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A multigrid approach to the average lattices of quasicrystals

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An average structure associated with a given quasilattice is a system composed of several average lattices that in reciprocal space produces strong main reflections. The average lattice of a quasicrystal is a useful concept closely related to the geometric description of the quasicrystal to crystal transformation and has been proved to be structurally significant. Here we calculate average structures for arbitrary two- and three-dimensional quasilattices using the dual generalized method. Additionally, closed analytical expressions for the coordinates of the average structure, the quasiperiodic lattice and its diffraction pattern are given.

1. Introduction

The concept of the average lattice was first introduced in the theory of incommensurate structures (see, for instance, Janner & Janssen, 1977). In quasicrystals, to define an average lattice has been proven to be possible and structurally significant (Duneau & Oguey, 1990; Wolny, 1998*a*; Xu & Mai, 1998; Steurer & Haibach, 1999; Steurer & Cervellino, 2001; Cervellino & Steurer, 2002). Here, we propose a general method to find average structures based on the so-called generalized dual method (GDM) to generate quasiperiodic lattices (Levine & Steinhardt, 1986; Socolar & Steinhardt, 1986). The proposed method allows us to obtain closed analytical expressions for the coordinates of the quasilattice, the average structure and its diffraction pattern. It is also shown that the average structure is composed of the superposition of average lattices and dominates the response for long-wave modes of the incident radiation.

To keep things as simple as possible, we introduce our formalism for two-dimensional quasilattices. So, we shall first use the GDM to obtain analytical expressions for the vertex coordinates of a two-dimensional quasiperiodic tiling. From the obtained formulae, it can be easily seen that the quasilattice can be expressed as an average structure plus small fluctuations. In some sense, this is a generalization of the observation made for the one-dimensional Fibonacci chain, where the positions can be written as an average lattice plus a fluctuation part (Naumis *et al.*, 1999), and in fact a unit cell can be defined by using a probabilistic approach (Wolny, 1998*b*). The behavior of the quasilattice for excitations of any kind with long-wave modes can be related to this average structure, and the complete diffraction pattern can be obtained from the expressions given by the GDM, and by using a Fourier series for the fluctuation part. The generalization of the method for three-dimensional quasilattices is given in §5.

2. Analytical expression for a quasilattice

By following the steps of the GDM to obtain plane quasiperiodic structures, we find an expression for the coordinates of the quasilattice. The GDM procedure is written in cursives; for further details, the reader is referred to Levine & Steinhardt (1986) and Socolar & Steinhardt (1986).

I. *Construct a star of N basis vectors* $\mathbf{e}_j$*, which contains the symmetry that the quasilattice is expected to have.*

For an octagonal tiling, for example, $N = 4$ and the basis vectors $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_4\}$ point to four vertices of a regular octagon.

II. *Construct a set of parallel lines perpendicular to each star vector to obtain a grid. These lines satisfy*

$$\mathbf{x}\cdot\mathbf{e}_j = n_j + \alpha_j,$$

where n_j *is an integer,* $\mathbf{x}$ *is a vector in 2D and* α_j *are shifts of the grid with respect to zero. The grid divides the space in open regions limited by planes. Each point in these spaces can be indexed by a set of integers corresponding to its ordinal position in the grid (given by* n_j*) for each* $\mathbf{e}_j$*, i.e., if a point in an open region lies between the planes* k_j *and* $k_j + 1$*, for the direction* $\mathbf{e}_j$*, we assign the number* k_j *to this region. A similar construction can be made for each star vector, to obtain the N ordinal coordinates* $(k_1, k_2, \ldots, k_N)$*.*

According to this step, regions to be mapped are defined by the intersection of two lines in 2D, which produces the four vertices of a cell. For each combination of star vectors, these intersections are the solutions of

$$\mathbf{x}\cdot\mathbf{e}_j = x_{n_j} = n_j + \alpha_j,$$
$$\mathbf{x}\cdot\mathbf{e}_k = x_{n_k} = n_k + \alpha_k,$$

where n_j and n_k are integers. The solutions of this system, the points $\mathbf{d}(jk)$, can be obtained by Kramer's rule and are given by

$$\mathbf{d}(jk) = x_{n_j}\mathbf{u}_{jk} + x_{n_k}\mathbf{u}_{kj},$$

where

$$\mathbf{u}_{jk} = \mathbf{e}_j^{\perp}/a_{jk}, \tag{1}$$

$\mathbf{e}_j^{\perp}$ is a vector perpendicular to $\mathbf{e}_j$ and a_{jk} is the area of the rhombus generated by $\mathbf{e}_j$ and $\mathbf{e}_k$.

Now consider the family of lines generated by the vectors $\mathbf{e}_j$ and $\mathbf{e}_k$. A close analysis shows that around each intersection there are four regions with ordinal coordinates $(n_j, n_k, f(n_j, n_k))$, $(n_j, n_k+1, f(n_j, n_k))$, $(n_j+1, n_k, f(n_j, n_k))$, $(n_j+1, n_k+1, f(n_j, n_k))$, where $f(n_j, n_k)$ are the ordinal coordinates with respect to the grid lines generated by the vectors that are different from $\mathbf{e}_j$ and $\mathbf{e}_k$. Each of these points generates a vertex of a rhombus. The function $f(n_j, n_k)$ can be obtained by the dot product between the point $\mathbf{d}(jk)$ with each star vector, and then by using the lowest integer function (denoted by $\lfloor x \rfloor$). Thus, for the direction $\mathbf{e}_l$, the corresponding ordinal coordinates are

$$k_l = \lfloor (x_{n_j}\mathbf{u}_{jk} + x_{n_k}\mathbf{u}_{kj})\cdot\mathbf{e}_l - \alpha_l \rfloor + 1, \tag{2}$$

where the one arises from the way in which one is labelling the space between grids.

III. *The quasilattice is obtained by using the dual transformation that associates with each open region the point*

$$\mathbf{t} = \sum_{j=1}^{N} k_j \mathbf{e}_j$$

in the dual space. The point $\mathbf{t}$ *is a vertex of a quasiperiodic packing of rhombic unit cells with an orientational symmetry corresponding to the star vectors* $\mathbf{e}_j$.

From (2), the dual transformation can be explicitly done to obtain one of the vertices associated with the intersection of lines j and k:

$$\mathbf{t}^0_{n_j,n_k} = n_j\mathbf{e}_j + n_k\ \mathbf{e}_k + \sum_{l\neq j\neq k}\{\lfloor (x_{n_j}\mathbf{u}_{jk} + x_{n_k}\mathbf{u}_{kj})\cdot\mathbf{e}_l - \alpha_l\rfloor + 1\}\mathbf{e}_l.$$

The complete set of vertices associated with the intersections are obtained by considering the $\binom{N}{2}$ pairs (jk). This, and (1), allows us to write the dual transformation as

$$\mathbf{t}^0_{n_j,n_k} = \sum_{k<j}^{N}\Bigg[n_j\mathbf{e}_j + n_k\mathbf{e}_k + \sum_{l\neq j\neq k}\left(\left\lfloor x_{n_j}\frac{b_{jl}}{a_{jk}} + x_{n_k}\frac{b_{kl}}{a_{jk}} - \alpha_l\right\rfloor + 1\right)\mathbf{e}_l\Bigg], \tag{3}$$

where $b_{ml} = \mathbf{e}_m^{\perp}\cdot\mathbf{e}_l$, $m = k, l$. The other three regions generate the remaining three vertices of each rhombus, with coordinates given by

$$\begin{aligned}\mathbf{t}^1_{n_j,n_k} &= \mathbf{t}^0_{n_j,n_k} - \mathbf{e}_j,\\ \mathbf{t}^2_{n_j,n_k} &= \mathbf{t}^0_{n_j,n_k} - \mathbf{e}_k,\\ \mathbf{t}^3_{n_j,n_k} &= \mathbf{t}^0_{n_j,n_k} - \mathbf{e}_j - \mathbf{e}_k.\end{aligned} \tag{4}$$

Equations (3) and (4) provide an analytical expression for the vertices of the quasilattice in two dimensions. Notice that, as a consequence of the dualization procedure, where a tile is associated with a single intersection of the grid, the expressions for each point in the quasilattice are not unique. A vertex of the tile can arise from Z different intersection points, where Z is the coordination number of the site. As we will see, this over-counting has an important effect in the definition of the average structure.

