 & -1 & 0 & -1 & -\tau \\ -1 & \tau & 0 & -\tau & 0 & -1 \\ 0 & -1 & \tau & -1 & -\tau & 0 \end{pmatrix}. \tag{21}$$

The splitting of E_6 into two three-dimensional spaces corresponds to the existence of a real six-dimensional reducible representation of A_5. The same method for the other two kinds of icosahedral module corresponds to a real ten-dimensional representation and a real fifteen-dimensional representation, with decompositions $10 = 4 \oplus 3 \oplus 3'$ and $15 = 5 \oplus 4 \oplus 3 \oplus 3'$.

The above example illustrates how an orthogonal $N \times N$ matrix $\mathbf{R}$ can be constructed out of the orthogonal representations of a group of order N. The orthogonality of the rows of a matrix $\mathbf{R}$ constructed in this way is guaranteed by equation (20) and the property

$$\sum_{g \in G} \Gamma^{\beta}_{\alpha}(g)\, \Gamma'^{b}_{a}(g) = 0 \tag{22}$$

of any pair of inequivalent irreducible representations of a group (Boerner 1963, Burrow 1965). It has been shown (Rokhsar *et al.* 1985) that there are just three quasilattices in E_3 obtainable by projection of a lattice in E_6, namely from the primitive, base-centred and face-centred hypercubic lattices.

We are here interested only in real matrices. However, any complex representation $\boldsymbol{\Gamma}$ is equivalent to a unitary representation ($\overline{\boldsymbol{\Gamma}}^{\mathrm{T}} = \boldsymbol{\Gamma}^{-1}$) and, from the matrices of an n-dimensional unitary representation, one can construct a $2n$-dimensional real orthogonal representation, by simply splitting every matrix $\boldsymbol{\Gamma}$ into its real and imaginary parts: $\boldsymbol{\Gamma} = \mathbf{A} + \mathrm{i}\mathbf{B}$. Then

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & \mathbf{A} \end{pmatrix}$$

is orthogonal. The complex conjugate representation $\overline{\boldsymbol{\Gamma}}$ gives a real $2n$-dimensional representation equivalent to that given by $\boldsymbol{\Gamma}$:

$$\mathbf{S}\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & \mathbf{A} \end{pmatrix}\mathbf{S}^{-1} = \begin{pmatrix} \mathbf{A} & -\mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{pmatrix}, \qquad \mathbf{S} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

8.2. *Example 2*

The irreducible representations of C_N are one dimensional. There are N of them. If N is odd, one of them (the trivial representation) is real and, if N is even, two of them are real. The rest are associated in conjugate complex pairs. Specifically, if $\mathbf{g}$ is the generator of the abstract group C_N ($g^N = e$), then g can be represented by a power of the Nth root of unity $\omega = \exp(i\theta)$, $\theta = 2\pi/N$. Take, for instance, the case

$N=5$. The five representations $\boldsymbol{\Gamma}_i$ $(i=1,\ldots,5)$ are given by taking $g=\omega^i$. Each pair of conjugate complex representations ($\boldsymbol{\Gamma}_1$, $\boldsymbol{\Gamma}_4$ or $\boldsymbol{\Gamma}_2$, $\boldsymbol{\Gamma}_3$) combines to give a real two-dimensional representation of the form

$$\mathbf{g}=\begin{pmatrix} c & s \\ -s & c \end{pmatrix},$$

one of them by taking $c=\cos(2\pi/5)=\sigma/2$ and $s=\sin(2\pi/5)=\beta\tau/2$. We obtain two orthogonal rows from the action of this representation on the vector $\mathbf{e}=[1,0]$. We obtain two more from the other two-dimensional representation, in which $c=\cos(4\pi/5)=-\tau/2$ and $s=\sin(4\pi/5)=\beta/2$. A fifth row comes from the trivial one-dimensional representation. Normalizing these rows to give them unit length gives us the orthogonal 5×5 matrix

$$\mathbf{R}=\frac{1}{10^{1/2}}\begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau \\ 2 & -\tau & -\sigma & -\sigma & -\tau \\ 0 & \beta & -\beta\tau & \beta\tau & \beta \\ 2^{1/2} & 2^{1/2} & 2^{1/2} & 2^{1/2} & 2^{1/2} \end{pmatrix}.$$

This generates a hypercubic lattice in E_5. The first two rows give the generating matrix for the C_5 module in $E_{\|}$ and the last three give a lattice in the three-dimensional perpendicular space E. If $\mathbf{R}$ and $\mathbf{M}$ are orthogonal N-dimensional matrices, then the $2N$-dimensional matrix

$$\mathbf{R}'=\frac{1}{2^{1/2}}\begin{pmatrix} \mathbf{R} & \mathbf{MR} \\ -\mathbf{M}^{\mathrm{T}}\mathbf{R} & \mathbf{R} \end{pmatrix}$$

is orthogonal. This observation can be exploited to construct modules by projection of hypercubic lattices on to subspaces. Let us consider a simple example in which $\mathbf{R}=\mathbf{I}_2$, $\mathbf{M}=(1/2^{1/2})\left(\begin{smallmatrix} 1 & 1 \\ -1 & 1 \end{smallmatrix}\right)$. $\mathbf{R}$ generates the square lattice in the plane and $\mathbf{M}$ is the matrix for a rotation through 45°:

$$\mathbf{R}'=\frac{1}{2^{1/2}}\begin{pmatrix} 2^{1/2} & 0 & 1 & 1 \\ 0 & 2^{1/2} & -1 & 1 \\ 1 & 1 & 2^{1/2} & 0 \\ -1 & 1 & 0 & 2^{1/2} \end{pmatrix}$$

generates a hypercubic lattice in E_4. Splitting this $\mathbf{R}'$ into two 2×4 matrices $\mathbf{E}$ and $\mathbf{F}$ according to equation (19) yields the prescription for obtaining the C_8 module by the projection method.