3. The average structure

By using the identity $x = \lfloor x\rfloor + \{x\}$ in (3), where $\{x\}$ denotes the decimal part of a number, we have

$$\begin{aligned}\mathbf{t}^0_{n_j,n_k} = \sum_{k<j}^{N}\Bigg[& n_j\mathbf{e}_j + n_k\mathbf{e}_k\\ &+ \sum_{l\neq j\neq k}\left[\left(x_{n_j}\frac{b_{jl}}{a_{jk}} + x_{n_k}\frac{b_{kl}}{a_{jk}} - \alpha_l\right) + \frac{1}{2}\right]\mathbf{e}_l\\ &+ \sum_{l\neq j\neq k}\left(\tfrac{1}{2} - \left\{x_{n_j}\frac{b_{jl}}{a_{jk}} + x_{n_k}\frac{b_{kl}}{a_{jk}} - \alpha_l\right\}\right)\mathbf{e}_l\Bigg],\end{aligned}$$

which can be written as

$$\mathbf{t}^0_{n_j,n_k} = \langle\mathbf{t}^0_{n_j,n_k}\rangle + \mathbf{f}^0_{n_j,n_k}. \tag{5}$$

The first term of the right side defines an average structure

$$\langle\mathbf{t}^0_{n_j,n_k}\rangle = \sum_{k<j}^{N}\Bigg[n_j\mathbf{e}_j + n_k\mathbf{e}_k + \sum_{l\neq j\neq k}\left(x_{n_j}\frac{b_{jl}}{a_{jk}} + x_{n_k}\frac{b_{kl}}{a_{jk}} - \alpha_l + \frac{1}{2}\right)\mathbf{e}_l\Bigg], \tag{6}$$

and the last one is a fluctuation part

$$\mathbf{f}^0_{n_j,n_k} = \sum_{k<j}^{N}\sum_{l\neq j\neq k}^{N}\left(\tfrac{1}{2} - \left\{x_{n_j}\frac{b_{jl}}{a_{jk}} + x_{n_k}\frac{b_{kl}}{a_{jk}} - \alpha_l\right\}\right)\mathbf{e}_l, \tag{7}$$

which we expect to have zero average in the sense that

$$\sum_{\mathbf{r}}(\langle\mathbf{r}\rangle - \mathbf{r}) = 0$$

because $\{\beta x\}$ covers in a dense and regular way the interval $[0, 1)$ if β is an irrational number.

The structure of $\langle\mathbf{t}^0_{n_j,n_k}\rangle$ is better appreciated if we rewrite (6) as

$$\langle\mathbf{t}^0_{n_j,n_k}\rangle = \sum_{k<j}^{N}(n_j\mathbf{a}_{jk} + n_k\mathbf{a}_{kj} + \mathbf{R}_{jk}), \tag{8}$$

where

$$\mathbf{a}_{jk} = \mathbf{e}_j + \sum_{l \neq j \neq k} b_{jl}/a_{jk}\mathbf{e}_l, \tag{9a}$$

$$\mathbf{a}_{kj} = \mathbf{e}_k + \sum_{l \neq j \neq k} b_{kl}/a_{jk}\mathbf{e}_l \tag{9b}$$

and

$$\mathbf{R}_{jk} = \sum_{l \neq j \neq k} \left(\alpha_j \frac{b_{jl}}{a_{jk}} + \alpha_k \frac{b_{kl}}{a_{jk}} - \alpha_l + \tfrac{1}{2} \right) \mathbf{e}_l. \tag{10}$$

Observe then that the average structure consists of a superposition of $\binom{N}{2}$ lattices with basis given by (9) plus shift terms given by (10). As in the case of the expressions for the quasilattice, the complete structure is obtained from (8) and

$$\begin{aligned} \langle \mathbf{t}^1_{n_j,n_k} \rangle &= \langle \mathbf{t}^0_{n_j,n_k} \rangle - \mathbf{e}_j, \\ \langle \mathbf{t}^2_{n_j,n_k} \rangle &= \langle \mathbf{t}^0_{n_j,n_k} \rangle - \mathbf{e}_k, \\ \langle \mathbf{t}^3_{n_j,n_k} \rangle &= \langle \mathbf{t}^0_{n_j,n_k} \rangle - \mathbf{e}_j - \mathbf{e}_k. \end{aligned} \tag{11}$$

As discussed at the end of the previous section, the dualization process introduces a degeneracy in (3) and (4) to generate the quasilattice. If a point $\mathbf{r}$ of the quasilattice is obtained from the intersection of two lines generated by the vectors $\mathbf{e}_j$ and $\mathbf{e}_k$, it can also be obtained from the intersection of two lines generated by two different vectors, say $\mathbf{e}_s$ and $\mathbf{e}_t$. When the average structure is considered, it turns out that these two intersection points do not necessarily produce the same point of the lattice. In fact, for each point in the quasilattice, we have Z points in the average structure. Since a quasilattice admits infinite average lattices (Cervellino & Steurer, 2002), one can always arbitrarily choose one of these Z points in order to define a possible average structure.

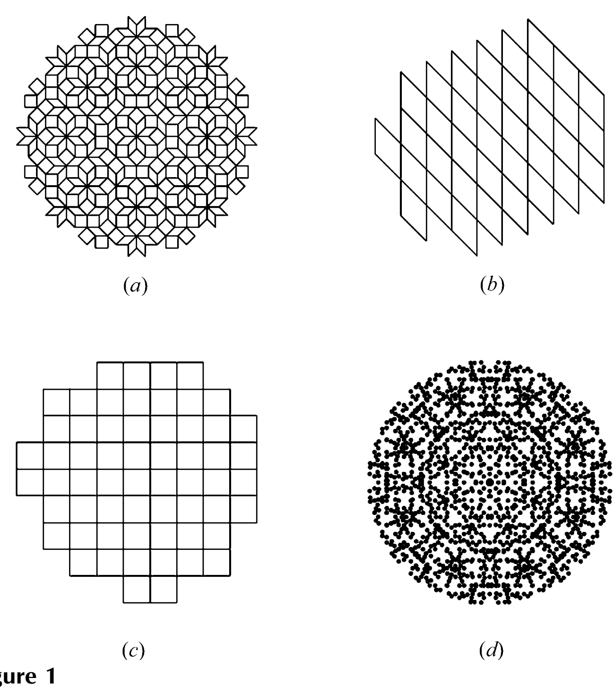

Figure 1
(*a*) The octagonal tiling obtained with equations (3) and (4), with shifts $\boldsymbol{\alpha} = (1/2, 1/2, 1/2, 1/2)$. Portions of the basic average lattices L_{21} (*b*) and L_{31} (*c*) that compose the average structure (*d*) of the octagonal tiling.

3.1. The average structure of the octagonal tiling

The octagonal tiling is generated with the star of vectors pointing to four vertices of a regular octagon:

$$\begin{aligned} \mathbf{e}_1 &= (1, 0), \\ \mathbf{e}_2 &= (1/2^{1/2})(1, 1), \\ \mathbf{e}_3 &= (0, 1), \\ \mathbf{e}_4 &= (1/2^{1/2})(-1, 1). \end{aligned}$$

In Fig. 1(*a*), a portion of the octagonal quasiperiodic tiling obtained with the above vectors and formulae (3) and (4), with shifts $\alpha = (1/2, 1/2, 1/2, 1/2)$, is shown.

According to (8), the average structure $\langle \mathbf{t}^0_{n_j,n_k} \rangle$ consists of the superposition of $\binom{4}{2} = 6$ average lattices plus the corresponding shift terms. By using the previous vectors and the shift $\boldsymbol{\alpha}$ in (8), we can deduce that these six average lattices fall into two basic classes generated by

$$\Lambda_1 = \{(0, 2 \times 2^{1/2}), (2, -2)\}$$

and

$$\Lambda_2 = \{(2, 0), (0, 2)\},$$

respectively. In particular, if $R_{\pi/4}$ denotes a rotation by $\pi/4$, the six possible average lattices are:

$$\begin{aligned} L_{21} &= Span\{\Lambda_1\}, \\ L_{32} &= Span\{R_{\pi/4}\Lambda_1\}, \\ L_{43} &= Span\{R^2_{\pi/4}\Lambda_1\}, \\ L_{41} &= Span\{R^3_{\pi/4}\Lambda_1\}, \\ L_{31} &= Span\{\Lambda_2\}, \\ L_{42} &= Span\{R_{\pi/4}\Lambda_2\}. \end{aligned} \tag{12}$$

By $Span\{\Lambda\}$, we mean that the term is generated by linear integer combinations of the basis Λ. The corresponding shift terms R_{jk} are obtained from (10) and are given by

$$\begin{aligned} \mathbf{R}_{21} &= \left(\frac{2 - 2^{1/2}}{4}, -1 + \frac{3}{2 \times 2^{1/2}} \right) \\ \mathbf{R}_{32} &= \left(-1 + \frac{3}{2 \times 2^{1/2}}, \frac{2 - 2^{1/2}}{4} \right), \\ \mathbf{R}_{43} &= \left(1 - \frac{3}{2 \times 2^{1/2}}, \frac{2 - 2^{1/2}}{4} \right), \\ \mathbf{R}_{41} &= \left(\frac{2 + 2^{1/2}}{4}, 1 + \frac{3}{2 \times 2^{1/2}} \right), \\ \mathbf{R}_{31} &= \left(\tfrac{1}{2}, \tfrac{1}{2} \right), \\ \mathbf{R}_{42} &= \left(0, \frac{1}{2^{1/2}} \right). \end{aligned}$$

The complete average structure is the superposition of these six lattices, with the corresponding shift terms, and those obtained with (11). Portions of the two basic average lattices L_{21} and L_{31} are shown in Figs. 1(*b*) and (*c*), respectively. In Fig.

1(d), a portion of the average structure of the octagonal quasilattice is shown.

As we will see in the next section, the importance of the average structure relies on its diffraction properties since it contains a significant fraction of the scattered intensity of the associated quasiperiodic structure. Also, it will be shown that the average structure dominates the response for long-wave modes of incident radiation.

4. Diffraction

The diffraction properties of the quasilattice and the average structure are associated with their Fourier transform. Using the decomposition (5), the Fourier transform of the quasilattice with vertices $\mathbf{t}$ is given by

$$F(\mathbf{q}) = \sum_{\mathbf{t}+\mathbf{f}} \exp(i\mathbf{q}\cdot\langle\mathbf{t}\rangle)\exp(i\mathbf{q}\cdot\mathbf{f}). \tag{13}$$

Since $\mathbf{f}$ is a vector with a norm smaller than one, it can be expanded as a power series for small $\mathbf{q}$:

$$\exp(i\mathbf{q}\cdot\mathbf{f}) \approx 1 + i\mathbf{q}\cdot\mathbf{f} + (\mathbf{q}\cdot\mathbf{f})^2/2 + \dots .$$

This suggests that the amplitudes are scaled as powers of $\mathbf{q}$, where the first-order contribution is given by the average structure. One then can conclude that, in many cases, the average structure dictates the response for long wavelengths of the probing particles, and the fluctuation part gives the corrections. At long wavelengths, the probe particle is not affected by the details of the quasiperiodic potential, and only feels an average effective potential.

The fluctuation term can be treated analytically owing to the periodic nature of the fractional part function. To make things easier, in what follows we set the shifts $\boldsymbol{\alpha}$ to zero since scattering intensities are not affected by this phase. Let us first write (13) as

$$F(\mathbf{q}) = \sum_{j<k}\sum_{n_j,n_k} h_{n_j,n_k}(\mathbf{q})\exp(i\mathbf{q}\cdot\langle\mathbf{t}^0_{n_j,n_k}\rangle)\exp(i\mathbf{q}\cdot\mathbf{f}^0_{n_j,n_k}), \tag{14}$$

where $h_{n_j,n_k}(\mathbf{q})$ is a factor that comes from (4), and is given by

$$h_{n_j,n_k}(\mathbf{q}) = \frac{1}{Z_{n_j,n_k}} + \frac{\exp(-i\mathbf{q}\cdot\mathbf{e}_j)}{Z_{n_j-1,n_k}} + \frac{\exp(-i\mathbf{q}\cdot\mathbf{e}_k)}{Z_{n_j,n_k-1}} + \frac{\exp[-i\mathbf{q}\cdot(\mathbf{e}_j+\mathbf{e}_k)]}{Z_{n_j-1,n_k-1}},$$

where Z_{n_j,n_k} is the local coordination in each site. This term is introduced to compensate for the overcounting. Since $\{x\}$ is a function with period one, the fluctuation $\mathbf{f}^0_{n_j,n_k}$ [see (7)] can be expressed as a Fourier series at $x = n_j$ and $y = n_k$:

$$S_l(x, y) \equiv \exp\left(-i\mathbf{q}\cdot\mathbf{e}_l\left\{x\frac{b_{jl}}{a_{jk}} + y\frac{b_{kl}}{a_{jk}}\right\}\right).$$

Thus,

$$S_l(x, y) = \sum_{f,g} B(f, g)\exp\left[2\pi i\left(\frac{fx}{T_1} + \frac{gy}{T_2}\right)\right],$$

where f and g are integers,

$$B(f, g) = \frac{1}{T_1T_2}\int_0^{T_1}\int_0^{T_2}\mathrm{d}x\,\mathrm{d}y \times \exp\left[-2\pi i\left(\frac{fx}{T_1} + \frac{gy}{T_2}\right) - i\mathbf{q}\cdot\mathbf{e}_l\left\{\frac{x}{T_1} + \frac{y}{T_2}\right\}\right]$$

and

$$T_1 = \frac{a_{jk}}{b_{jl}}, \quad T_2 = \frac{a_{jk}}{b_{kl}}.$$

$B(f, g)$ can be evaluated using the relationship $\{x + y\} = x + y$ when $\{x\} + \{y\} < 1$, provided that special care is taken with the integration limits to always fulfil this condition. After some lengthy calculations, we obtain

$$B(g) \equiv B(f, g) = \begin{cases} 0 & \text{if } f \neq g \\ \dfrac{-i\exp(-i\mathbf{q}\cdot\mathbf{e}_l) - 1}{2\pi g + \mathbf{q}\cdot\mathbf{e}_l} & \text{if } f = g. \end{cases}$$