For a less trivial example, let $\mathbf{R}$ be the 5×5 matrix

$$\frac{1}{10^{1/2}}\begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau \\ 2^{1/2} & 2^{1/2} & 2^{1/2} & 2^{1/2} & 2^{1/2} \\ 2 & -\tau & -\sigma & -\sigma & -\tau \\ 0 & \beta & -\beta\tau & \beta\tau & -\beta \end{pmatrix}.$$

The first three rows give a 3×5 matrix that generates a C_5 module in E_3. If $\mathbf{M}^2=\mathbf{I}$, then $\mathbf{R}'$ gives a hypercubic lattice in E_{10} that projects to a D_5 module in E_3. There is a variety of different choices for $\mathbf{M}$ that give rise to modules in E_3 with various point symmetries.

If the matrix $\mathbf{F}$ in equation (19) is replaced by a rational matrix, the projection method gives rise to a periodic structure in $E_{\|}$. Linear dependence relations among the rows of $\mathbf{F}$ (with integer coefficients) correspond to periods of the structure in $E_{\|}$. This underlies the theoretical treatment of approximants of quasilattices and quasicrystals by projection methods. Orthorhombic approximants to the standard icosahedral quasilattice, for example, are obtained by replacing τ in each of the last three rows of equation (21) by Fibonacci approximants (p/q) where p and q are successive terms of the Fibonacci sequence. Taking out irrelevant overall factors from the resulting rows gives

$$\mathbf{F} = \begin{pmatrix} p_1 & 0 & -q_1 & 0 & -q_1 & -p_1 \\ -q_2 & p_2 & 0 & -p_2 & 0 & -q_2 \\ 0 & -q_3 & p_3 & -q_3 & -p_3 & 0 \end{pmatrix}.$$

Other types of periodic approximant arise from different choices of the rationalized $\mathbf{F}$ (Ishii 1991). The problem of relating the six-integer indexing scheme of the module to the ordinary crystallographic three-integer scheme appropriate to the approximant has been investigated by Quiquandon *et al.* (1999).

§ 9. Layered modules

The reducible three-dimensional representation of C_5, applied to a general vector $\mathbf{e}$, gives five vectors that do not all lie in a plane. Without loss of generality we may take them to be given by the columns of

$$\mathbf{E} \sim \begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau \\ z & z & z & z & z \end{pmatrix}. \tag{23}$$

(Here and in what follows the symbol $\sim$ will denote equality to within a normalization factor). These five vectors form a pyramidal configuration. An indexing scheme for decagonal quasicrystals based on this module has been proposed (Ho 1986). The three-dimensional module generated by this matrix consists of layers of a two-dimensional E_2 submodule and is periodic along the z axis with period $5z$ and has fivefold screw axes. Its point symmetry is $\bar{5}m$. It is quite different from the direct sum module generated by

$$\mathbf{E} \sim \begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma & 0 \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau & 0 \\ 0 & 0 & 0 & 0 & 0 & z \end{pmatrix}, \tag{24}$$

which consists of layers related by translation along the z axis and has period z. Its points symmetry is $10/mmm$. The indexing scheme for decagonal quasicrystals that this module provides (Choy *et al.* 1988, Fitz Gerald *et al.* 1988) has recently been successfully exploited (Singh and Ranaganathan 1996, Ranganathan *et al.* 1997).

The analogues of these two modules for $N = 3$ are the rhombohedral trigonal and the hexagonal Bravais lattices, respectively.

§ 10. The rank of a module

A vector $\mathbf{x} = \mathsf{E}x$ is not, in general, associated with a unique set of indices x. Since $\mathsf{EQ} = 0$, x and $x + \mathsf{Q}z$ label the same point $\mathbf{x}$. (We are, of course, concerned only with linear combinations $\mathsf{Q}z$ of the columns of Q that have integer components.) This redundancy can be removed by imposing conditions on the index sets x. Consider for example the C_3 module which is simply the plane hexagonal lattice. We have

$$\mathsf{E} = \tfrac{1}{2}\begin{pmatrix} 2 & -1 & -1 \\ 0 & 3^{1/2} & -3^{1/2} \end{pmatrix}.$$

The lattice points in the plane are specified by index sets $x = [x^1, x^2, x^3]$. For all integers m, $[x^1 + m, x^2 + m, x^3 + m]$ all specify the same lattice point $\mathbf{x} = \mathsf{E}x$. This redundancy is removed by requiring that $x^1 + x^2 + x^3 = 0$. The reciprocal indices k necessarily satisfy $k^1 + k^2 + k^3 = 0$ because of the identify $k\mathsf{Q} = 0$. In this example, k is rational; so we can take $\kappa = k$. (There are only 'trivial' inflation rules; inflation by integers; there is an inflation matrix $\mathsf{T} = \mathrm{cycl}\,(0 - 1 - 1)$ with 'inflation factor' $\lambda = 1$.) This example is, of course, Frank's scheme for indexing the hexagonal lattices. An alternative response to the redundancy is to reduce the number of base vectors.