Since for each l in (3) we can write a similar expression, we define a vector $\mathbf{g} = (g_1, g_2, \dots, g_N)$, where each component is an arbitrary integer. With this vector, the fluctuation part of the FT is

$$\sum_{\mathbf{g}}\left(\prod_{l\neq j\neq k} B(g_l)\right)\exp\left[\sum_{l\neq j\neq k} 2\pi i g_l\left(n_j\frac{b_{jl}}{a_{jk}} + n_k\frac{b_{kl}}{a_{jk}}\right)\right].$$

Consequently, using (14), (6) and this last result, the total FT is

$$F(\mathbf{q}) = \sum_{n_j,n_k,g_l} h_{n_j,n_k}(\mathbf{q})\left(\prod_{l\neq j\neq k} B(g_l)\right)\exp\left[i\mathbf{q}\cdot\left(n_j\mathbf{e}_j + n_k\mathbf{e}_k\right) + i\sum_{l\neq j\neq k}\left(n_j\frac{b_{jl}}{a_{jk}} + n_k\frac{b_{kl}}{a_{jk}}\right)(\mathbf{q}\cdot\mathbf{e}_l + 2\pi g_l)\right]. \tag{15}$$

A clear drawback of this formula is that the coordination Z_{n_j,n_k} of each site must be known. Although it has this analytical difficulty, the method is much more efficient than the cut-and-projection method, where a complicated algorithm for determining the volume of the acceptance domain is needed. Equation (15) can be approximated by considering the fluctuations of the local coordination ($\Delta Z_{n_j,n_k}$) with respect to the average coordination number $\langle Z\rangle$ as follows:

$$\frac{1}{Z_{n_j,n_k}} = \frac{1}{\langle Z\rangle + \Delta Z_{n_j,n_k}} \simeq \frac{1}{\langle Z\rangle}\left(1 - \frac{\Delta Z_{n_j,n_k}}{\langle Z\rangle}\right).$$

As an approximation, we retain only the first term, in such a way that the coordination of each site is replaced by an average coordination. The effect of this truncation is that the amplitudes in each diffraction spot are changed but the positions of the spots, in the reciprocal space, are not altered. A very rough estimation of the error introduced with this approximation can be given if we observe that $\Delta Z_{n_j,n_k}$ has a certain distribution. Since each type of vertex has a concentration $P(Z)$ in the lattice, the magnitude of the error is of the order of the standard deviation of $P(Z)$:

$$\frac{\Delta Z_{n_j,n_k}}{\langle Z\rangle} \sim \frac{(\Delta Z)^{-2}}{\langle Z\rangle} = \frac{1}{\langle Z\rangle}\left[\sum_{\mu} P(Z_\mu)(Z_\mu - \langle Z\rangle)^2\right]^{1/2},$$

where μ is the kind of vertex. For example, in the octagonal tiling, discussed in §3.1, $\mu = 3, 4, 5, 6, 7, 8$, each occurring with frequencies $f_3 = \omega$, $f_4 = 2\omega^2$, $f_5 = 2\omega^3$, $f_6 = 2\omega^4$, $f_7 = \omega^5$ and $f_8 = \omega^4$, $\omega = 2^{1/2} - 1$. The average coordination is, then, $\langle Z\rangle = \sum_{i=3}^{8} i f_i = 4$. The maximum deviation is $\Delta Z_{n_j,n_k} = 4$, which corresponds to $Z = 8$. The concentration of these vertices is, however, very low (2.9%) since the more frequent vertices are those with coordination $Z = 3$, $Z = 4$ and $Z = 5$ (41.4, 34.3 and 14.2%, respectively).

By use of the Fourier series of the δ function in (15), the sum over n_j and n_k can be carried out, and using this result in (13) we finally get

$$F(\mathbf{q}) = \sum_{j<k,\mathbf{g}} h_{jk}(\mathbf{q}) \left(\prod_{l\neq j\neq k} B(g_l) \right) \times \delta\left(\mathbf{q}\cdot\mathbf{e}_j + \sum_{l\neq j\neq k} \frac{b_{jl}}{a_{jk}} (\mathbf{q}\cdot\mathbf{e}_l + 2\pi g_l) + 2\pi m_j \right) \times \delta\left(\mathbf{q}\cdot\mathbf{e}_k + \sum_{l\neq j\neq k} \frac{b_{kl}}{a_{jk}} (\mathbf{q}\cdot\mathbf{e}_l + 2\pi g_l) + 2\pi m_k \right),$$

where m_j and m_k are integers. The function $h_{jk}(\mathbf{q})$ is similar to $h_{n_j,n_k}(\mathbf{q})$ except for the fact that the local coordination has been replaced by the average coordination. Notice that the two δ functions define the positions of the diffraction spots, thus defining the reciprocal lattice of the quasicrystal, as will be clarified in what follows.

$F(\mathbf{q})$ is different from zero if the two δs are satisfied simultaneously for a given value of the probe wavevector $\mathbf{q}$. Thus, $\mathbf{q}$ must satisfy the following set of equations:

$$\mathbf{q}\cdot\left(a_{jk}\mathbf{e}_j + \sum_{l\neq j\neq k} b_{jl}\mathbf{e}_l \right) = -2\pi\left(a_{jk} m_j + \sum_{l\neq j\neq k} b_{jl} g_l \right),$$
$$\mathbf{q}\cdot\left(a_{jk}\mathbf{e}_k + \sum_{l\neq j\neq k} b_{kl}\mathbf{e}_l \right) = -2\pi\left(a_{jk} m_k + \sum_{l\neq j\neq k} b_{kl} g_l \right),$$

which has as solution the vector $\mathbf{q} = \mathbf{Q}$,

$$\mathbf{Q} = \sum_{k<j} \sum_{m_k,m_j} \left[\left(a_{jk} m_j + \sum_{l\neq j\neq k} b_{jl} g_l \right) \mathbf{Q}_{jk}^{(1)} + \left(a_{jk} m_k + \sum_{l\neq j\neq k} b_{kl} g_l \right) \mathbf{Q}_{jk}^{(2)} \right], \quad (16)$$

where $\mathbf{Q}_{jk}^{(1)}$ and $\mathbf{Q}_{jk}^{(2)}$ are vectors that define the basis in the two-dimensional reciprocal space,

$$\mathbf{Q}_{jk}^{(1)} = \frac{2\pi[|\mathbf{v}_{jk}|^2 \mathbf{u}_{jk} - (\mathbf{u}_{jk}\cdot\mathbf{v}_{jk})\mathbf{v}_{jk}]}{|\mathbf{u}_{jk}|^2 |\mathbf{v}_{jk}|^2 - (\mathbf{u}_{jk}\cdot\mathbf{v}_{jk})^2}, \quad (17a)$$

$$\mathbf{Q}_{jk}^{(2)} = \frac{2\pi[|\mathbf{u}_{jk}|^2 \mathbf{v}_{jk} - (\mathbf{u}_{jk}\cdot\mathbf{v}_{jk})\mathbf{u}_{jk}]}{|\mathbf{u}_{jk}|^2 |\mathbf{v}_{jk}|^2 - (\mathbf{u}_{jk}\cdot\mathbf{v}_{jk})^2}, \quad (17b)$$

where $\mathbf{u}_{jk} = a_{jk}\mathbf{e}_j + \sum_{l\neq j\neq k} b_{jl}\mathbf{e}_l$ and $\mathbf{v}_{jk} = a_{jk}\mathbf{e}_k + \sum_{l\neq j\neq k} b_{kl}\mathbf{e}_l$. Notice that we can arrive at this last result by calculating the reciprocal vectors of the set (8) with shifts $\alpha_l = 0$.

Finally, the diffraction pattern of the quasicrystalline lattice is given by the amplitude of the FT,

$$I(\mathbf{q}) = \sum_{\mathbf{Q}} \|h_{jk}(\mathbf{q})\|^2 \left(\prod_{l\neq j\neq k} \frac{4\sin^2(\mathbf{q}\cdot\mathbf{e}_l/2)}{(2\pi g_l + \mathbf{q}\cdot\mathbf{e}_l)^2} \right) \delta(\mathbf{q} - \mathbf{Q}). \quad (18)$$

We observe that maxima in amplitude are produced when

$$\mathbf{q}\cdot\mathbf{e}_l \sim -2\pi g_l, \quad (19)$$

which is similar to the Laue condition for diffraction that holds in periodical lattices, but here it refers to a lattice in a higher dimension. It is also interesting to note that the more intense peaks are those with $g_l = 0$, and the corresponding vectors $\mathbf{Q}$ are the reciprocal vectors of the average structure of the quasicrystal. Consequently, the average structure produces strong main reflections of the quasilattice. When we consider integer values $g_l \neq 0$, new Bragg peaks appear that can be considered satellites of the reciprocal average structure. Formally, the reciprocal space is densely filled (as expected for a quasiperiodic structure) when all possible integer values of g_l are taken into account.

4.1. The diffraction pattern of the octagonal tiling

Let us consider again the example of the octagonal tiling discussed in §3.1 The reciprocal vectors are defined by the superposition of six periodic lattices with bases $\{\mathbf{Q}_{21}^{(1)}, \mathbf{Q}_{21}^{(2)}\}$, $\{\mathbf{Q}_{31}^{(1)}, \mathbf{Q}_{31}^{(2)}\}$, $\{\mathbf{Q}_{32}^{(1)}, \mathbf{Q}_{32}^{(2)}\}$, $\{\mathbf{Q}_{41}^{(1)}, \mathbf{Q}_{41}^{(2)}\}$, $\{\mathbf{Q}_{42}^{(1)}, \mathbf{Q}_{42}^{(2)}\}$ and $\{\mathbf{Q}_{43}^{(1)}, \mathbf{Q}_{43}^{(2)}\}$, respectively [see (17)]. By using the star vector of the octagonal lattice, we can see that these basis vectors fall into two basic classes generated by:

$$\mathbf{Q}_{21} = \{\mathbf{Q}_{21}^{(1)}, \mathbf{Q}_{21}^{(2)}\} = \{(\pi,\pi), (2^{1/2}\pi, 0)\}$$

and

$$\mathbf{Q}_{31} = \{\mathbf{Q}_{31}^{(1)}, \mathbf{Q}_{31}^{(2)}\} = \{(0,\pi), (\pi, 0)\},$$

such that the remaining basis vectors are obtained as $\mathbf{Q}_{32} = R_{\pi/4}\mathbf{Q}_{21}$, $\mathbf{Q}_{43} = R_{\pi/4}^2\mathbf{Q}_{21}$, $\mathbf{Q}_{41} = R_{\pi/4}^3\mathbf{Q}_{21}$, $\mathbf{Q}_{42} = R_{\pi/4}\mathbf{Q}_{31}$, where $R_{\pi/4}$ is a rotation by $\pi/4$. As discussed at the end of the previous section, the complete reciprocal vectors are obtained with (16) by running over m_j and m_k and considering arbitrary integer values g_l. As an example, Fig. 2(*a*) shows a portion of the reciprocal vectors obtained with (16) for $g_l = 0$, $l = 1, 2, 3, 4$, which corresponds to the reciprocal of the average structure. In order to exemplify how the reciprocal space is filled, Fig. 2(*b*) shows the superposition of the previous reciprocal vectors with that obtained with $g_l = 1$, $l = 1, 2, 3, 4$, and displayed with smaller dots. Observe that the new $\mathbf{Q}$ vectors appear as satellites of the vectors corresponding to the reciprocal of the average structure. This effect is also displayed in Fig. 2(*c*), where the reciprocal vectors for $g_l = 2$, $l = 1, 2, 3, 4$, are superimposed, with even smaller dots, on the previous ones. Fig. 2(*d*) shows a portion of the diffraction pattern of the average structure ($g_l = 0$) with intensities calculated using (18). The black spots are reflections with high intensity that fulfils (19). The remaining reflections of the average structure are shown using gray dots with radius proportional to their intensity. The reciprocal of the average structure contains, therefore, a significant fraction of the scattered intensity of the quasiperiodic structure.

For comparison purposes, in Fig. 3 we show the diffraction pattern of the octagonal quasiperiodic tiling compared with those of the average structure. The former is shown with circles with radius equal to the intensity calculated using the cut-and-projection method (see, for instance, Aragón *et al.*, 1989); four-dimensional points between -13 and 13 were mapped and the maximum calculated intensity is $I_{\max} = 28.0517$, in arbitrary units. A cutoff of 2.0 was used to display the pattern. The diffraction pattern of the average structure is superimposed using filled squares with edge length equal to twice the intensity calculated using (18). To properly compare, intensities were scaled as follows. Since, according to (18), the reciprocal vectors that fulfil the Laue condition (19) have infinite intensity, these intensities were set to $I_{\max}$. Next, the intensities of the remaining reciprocal vectors were scaled such that the maximum obtained equals the next maximum $I < I_{\max}$ of the octagonal diffraction pattern. As can be seen, the values of the intense peaks fit very well and the average structure accounts for a large portion of the most intense peaks observed.

5. Three-dimensional quasilattices

The results presented in previous sections can be generalized to the case of three-dimensional quasilattices in a straightforward manner. Here, we present a survey of the main equations without further details.

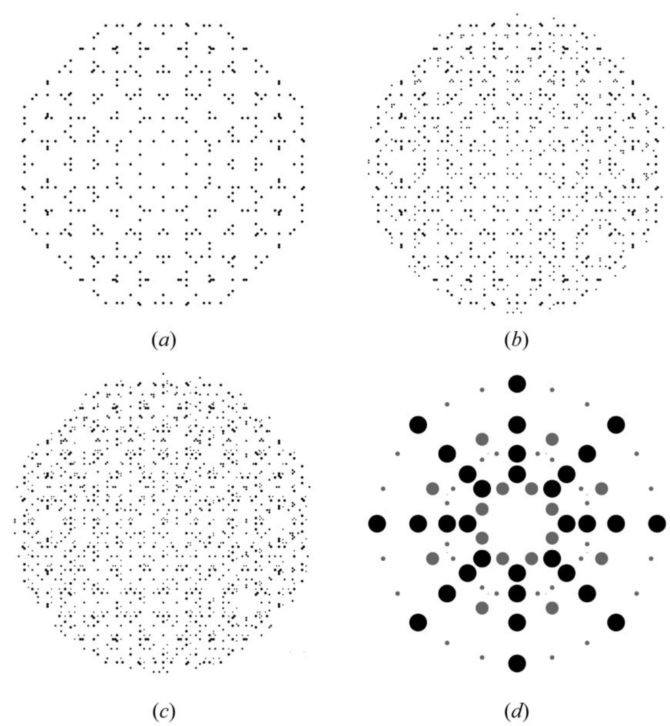

Figure 2
The reciprocal space of the octagonal quasiperiodic tiling. (*a*) Reciprocal vectors obtained with $\mathbf{g} = (0, 0, 0, 0)$, which corresponds to the reciprocal of the average structure shown in Fig. 1(*d*). The reciprocal vectors corresponding to $\mathbf{g} = (1, 1, 1, 1)$, with smaller dots, and $\mathbf{g} = (2, 2, 2, 2)$, with even smaller dots, are superimposed and shown in (*b*) and (*c*), respectively. (*d*) Diffraction pattern of the average structure. Black spots are reflections that fulfil equation (19). The remaining reflections are shown using gray dots with radius proportional to their intensity.