The *rank* of a module generated by a matrix E (not to be confused with the rank of the matrix E) is the smallest number of base vectors that will generate it. For example, the C_N modules can be generated by fewer than N vectors. The identity $\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3 + \cdots + \mathbf{e}_N = \mathbf{0}$ shows immediately that at most $N - 1$ vectors are needed. If N is even, the module can be generated by only $N/2$ vectors, because $\mathbf{e}_0 = -\mathbf{e}_{N/2}$ & cycl. (here, the subscript labels are integers modulo N). If N is divisible by 3, we have $\mathbf{e}_0 + \mathbf{e}_{N/3} + \mathbf{e}_{2N/3} = \mathbf{0}$ & cycl. These obvious geometrical properties of regular N-gons enable us to deduce the following values for the ranks of the C_N-modules:

N odd, not divisible by 3: rank $N - 1$,

N odd, divisible by 3: rank $2N/3$,

N even, not divisible by 4: the C_N module is the same as the $C_{N/2}$ module,

N divisible by 4 but not by 3: rank $N/2$,

N divisible by 12: rank $N/3$.

A module of rank r generated by an $n \times N$ matrix E can equally well be generated by an $n \times r$ matrix E'. The four-index scheme for the planar C_5 module (Ostlund and Wright 1986) has been adopted by many researchers, in spite of the disadvantage that the fivefold symmetry is not self-evident in the notation.

The columns of E' are just r of the columns of E, and the remaining columns of E are linear combinations of them with integer coefficients. This relationship can be written $\mathsf{E} = \mathsf{E}'\mathsf{J}$, where J is $r \times N$. Similarly, there will be a reduced matrix E'' and an $N \times r$ matrix J' satisfying $\mathsf{E}^* = \mathsf{J}'\mathsf{E}''$. One can therefore employ reduced index sets x' and κ', satisfying $x' = \mathsf{J}x$, $\kappa' = \kappa\mathsf{J}'$. In terms of these reduced index sets, the zone law is

$$\kappa'\mathsf{P}'x' = 0, \qquad \mathsf{P} = \mathsf{E}''\mathsf{E}'.$$

10.1. *Examples*

$$C_5\text{:}\quad \mathbf{E}' = \tfrac{1}{2}\begin{pmatrix} -\sigma & -\tau & -\tau & -\sigma \\ \beta\tau & \beta & -\beta & -\beta\tau \end{pmatrix},\qquad \mathbf{J} = (\mathbf{J}')^{\mathrm{T}} = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Hence

$$\mathbf{P}' \sim \begin{pmatrix} 2 & -\sigma & -\tau & -\tau \\ -\sigma & 2 & -\sigma & -\tau \\ -\tau & -\sigma & 2 & -\sigma \\ -\tau & -\tau & -\tau & 2 \end{pmatrix},$$

giving the rational pair of zone laws

$$2(\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4) - (12) - (23) - (34) = 0,$$

$$(12) + (23) + (34) - (13) - (34) - (41) = 0.$$

$$C_8\text{:}\quad \mathbf{E}' = \tfrac{1}{2}\begin{pmatrix} 2 & 2^{1/2} & 0 & -2^{1/2} \\ 0 & 2^{1/2} & 2 & 2^{1/2} \end{pmatrix},\quad \mathbf{J} = (\mathbf{J}')^{\mathrm{T}} = (\mathbf{I}_4\ \ -\mathbf{I}_4).$$

$$\mathbf{P}' = \tfrac{1}{4}\begin{pmatrix} 2 & 2^{1/2} & 0 & -2^{1/2} \\ 2^{1/2} & 2 & 2^{1/2} & 0 \\ 0 & 2^{1/2} & 2 & 2^{1/2} \\ -2^{1/2} & 0 & 2^{1/2} & 2 \end{pmatrix},$$

giving the rational pair of zone laws

$$\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4 = 0,$$
$$(12) + (23) + (34) - (14) = 0.$$

$$C_{12}\text{:}\quad \mathbf{E}' \sim \begin{pmatrix} 1 & 3^{1/2} & 3^{1/2} & 1 \\ -3^{1/2} & -1 & 1 & 3^{1/2} \end{pmatrix},$$

$$\mathbf{J} = (\mathbf{J}')^{\mathrm{T}} = (\mathbf{K}\ \ -\mathbf{K}),\qquad \mathbf{K} = \begin{pmatrix} 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 & -1 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathbf{P}' = \tfrac{1}{4}\begin{pmatrix} 2 & 3^{1/2} & 0 & -1 \\ 3^{1/2} & 2 & 1 & 0 \\ 0 & 1 & 2 & 3^{1/2} \\ -1 & 0 & 3^{1/2} & 2 \end{pmatrix},$$