According to the GDM, a three-dimensional quasilattice is constructed by means of a set of parallel planes perpendicular to a three-dimensional star of vectors. For each combination of the star vectors, the intersections of these planes are the solutions of the equations

$$\begin{aligned}\mathbf{x}\cdot\mathbf{e}_s &= x_{n_s} = n_s + \alpha_s,\\ \mathbf{x}\cdot\mathbf{e}_j &= x_{n_j} = n_j + \alpha_j,\\ \mathbf{x}\cdot\mathbf{e}_k &= x_{n_k} = n_k + \alpha_k,\end{aligned}$$

where n_s, n_j and n_k are integers. The solutions of this system are of the form

$$\mathbf{d}(sjk) = x_{n_s}\mathbf{u}_{ksj} + x_{n_j}\mathbf{u}_{sjk} + x_{n_k}\mathbf{u}_{jks},$$

where

$$\mathbf{u}_{sjk} = \frac{\mathbf{e}_j \times \mathbf{e}_k}{\mathbf{e}_s \cdot (\mathbf{e}_j \times \mathbf{e}_k)} = \frac{\mathbf{e}_j \times \mathbf{e}_k}{V_{sjk}}$$

and

$$V_{sjk} = \mathbf{e}_s \cdot (\mathbf{e}_j \times \mathbf{e}_k)$$

is the volume of a rhombohedron with sides $\mathbf{e}_s$, $\mathbf{e}_j$ and $\mathbf{e}_k$.

The ordinal coordinates of regions in the multigrid, along the direction $\mathbf{e}_l$, are

$$k_l = \lfloor (x_{n_s}\mathbf{u}_{ksj} + x_{n_j}\mathbf{u}_{sjk} + x_{n_k}\mathbf{u}_{jks}) \cdot \mathbf{e}_l - \alpha_l \rfloor + 1.$$

Using these coordinates, the dual transformation leads us to the formula for the coordinates of the vertices of a three-dimensional quasilattice:

$$\begin{aligned}\mathbf{t}^0_{n_s,n_j,n_k} = \sum_{k<j<s}^{N} \Bigg[& n_s\mathbf{e}_s + n_j\mathbf{e}_j + n_k\mathbf{e}_k \\ & + \sum_{l\neq j\neq k\neq s} \left(\left\lfloor x_{n_s}\frac{V_{lsj}}{V_{sjk}} + x_{n_j}\frac{V_{ljk}}{V_{sjk}} + x_{n_k}\frac{V_{slk}}{V_{sjk}} - \alpha_l \right\rfloor + 1 \right)\mathbf{e}_l \Bigg],\end{aligned}$$

where one has to consider the $\binom{N}{3}$ triplets s, j and k. The remaining seven vertices of each rhombohedron are

$$\begin{aligned}\mathbf{t}^1_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_s,\\ \mathbf{t}^2_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_j,\\ \mathbf{t}^3_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_k,\\ \mathbf{t}^4_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_j - \mathbf{e}_k,\\ \mathbf{t}^5_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_s - \mathbf{e}_j,\\ \mathbf{t}^6_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_s - \mathbf{e}_k,\\ \mathbf{t}^7_{n_s,n_j,n_k} &= \mathbf{t}^0_{n_s,n_j,n_k} - \mathbf{e}_j - \mathbf{e}_k - \mathbf{e}_s.\end{aligned}$$

For each of these vectors, by using the identity, $x = \lfloor x \rfloor + \{x\}$, the expression for the points in the quasilattice can be written as the sum of an average structure,

$$\langle \mathbf{t}^0_{n_s,n_j,n_k} \rangle = \sum_{k<j<s}^{N} (n_s\mathbf{a}_{sjk} + n_j\mathbf{a}_{jks} + n_k\mathbf{a}_{ksj} + \mathbf{R}_{jks}),$$

where

$$\mathbf{a}_{sjk} = \mathbf{e}_s + \sum_{l\neq j\neq k\neq s} (V_{lsj}/V_{sjk})\mathbf{e}_l,$$
$$\mathbf{a}_{jks} = \mathbf{e}_j + \sum_{l\neq j\neq k\neq s} (V_{ljk}/V_{sjk})\mathbf{e}_l,$$
$$\mathbf{a}_{ksj} = \mathbf{e}_k + \sum_{l\neq j\neq k\neq s} (V_{slk}/V_{sjk})\mathbf{e}_l$$

and

$$\mathbf{R}_{jks} = \sum_{l\neq j\neq k\neq s} \left(\alpha_s \frac{V_{lsj}}{V_{sjk}} + \alpha_j \frac{V_{ljk}}{V_{sjk}} + \alpha_k \frac{V_{slk}}{V_{sjk}} - \alpha_l - \tfrac{1}{2}\right)\mathbf{e}_l,$$

plus a fluctuation part:

$$\mathbf{f}^0_{n_s,n_j,n_k} = \sum_{k<j<s}^{N} \sum_{l\neq j\neq k\neq s}^{N} \left(\tfrac{1}{2} - \left\{x_{n_s}\frac{V_{lsj}}{V_{sjk}} + x_{n_j}\frac{V_{ljk}}{V_{sjk}} + x_{n_k}\frac{V_{slk}}{V_{sjk}} - \alpha_l\right\}\right)\mathbf{e}_l.$$

In three dimensions, the average structure then consists of a superposition of $\binom{N}{3}$ lattices plus the corresponding shift terms.