giving the rational pair of zone laws

$$2(\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4) + (23) - (14) = 0,$$

$$(12) + (34) = 0.$$

Scaling laws for these three cases are

$$C_5: \quad \mathbf{T} = \begin{pmatrix} 0 & 0 & -1 & -1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ -1 & -1 & 0 & 0 \end{pmatrix}, \quad \lambda = \tau,$$

$$C_8: \quad \mathbf{T} = \begin{pmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{pmatrix}, \quad \lambda = 2^{1/2},$$

$$C_{12}: \quad \mathbf{T} = \begin{pmatrix} 0 & 2 & 1 & 0 \\ 2 & 0 & 0 & -1 \\ -1 & 0 & 0 & 2 \\ 0 & 1 & 2 & 0 \end{pmatrix}, \quad \lambda = 3^{1/2}.$$

As we have noted, three kinds of icosahedral module can be identified, corresponding to $N = 6$, 10 and 15. All three icosahedral modules have rank six. Consider the 3×10 generating matrix

$$\mathbf{E} \sim \begin{pmatrix} -\sigma & \tau & 0 & 1 & -1 & 1 & 0 & \sigma & \tau & 1 \\ 0 & -\sigma & \tau & 1 & 1 & -1 & \tau & 0 & \sigma & 1 \\ \tau & 0 & -\sigma & -1 & 1 & 1 & \sigma & \tau & 0 & 1 \end{pmatrix}$$

(in which the columns correspond to the threefold axes of an icosahedron). For simplicity we denote the vectors $\mathbf{e}_i$ simply by their labels. They satisfy the identities

$$1 = 2 + 5 - 7 = 3 - 5 + 9 \text{ \& cycl.},$$

$$4 = -1 + 3 + 9 = -5 - 6 + 10 \text{ \& cycl.},$$

$$7 = -1 + 2 + 5 = -8 - 9 + 10 \text{ \& cycl.},$$

$$10 = 7 + 8 + 9.$$

(& cycl. in this context denotes the set of relations obtained by applying the permutation (123)(456)(789).) From these relations we select the four relations

$$7 = -1 + 2 + 5, \qquad 8 = -2 + 3 + 6, \qquad 9 = -3 + 1 + 4, \qquad 10 = 4 + 5 + 6.$$

That is, all ten vectors of the module are linear combinations, with integer coefficients, of the six vectors $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, $\mathbf{e}_4$, $\mathbf{e}_5$ and $\mathbf{e}_6$, and we have the reduced generating matrix

$$\mathsf{E} \sim \begin{pmatrix} -\sigma & \tau & 0 & 1 & -1 & 1 \\ 0 & -\sigma & \tau & 1 & 1 & -1 \\ \tau & 0 & -\sigma & -1 & 1 & 1 \end{pmatrix}.$$

The three rows are (apart from a normalization factor) orthonormal. Hence the module is a projection of a hypercubic lattice in E_6.

For the $N = 15$ case, we can take

$$\mathsf{E} = \begin{pmatrix} \tau & \tau & \tau & \tau & 1 & 1 & 1 & 1 & -\sigma & -\sigma & -\sigma & -\sigma & 2 & 0 & 0 \\ 1 & 1 & -1 & -1 & -\sigma & -\sigma & \sigma & \sigma & \tau & \tau & -\tau & -\tau & 0 & 2 & 0 \\ \sigma & -\sigma & -\sigma & \sigma & -\tau & \tau & \tau & -\tau & -1 & 1 & 1 & -1 & 0 & 0 & 2 \end{pmatrix}$$

(corresponding to the twofold axes of an icosahedron). The 15 vectors $\mathbf{e}_i$ satisfy

$$1 = 18 + 10, \qquad 2 = 7 + 9, \qquad 3 = 6 + 12, \qquad 4 = 5 + 11,$$

$$13 = 5 + 7 = 6 + 8, \qquad 14 = 1 - 4 = 2 - 3, \qquad 15 = 10 - 9 = 11 - 12.$$

It follows from these identities that all 15 vectors are linear combinations, with integer coefficients, of only six of them: choosing $\{\mathbf{e}_2, \mathbf{e}_6, \mathbf{e}_{10}, \mathbf{e}_{13}, \mathbf{e}_{14}, \mathbf{e}_{15}\}$ as the linearly independent basis, we have

$$\begin{pmatrix} 8 \\ -3 \\ -9 \\ 1 \\ -12 \\ 7 \\ -4 \\ 5 \\ 11 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 0 & 1 & -1 & -1 & 1 & 0 \\ -1 & 0 & 1 & 1 & 0 & -1 \\ 1 & -1 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 6 \\ 10 \\ 13 \\ 14 \\ 15 \end{pmatrix}.$$

The reduced matrix E in this case has orthogonal rows; the module generated by the six vectors is not in this case a projection from a six-dimensional hypercubic lattice.

§ 11. The decagonal modules

Consider again the module generated by equation (24):

$$\mathsf{E} = \begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma & 0 \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau & 0 \\ 0 & 0 & 0 & 0 & 0 & z \end{pmatrix}.$$

There is no inflation rule; the τ inflation rule of the layers is not compatible with the periodicity in the z direction, but the planes of the module can nevertheless be indexed by six integers. How this comes about is outlined below.

Take any two points $\mathbf{x} = \mathsf{E}x$ and $\mathbf{y} = \mathsf{E}y$, determining two zone axes and the plane containing them, with normal $\mathbf{k} = \mathbf{x} \times \mathbf{y}$. The (irrational) index set $k = \mathbf{k}\mathsf{E}$ is, apart from an overall factor, of the form $a + b\tau$, in which a and b are sextuples of integers. The important point to note is that the arbitrary number z is factored out at this stage. Multiplying k by $-(a_6 + b_6) + b_6\tau$, we obtain a k with its sixth component rational.

The projection matrix $\mathbf{P} = \mathbf{E}^*\mathbf{E}$ is, in terms of the corresponding 5×5 matrix $\mathbf{P}' = \frac{1}{5}\,\mathrm{cycl}\,(2 - \sigma - \tau - \tau - \sigma)$.

$$\mathbf{P} = \begin{pmatrix} \mathbf{P}' & 0 \\ 0 & \mathbf{1} \end{pmatrix}.$$

Thus, we obtain a set κ of six integers, $\kappa_6 = k_6 = a_6$ and $\kappa_i = a_i + b_j \mathbf{T}_i^j$, $i = 1, \ldots, 5$ ($\mathbf{T}$ is the inflation matrix (14) for the two-dimensional C_5 module). The zone law is (Singh and Ranganathan 1996)

$$\begin{aligned} &5\kappa_6 x^6 + 2(\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4 + \kappa_5 x^5) \\ &\quad - (12) - (23) - (34) - (45) - (51) \\ &\quad + \tau[(12) + (23) + (34) + (45) + (51) - (13) - (24) - (35) - (41) - (52)] = 0, \end{aligned} \tag{25}$$

giving a pair of rational zone laws.

11.1. *Example*

For the two points of the decagonal module indexed by $x = (110000)$ and $y = (100001)$ we find that $\mathbf{x} \sim [2 - \sigma,\ \beta\tau,\ 0]$, $\mathbf{y} \sim [2, 0, \gamma]$ and hence $\mathbf{k} \sim (z\beta\tau,\ z(\sigma - 2),\ -2\beta\tau)$. Then

$$k = \mathbf{kE} \sim (1\ \ -1\ 0\ 0\ 0\ \ -1) + \tau(0\ 0\ -1\ 0\ 1\ 0)$$

(b_6 already happens to be zero). Now, $(0\ 0\ -1\ 0\ 1)\ \mathbf{T} = (1\ -1\ -1\ 0\ 1\ 0)$; so we obtain

$$\kappa = (1\ \ -1\ 0\ 0\ 0\ \ -1) + (1\ \ -1\ \ -1\ 0\ 1\ 0) = (2\ \ -2\ \ -1\ 0\ 1\ \ -1).$$

§ 12. Redundancy of indices

An indexing scheme for a module of rank r that employs index sets with more than r indices has, *a priori*, a built-in redundancy; the vectors $\mathbf{x}$ and the reciprocal vectors $\mathbf{k}$ do not possess unique sets of integer indices. Because $\mathbf{EQ} = 0$ and $\mathbf{QE}^* = 0$, $\mathbf{x}$ and $\mathbf{k}$ with rational index sets x and κ such that

$$\mathbf{x} = \mathbf{E}x, \qquad \mathbf{k} = \kappa\mathbf{E}^*,$$

are also associated with the index sets $x + j$ and $\kappa + j'$ where j and j' are any rational sets that are linear combinations of the columns or rows of $\mathbf{Q}$.

As we have seen, this redundancy is absent in a scheme obtained from a reduced matrix $\mathbf{E}$ having only r columns. The use of a four-index scheme for the C_5 module in E_2 is quite common in the literature. The disadvantage of such a scheme is the loss of the straightforward role of the M–P inverse $\mathbf{E}^*$ as the generating matrix for the reciprocal module, and the fact that the point symmetries of the module act on the index sets in a clumsy and unnatural way.

An alternative approach to the redundancy is to impose restrictions on the index sets, without reducing the number of indices. A completely general statement of this method is the following. Let $\mathbf{J}$ be an $N \times (N - r)$ rational matrix whose columns are

$N-r$ linear combinations of the rows of $\mathbf{Q}$. Then, for any arbitrary rational index sets x and κ, we can apply the transformations

$$x \to x - \mathbf{JJ}^* x, \tag{26}$$

$$\kappa \to \kappa - \kappa \mathbf{JJ}^*. \tag{27}$$

We obtain, then, a unique set of indices for every vector **x** and every reciprocal vector **k** that satisfies

$$\mathbf{J}^* x = 0,$$

$$\kappa \mathbf{J} = 0.$$

12.1. *Example 1*

For a hexagonal lattice in E_3.

$$\mathbf{E} \sim \begin{pmatrix} 2 & -1 & -1 & 0 \\ 0 & 3^{1/2} & -3^{1/2} & 0 \\ 0 & 0 & 0 & z \end{pmatrix}.$$