The diffraction pattern of the three-dimensional quasilattice, written as

$$\mathbf{t}^0_{n_s,n_j,n_k} = \langle \mathbf{t}^0_{n_s,n_j,n_k}\rangle + \mathbf{f}^0_{n_s,n_j,n_k},$$

is calculated in a similar way to that exposed in §4. The total FT of the three-dimensional quasilattice is

$$F(\mathbf{q}) = \sum_{n_s,n_j,n_k,g_l} h_{n_s,n_j,n_k}(\mathbf{q}) \left(\prod_{l\neq j\neq k\neq s} B(g_l)\right) \times \exp\Bigg[i\mathbf{q}\cdot(n_s\mathbf{e}_s + n_j\mathbf{e}_j + n_k\mathbf{e}_k) + i\sum_{l\neq j\neq k\neq s}\left(n_s\frac{V_{lsj}}{V_{sjk}} + n_j\frac{V_{ljk}}{V_{sjk}} + n_k\frac{V_{slk}}{V_{sjk}}\right)(\mathbf{q}\cdot\mathbf{e}_l + 2\pi g_l)\Bigg],$$

where

$$B(g) \equiv B(e,f,g) = \begin{cases} 0 & \text{if } e\neq f\neq g \\ \dfrac{-i\exp(-i\mathbf{q}\cdot\mathbf{e}_l) - 1}{2\pi g + \mathbf{q}\cdot\mathbf{e}_l} & \text{if } e = f = g \end{cases}$$

and

$$h_{n_s,n_j,n_k}(\mathbf{q}) = \frac{1}{Z_{n_s,n_j,n_k}} + \frac{\exp(-i\mathbf{q}\cdot\mathbf{e}_s)}{Z_{n_s-1,n_j,n_k}} + \frac{\exp(-i\mathbf{q}\cdot\mathbf{e}_j)}{Z_{n_s,n_j-1,n_k}} + \frac{\exp(-i\mathbf{q}\cdot\mathbf{e}_k)}{Z_{n_s,n_j,n_k-1}} + \frac{\exp[-i\mathbf{q}\cdot(\mathbf{e}_s+\mathbf{e}_k)]}{Z_{n_s-1,n_j,n_k-1}} + \frac{\exp[-i\mathbf{q}\cdot(\mathbf{e}_j+\mathbf{e}_k)]}{Z_{n_s,n_j-1,n_k-1}} + \frac{\exp[-i\mathbf{q}\cdot(\mathbf{e}_s+\mathbf{e}_j)]}{Z_{n_s-1,n_j-1,n_k}} + \frac{\exp[-i\mathbf{q}\cdot(\mathbf{e}_s+\mathbf{e}_j+\mathbf{e}_k)]}{Z_{n_s-1,n_j-1,n_k-1}}.$$

With the use of the average coordination in the previous equation, the sum over n_j, n_k and n_s can be carried out in the equation for the total FT, and it turns out that $F(\mathbf{q})$ is different from zero at vectors $\mathbf{q} = \mathbf{Q}$, where

$$\mathbf{Q} = \sum_{k<j<s}\sum_{m_s,m_k,m_j}\left[\left(V_{sjk}m_s + \sum_{l\neq j\neq k\neq s} V_{lsj}g_l\right)\mathbf{Q}^{(1)}_{sjk} + \left(V_{sjk}m_j + \sum_{l\neq j\neq k\neq s} V_{ljk}g_l\right)\mathbf{Q}^{(2)}_{sjk} + \left(V_{sjk}m_k + \sum_{l\neq j\neq k\neq s} V_{skl}g_l\right)\mathbf{Q}^{(3)}_{sjk}\right].$$

$\mathbf{Q}^{(1)}_{sjk}$, $\mathbf{Q}^{(2)}_{sjk}$ and $\mathbf{Q}^{(3)}_{sjk}$ are vectors that define the basis in the reciprocal space, and are given by

$$\mathbf{Q}^{(1)}_{sjk} = \frac{2\pi(\mathbf{v}\times\mathbf{w})}{\mathbf{u}\cdot(\mathbf{v}\times\mathbf{w})}, \quad \mathbf{Q}^{(2)}_{sjk} = \frac{2\pi(\mathbf{w}\times\mathbf{u})}{\mathbf{u}\cdot(\mathbf{v}\times\mathbf{w})}, \quad \mathbf{Q}^{(3)}_{sjk} = \frac{2\pi(\mathbf{u}\times\mathbf{v})}{\mathbf{u}\cdot(\mathbf{v}\times\mathbf{w})},$$

where

$$\mathbf{u} = V_{sjk}\mathbf{e}_s + \sum_{l\neq j\neq k\neq s} V_{lsj}\mathbf{e}_l,$$
$$\mathbf{v} = V_{sjk}\mathbf{e}_j + \sum_{l\neq j\neq k\neq s} V_{ljk}\mathbf{e}_l,$$
$$\mathbf{w} = V_{sjk}\mathbf{e}_k + \sum_{l\neq j\neq k\neq s} V_{slk}\mathbf{e}_l.$$

Finally, the amplitude of the FT is

$$I(\mathbf{q}) = \sum_{\mathbf{Q}} \|h_{sjk}(\mathbf{q})\|^2 \left(\prod_{l\neq j\neq k\neq s} \frac{4\sin^2(\mathbf{q}\cdot\mathbf{e}_l/2)}{(2\pi g_l + \mathbf{q}\cdot\mathbf{e}_l)^2}\right)\delta(\mathbf{q}-\mathbf{Q}).$$

The function $h_{sjk}(\mathbf{q})$ is the same as $h_{n_s,n_j,n_k}(\mathbf{q})$ but the local coordination has been replaced by the average coordination.

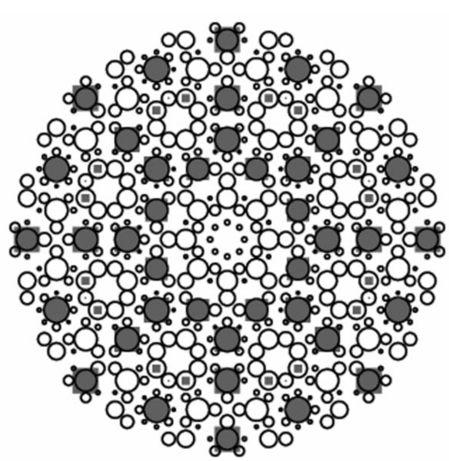

Figure 3
Comparison between the diffraction patterns of the octagonal quasiperiodic tiling, calculated using the cut-and-projection method, and the average structure, obtained from (16) and (18). The former is shown with circles with radius equal to the calculated intensity. The pattern of the average structure is superimposed using filled squares with edge length equal to twice the calculated intensity.

6. Relationship with the cut-and-projection method

For completeness, we shall briefly discuss the relationship of the present approach with the cut-and-projection method (Duneau & Katz, 1985). It is directly related to non-orthogonal projections, originally proposed to describe continuous transformations from quasiperiodic to periodic structures using the cut-and-projection method (Torres *et al.*, 1989). Let us consider the case of the Fibonacci sequence, which is the most simple quasiperiodic structure in one dimension. The coordinate of the nth vertex of the quasiperiodic sequence of vertices is given by

$$t_m = mS + \frac{1}{\tau}\left\lfloor\frac{m}{\tau}\right\rfloor S.$$

It produces a Fibonacci sequence of short (S) and long ($L = \tau S$) intervals. By decorating the sequence t_m with atoms at the vertices, we obtain the most studied example of a quasicrystal in one dimension. As described in §3, the substitution $\lfloor x\rfloor = x - \{x\}$ gives

$$\begin{aligned} t_m &= mS + \frac{1}{\tau}\left(\frac{m}{\tau} - \left\{\frac{m}{\tau}\right\}\right)S \\ &= m(3-\tau)S - \left\{\frac{m}{\tau}\right\}\frac{S}{\tau}. \end{aligned}$$

We then have, as usual, an average periodic structure with period $\overline{a} = (3-\tau)S$ and the last term is the fluctuation part. The average property of $(3-\tau)S$ can be better appreciated by noticing that the fluctuation part in t_m is always less that 1 so, for large m, the dominant term is $m(3-\tau)S$. Under this condition, we have $t_m/m = \langle t_m\rangle = (3-\tau)S$.