In this case there is (apart from an overall factor) only one rational combination of the rows of $\mathbf{Q}$, namely $j=[1110]$, and the transformations (26) and (27) become

$$x \to x - \frac{j(j^{\mathrm{T}}x)}{(j^{\mathrm{T}}j)}, \tag{28}$$

$$\kappa \to \kappa - \frac{(\kappa j)j^{\mathrm{T}}}{(j^{\mathrm{T}}j)}. \tag{29}$$

The restricted index sets satisfy $j^{\mathrm{T}}x=0$ and $\kappa j=0$, i.e.,

$$x^1 + x^2 + x^3 = 0, \qquad \kappa_1 + \kappa_2 + \kappa_3 = 0.$$

This is, of course, Frank's scheme for indexing hexagonal lattices. For purposes of illustration, consider the two arbitrary index sets $x=[1101]$ and $y=[2100]$. The transformation (28) gives

$$x \to [1101] - \tfrac{2}{3}[1110] = \tfrac{1}{3}[11\bar{2}3] \sim [11\bar{2}3],$$

$$y \to [2100] - [1110] = [10\bar{1}0]$$

(which satisfy $x^1+x^2+x^3=0$ and $y^1+y^2+y^3=0$). The corresponding zone axes are $\mathbf{x} \sim [1, 3^{1/2}, z]$, $\mathbf{y} \sim [3, 3^{1/2}, 0]$ and hence $\mathbf{k} = \mathbf{x} \times \mathbf{y} \sim (-3^{1/2}z, 3z, -2 \times 3^{1/2})$. Therefore $\kappa = k = \mathbf{kE} \sim (\bar{1}2\bar{1}\bar{1})$ (which satisfies $\kappa_1+\kappa_2+\kappa_3=0$ necessarily, because, by definition, $kQ=0$).

An analogous treatment can be applied to Fitz Gerald's scheme for the layered decagonal module, for which

$$\mathbf{E} \sim \begin{pmatrix} 2 & -\sigma & -\tau & -\tau & -\sigma & 0 \\ 0 & \beta\tau & \beta & -\beta & -\beta\tau & 0 \\ 0 & 0 & 0 & 0 & 0 & z \end{pmatrix}.$$

Again, there is (apart from an overall factor) only one rational linear combination of the columns of $\mathbf{Q}$: $j=[111110]$. The transformations (28) and (29) applied to arbitrary sets of integers x and κ give rise to unique labels for the vectors $\mathbf{x}$ and $\mathbf{k}$ that satisfy

$$x^1 + x^2 + x^3 + x^4 + x^5 = 0, \qquad \kappa_1 + \kappa_2 + \kappa_3 + \kappa_4 + \kappa_5 = 0.$$

Note that the indices κ defined from equation (14) with the aid of the τ inflation rule of the C_5 module necessarily satisfy this condition, because $k\mathbf{Q} = 0$ for the (irrational) index sets $k = \mathbf{kE}$, and so $kj = 0$.

12.2. *Example 2*

Consider the index sets $x = [110100]$ and $y = [210001]$. Application of equation (28) converts them to $x' \sim [22\bar{3}230]$ and $y' \sim [33\bar{2}\bar{2}25]$. The directions referred to by these index sets are $\mathbf{x} = \mathbf{E}x \sim (1, -\beta\sigma, 0)$ and $\mathbf{y} = \mathbf{E}y \sim (\tau^2, \beta\tau, 0)$. $\mathbf{k} = \mathbf{x} \times \mathbf{y} = [\beta\sigma, 1, 0]$ is perpendicular to both. Its corresponding (irrational) index set is $k \sim [\sigma, -\sigma, 1, 0, -1, 0]$ and the rational set obtained (on account of the τ inflation rule for the submodules perpendicular to the periodic axis; see § 6) is $\kappa = [1\bar{1}20\bar{2}0]$.

§ 13. Fibonacci sequences

We review here the methods developed by Singh and Ranganathan (1996) for dealing with the indexing problem posed by decagonal quasicrystals. Fibonacci-type sequences of indices are identified, and the complicated zone laws for the layered decagonal module can be shown to be approximated by the simple expression

$$\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4 + \kappa_5 x^5 + \kappa_6 x^6 = 0 \tag{30}$$

when the inflation factor is sufficiently large. We shall then show how the approach of Singh and Ranganathan can be modified to deal with octagonal and dodecagonal quasicrystals.

The τ inflation matrix $\mathbf{T} = \mathrm{cycl}\,(00\bar{1}\bar{1}0)$ for the C_5 module in E_2 satisfies

$$\mathbf{T}^2 = \mathbf{T} + \mathbf{I} + \mathbf{U},$$

where $\mathbf{U}$ is the matrix all of whose elements are 1: $\mathbf{U} = \mathrm{cycl}\,(11111)$. Hence, if we employ indices κ for the reciprocal vectors that satisfy $\kappa\mathbf{U} = 0$, that is

$$\kappa_1 + \kappa_2 + \kappa_3 + \kappa_4 + \kappa_5 = 0, \tag{31}$$

then the repeated application of the τ inflation of a reciprocal vector $\mathbf{k}$ corresponds to a sequence of index sets $\kappa(0) = \kappa$, $\kappa(1) = \kappa\mathbf{T}$, $\kappa(2) = \kappa\mathbf{T}^2, \ldots$, in which each index set is the sum of the two previous sets: $\kappa(n+1) = \kappa(n) + \kappa(n-1)$. For example, starting from $[1\bar{1}000]$, we obtain the sequence

$$\begin{array}{llllll}
\kappa(0): & 1 & \bar{1} & 0 & 0 & 0, \\
\kappa(1): & 0 & 0 & \bar{1} & 0 & 1, \\
\kappa(2): & 1 & \bar{1} & \bar{1} & 0 & 1, \\
\kappa(3): & 1 & \bar{1} & \bar{2} & 0 & 2, \\
\kappa(4): & 2 & \bar{2} & \bar{3} & 0 & 3, \\
\kappa(5): & 3 & \bar{3} & \bar{5} & 0 & 5, \\
\kappa(6): & 5 & \bar{5} & \bar{8} & 0 & 8, \\
\vdots & & & & &
\end{array}$$

The numbers appearing in this sequence are the Fibonacci numbers

$$1 \quad 1 \quad 2 \quad 3 \quad 5 \quad 8 \quad 13 \quad 21 \ldots$$

generated by the recursion relation $F_{n+1} = F_{n-1} + F_n$. Thus $\kappa(n) = (F_{n-1}, -F_{n-1}, -F_n, 0, F_n)$. The limit of F_{n+1}/F_n is the 'golden number' τ; so we have

$$\lim_{n\to\infty}\left(\frac{\kappa(n)}{F_n}\right) = (\,-\sigma \;\; \sigma \;\; -1 \;\; 0 \;\; 1\,) = \frac{\kappa(0)}{5^{1/2}}\mathbf{P} \tag{32}$$

where $\mathbf{P}$ is the matrix

$$\mathbf{P} = \frac{1}{5^{1/2}}\,\mathrm{cycl}(\,2 \;\; -\sigma \;\; -\tau \;\; -\tau \;\; -\sigma\,).$$

Similarly, it can be established that this relation holds when $\kappa(0)$ is any one of the index sets $(1\bar{1}000)$, $(01\bar{1}00)$, $(001\bar{1}0)$, $(0001\bar{1})$ or $(\bar{1}0001)$. However, any 5-tuple satisfying equation (31) is a linear combination of these, so that equation (32) is true in general for the sequences generated from any 5-tuple $\kappa(0)$ satisfying equation (31). If follows, then (because $\mathbf{P}^2 = \mathbf{P}$), that for the higher terms in these sequences the expression $\kappa(n)\mathbf{P}$ is approximately equal to $\kappa(n)$. This in turn implies that the complicated zone law (25) for the layered decagonal module can be approximated by the simpler expression (30) if the inflation factor is sufficiently large.

Similar methods are possible for octagonal and dodecagonal quasicrystals. The C_8 module in E_2 has a $2^{1/2}$ inflation rule. This does not provide a scheme analogous to that described above for the C_5 module. However, consider the $1 + 2^{1/2}$ inflation rule. For the 2×4 generating matrix for the C_8 module given in § 10, the inflation matrix for the inflation factor $\lambda = 1 + 2^{1/2}$ is

$$\mathbf{T} = \begin{pmatrix} 1 & 1 & 0 & \bar{1} \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ \bar{1} & 0 & 1 & 1 \end{pmatrix}.$$

Starting with $\kappa(0) = (1000)$, successive multiplication by $\mathbf{T}$ gives the sequence

$$\begin{array}{lcccc}
\kappa(1): & 1 & 0 & 0 & 0, \\
\kappa(2): & 1 & 1 & 0 & \bar{1}, \\
\kappa(3): & 3 & 2 & 0 & \bar{2}, \\
\kappa(4): & 7 & 5 & 0 & \bar{5}, \\
\kappa(5): & 17 & 12 & 0 & \bar{1}\bar{2}, \\
\vdots & & & &
\end{array}$$

Since $\lambda^2 = 1 + 2\lambda$, number sequences generated by the recursion relation $F_{n+1} = F_n + 2F_{n-1}$ have the limit property $\lim(F_{n+1}/F_n) = \lambda$. Denoting the nth terms in the two sequences

$$1 \quad 1 \quad 3 \quad 7 \quad 17 \quad 41 \quad 99 \ldots,$$

$$0 \quad 1 \quad 2 \quad 5 \quad 12 \quad 29 \quad 70 \ldots,$$

by F_n and G_n respectively, a further relation is $F_n = G_n + G_{n-1}$ from which it follows that $F_n/G_n = 1 + G_{n-1}/G_n$. Taking the limit,

$$\lim_{n\to\infty}\left(\frac{F_n}{G_n}\right) = 2^{1/2}.$$

The nth term in the sequence of index sets is clearly $\kappa(n) = (F_n, G_n, 0, -G_n)$, so that

$$\lim_{n\to\infty}\left(\frac{\kappa(n)}{F_n}\right) = 2\kappa(0)\mathbf{P}, \tag{33}$$