In the cut-and-projection approach, the sequence t_m is generated by projecting certain vertices of a two-dimensional square periodic structure onto an adequately selected space $E^{\parallel}$ (Duneau & Katz, 1985). In particular, let $\Lambda = \mathbb{Z}^2$ be the square lattice in $\mathbb{R}^2$, generated by the standard canonical basis, with unitary square Γ_2. Let $E^{\parallel}$ be the one-dimensional space, where the sequence is generated, and $E^{\perp}$ the orthogonal complement. Denote by $P^{\parallel}$ and $P^{\perp}$ the two complementary projectors onto $E^{\parallel}$ and $E^{\perp}$, respectively; $E^{\parallel} = P^{\parallel}(\mathbb{R}^2)$, $E^{\perp} = P^{\perp}(\mathbb{R}^2)$ and $\mathbb{R}^2 = E^{\parallel} \oplus E^{\perp}$. A strip $\mathbf{S}$ is generated by shifting Γ_2 along $E^{\parallel}$. The orthogonal projection onto $E^{\parallel}$ of the points that fall inside the strip produces the vertices of a non-periodic sequence $\mathcal{Q} = P^{\parallel}(\mathbf{S} \cap \Lambda)$, provided that the slope of $E^{\parallel}$, with respect to the canonical basis of $\mathbb{R}^2$, is an irrational number. The Fibonacci sequence is obtained if $\tan\theta = 1/\tau$, τ is the golden ratio. Under this condition, the large and short segments are $L = \cos\theta$ and $S = \sin\theta$. By changing the slope of $E^{\parallel}$ so that $\tan\theta$ equals a rational approximant of τ, one obtains structures formed by a periodically repeated sequence of segments (Torres *et al.*, 1989). An alternative and equivalent procedure consists of maintaining the slope of $E^{\parallel}$ but using instead a non-orthogonal projection. By following this last approach, Duneau & Oguey (1990) demonstrated that, under certain conditions, an average lattice, obtained by means of an oblique projection, can be associated with the quasiperiodic structure. In the above discussed case of the Fibonacci sequence, the average lattice is obtained by projecting, onto $E^{\parallel}$, the vertices of Λ inside the strip along the direction parallel to the vector $(-1, 1)$ in $\mathbb{R}^2$, as described in detail by Duneau (1991) and Steurer & Haibach (1999). In Fig. 4, we show a simplified version of a portion of this scheme. The orthogonal projection onto $E^{\parallel}$ of the vertices of Λ inside the strip $\mathbf{S}$ produces the quasiperiodic sequence of long and short intervals. The projection along one of the square diagonals ($\beta = \pi/4$) yields the average lattice represented by bold dots along $E^{\parallel}$. The period $\overline{a}$ of this structure can be obtained by noticing that

$$\overline{a} = L - \tan(\pi/4 - \theta)S.$$

By using the facts that $L = \tau S$ and $\tan\theta = 1/\tau$, we get

$$\overline{a} = \left(\tau - \frac{1 - 1/\tau}{1 + 1/\tau}\right)S = (3-\tau)S,$$

as expected.

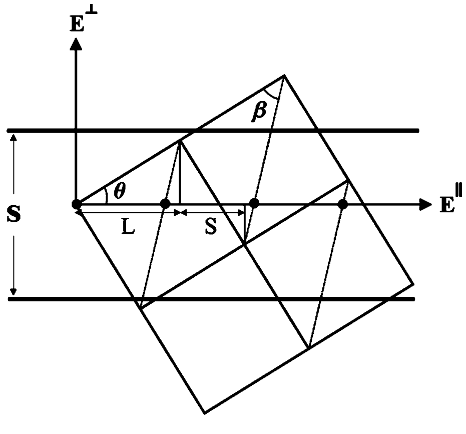

Figure 4
A portion of the cut-and-projection scheme to illustrate the oblique projection that leads to the average lattice of the Fibonacci chain, represented by bold dots along the $E^{\parallel}$ line.

The cut-and-projection method is easily generalizable to obtain quasilattices in n dimensions by projecting vertices of an N-dimensional lattice (Duneau & Katz, 1985). In this case, the periodic hyperstructure is $\Lambda = \mathbb{Z}^N$ with unitary hypercell Γ_N. $\mathrm{Dim}(E^{\parallel}) = n$ and $\mathrm{Dim}(E^{\perp}) = N - n$. The procedure follows the same lines as in the above-described case for $N = 2$, $n = 1$. The generalization of the oblique projection technique to more dimensions is as follows (Duneau & Oguey, 1990; Xu & Mai, 1998). Let W be the projection of the unit hypercube Γ_N onto $E^{\perp}$ (the so-called window or acceptance domain). If W tiles the orthogonal space (*i.e.* W is a prototile), then an average lattice is associated with the quasilattice by the oblique projection (Duneau & Oguey, 1990). If this condition over W is not fulfilled, then let us assume that the window can be divided into $W_1, W_2, \ldots, W_k$ disjoint cells, such that each W_i tiles the orthogonal space. The strip $\mathbf{S}$ is then subdivided into k substrips $\mathbf{S}_1, \mathbf{S}_2, \ldots, \mathbf{S}_k$ and the quasilattice $\mathcal{Q}$ is also partitioned into $\mathcal{Q}_1, \mathcal{Q}_2, \ldots, \mathcal{Q}_k$. To each $\mathcal{Q}_i$ an average lattice can be associated by means of an oblique projection of the vertices of Λ falling inside the corresponding substrip $\mathbf{S}_i$.

Without further details, we just compare our results of §3.1 with those obtained by Xu & Mai (1998) using the oblique projection. The octagonal quasiperiodic structure is generated by projecting points in $\Lambda = \mathbb{Z}^4$. The window $W = P^{\perp}(\Gamma_4)$ is a regular octagon. Since the octagon is not a prototile, W is divided into six disjoint subwindows $W_1, W_2, \ldots, W_6$: two squares and four 45° rhombuses (see Fig. 1 in Xu & Mai, 1998). The quasilattice $\mathcal{Q}$ is then subdivided into

$\mathcal{Q}_1, \mathcal{Q}_2, \ldots, \mathcal{Q}_6$ substructures and an average lattice is associated with each $\mathcal{Q}_i$ by means of the oblique projection. Given the structure of the window, the six average lattices obtained are two square and four 45° rhombohedral lattices, which coincides with our results in §3.1 [equation (12)]. The one-to-one correspondence between the octagonal quasiperiodic structure and the rhombohedral average lattice L_{21}, shown in Fig. 1(*b*), is depicted in Fig. 5 of Duneau & Oguey (1990).

7. Summary and discussion

In this work, we show that a quasiperiodic lattice can be separated into two parts: an average structure plus a factor that considers the fluctuations from the average positions. The average structure of a given quasilattice is calculated using the dual generalized method and it turns out that it is composed by several average lattices. The importance of the average structures in quasicrystals relies on the facts that the reciprocal of the average structure contains a significant fraction of the scattered intensity of the quasiperiodic structure and that the average structure dominates the response for long-wave modes of incident radiation. A possible consequence of these properties is that the average structure can be useful to determine the main terms that contribute to define a physically relevant Brillouin zone.

The use of the dual generalized method allows us to write explicit analytical expressions for the vertex coordinates of the quasilattice, the average structure and their diffraction pattern. These expressions provide a useful procedure to generate quasiperiodic tilings in an efficient and general way, avoiding the computational problems of the pure GDM and the cut-and-projection methods (for the last case, see Aragón *et al.*, 1989; Vogg & Ryder, 1996). Also, a useful frame to understand the reciprocal-space properties of quasiperiodic structures is provided. The particular example of the octagonal quasiperiodic tiling is worked out.

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