where $\mathbf{P}$ is the projection matrix

$$\mathbf{P} = \tfrac{1}{4}\begin{pmatrix} 2 & 2^{1/2} & 0 & -2^{1/2} \\ 2^{1/2} & 2 & 2^{1/2} & 0 \\ 0 & 2^{1/2} & 2 & 2^{1/2} \\ -2^{1/2} & 0 & 2^{1/2} & 2 \end{pmatrix}$$

for the C_8 module. Similarly, it is easily established that equation (33) is also valid for the values (1000), (0100), (0010) and (0001) of $\kappa(0)$ and hence for any choice of $\kappa(0)$. Hence, for the five-index scheme for the layered octagonal module in E_3 (analogous to Fitz Gerald's scheme for the decagonal module) the complicated zone law can be approximated by

$$\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4 + \kappa_5 x^5 = 0.$$

For the layered C_{12} module we find that a similar scheme works if we employ six vectors perpendicular to the periodic axis, although the rank of the planar C_{12} module is in fact only four. That is, we choose

$$\mathbf{E} \sim \begin{pmatrix} 2 & 3^{1/2} & 1 & 0 & -1 & -3^{1/2} \\ 0 & 1 & 3^{1/2} & 2 & 3^{1/2} & 1 \end{pmatrix}$$

as the generating matrix for the planar C_{12} module. Then

$$\mathbf{P} = \tfrac{1}{6}\begin{pmatrix} 2 & 3^{1/2} & 1 & 0 & -1 & -3^{1/2} \\ 3^{1/2} & 2 & 3^{1/2} & 1 & 0 & -1 \\ 1 & 3^{1/2} & 2 & 3^{1/2} & 1 & 0 \\ 0 & 1 & 3^{1/2} & 2 & 3^{1/2} & 1 \\ -1 & 0 & 1 & 3^{1/2} & 2 & 3^{1/2} \\ -3^{1/2} & -1 & 0 & 1 & 3^{1/2} & 2 \end{pmatrix}.$$

Because the rank of the module is only four, the sets of reciprocal indices κ are not independent. They satisfy

$$\kappa_5 = \kappa_3 - \kappa_1, \qquad \kappa_6 = \kappa_4 - \kappa_2. \tag{34}$$

We have a $\lambda = 1 + 3^{1/2}$ inflation rule with inflation matrix

$$\mathbf{T} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & \bar{1} \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ \bar{1} & 0 & 0 & 0 & 1 & 1 \end{pmatrix}.$$

Any index set κ satisfying equation (34) is a linear combination of the index sets

$$(1000\bar{1}0),\ (01000\bar{1}),\ (001010),\ (000101). \tag{35}$$

Applying the matrix $\mathbf{T}$ repeatedly to any one of these four sets, we obtain a sequence in which each set is twice the sum of the previous two, corresponding to the property $\lambda^2 = 2(\lambda+1)$ of the inflation factor. For example,

$$\begin{array}{lrrrrrr}
\kappa(1): & 1 & 0 & 0 & 0 & \bar{1} & 0, \\
\kappa(2): & 1 & 1 & 0 & \bar{1} & \bar{1} & \bar{2}, \\
\kappa(3): & 4 & 2 & 0 & \bar{2} & \bar{4} & \bar{4}, \\
\kappa(4): & 10 & 6 & 0 & \bar{6} & \overline{10} & \overline{12}, \\
\kappa(5): & 28 & 16 & 0 & \overline{16} & \overline{28} & \overline{32}, \\
\vdots & & & & & &
\end{array}$$

In terms of the two sequences F and G,

$$\begin{array}{cccccc}
1 & 1 & 4 & 10 & 28 & 76\ldots, \\
0 & 1 & 2 & 6 & 16 & 44\ldots,
\end{array} \tag{36}$$

generated by the recursion relation $F_{n+1} = 2(F_n + F_{n-1})$,

$$\kappa(n) = (F_n, G_n, 0, -G_n, -F_n, -2G_n).$$

Other sequences can be generated similarly from the other sets given in equation (35). It readily follows, from the property

$$\lim\left(\frac{F_n}{G_n}\right) = 3^{1/2}$$

of the two number sequences (36) that, for any index set $\kappa(0)$ satisfying (33),

$$\lim_{n\to\infty}\left(\frac{\kappa(n)}{F_n}\right) = 2\kappa(0)\mathbf{P}.$$

Since $\mathbf{P}^2 = \mathbf{P}$, the terms $\kappa(n)\mathbf{P}$ occurring in the zone law for the layered C_{12} module in E_3 can, as in the previous cases C_5 and C_8, be approximated by $\kappa(n)$, and the complicated zone law has, correspondingly, this simple approximation

$$\kappa_1 x^1 + \kappa_2 x^2 + \kappa_3 x^3 + \kappa_4 x^4 + \kappa_5 x^5 + \kappa_6 x^6 + \kappa_7 x^7 = 0.$$

(The seventh term, of course, refers to the periodic axis.)

Acknowledgements

I thank Professor S. Ranganathan, for his interest in my work and for making the facilities of the Department of Metallurgy, Indian Institute of Science, available to me. Financial support from the Department of Science and Technology, New Delhi, the Office of Naval Research and the Defence, Research and Development Organisation, Ministry of Defence, Government of India is gratefully acknowledged.

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