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General periodic average structures of decagonal quasicrystals

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The concept of periodic average structure is mutuated from the theory of incommensurately modulated structures. For quasicrystals, this concept (up to now explored only in few cases) is becoming increasingly useful to understand their properties and to interpret some important structural features. The peculiar property of quasicrystals is that they admit not one but many (infinite) possible different average structures. Few of them, however, will be meaningful. Here are given a simple method (based on reciprocal space) for generating all the possible periodic average structures of decagonal quasicrystals and some new ideas about their meaning. By this method, the most significant average structures can be recognized from the diffraction pattern.

1. Introduction

The concept of periodic average structure (PAS hereafter) stems from the theory of incommensurately modulated structures and composite structures [in short IMS, CS, respectively (see Steurer & Haibach, 2001, for details)]. In IMS, a *main* periodic lattice is perturbed by weak modulations incommensurate to it; this is clearly visible in reciprocal space, showing a lattice of strong *main* reflections accompanied by a multitude of incommensurate weaker *satellite* peaks. In CS, two or more incommensurate periodic phases coexist and the same number of incommensurate main reciprocal lattices form the diffraction pattern. The description of quasicrystals (QCs in this work) as IMSs has been proven to be possible (Steurer & Haibach, 1999*b*; Steurer, 1999, 2000) and structurally significant (Steurer & Cervellino, 2001; Cervellino *et al.*, 2002). In QCs, however, there is no clearcut distinction between main and satellite reflections, and there are several possible main reflections lattices, as in CS. However, there is intermodulation between different possible PASs, as in IMS. In fact, as we will show, any periodic sublattice of the QC's reciprocal lattice may be chosen as the main reflections lattice. Two possible choices for a decagonal QC (basic Ni-rich d-Al–Co–Ni) are given in Steurer & Cervellino (2001).

Let us first clarify the meaning of PAS. The comparison of QCs with analogous periodic phases has previously been developed in the framework of the *approximant* phases (see Quiquandon *et al.*, 1999; Steurer & Haibach, 1999*a*, 2001, and references therein); their relation to QCs is quite different from the QC–PAS relation. In fact, to compare QCs with approximants one has to introduce unbounded atomic displacements, with consequent difficulties of interpretation (Steurer, 2000). In the PAS approach, conversely, the atomic displacement field is bounded.

Different methods to obtain PAS of QCs have been considered. In the approach of Duneau & Oguey (1990), Duneau (1991) and Xu & Mai (1998), no real average structure is involved. There a QC is partitioned as a CS with intermodulation of the different components, combining concepts from IMS and CS theory. However, there the different intermodulating periodic structures are obtained by a tricky geometric partition of the acceptance window. The method is very complex to generalize. Furthermore, it yields little information on the global relationship between QC and existing similar periodic phases.

The approach of Wolny (1998, see also references therein) is more meaningful. The formalism developed there, based on reciprocal-space analysis, is very useful because it defines properly the concept of PAS for any scattering system (periodic, quasiperiodic and disordered; static and dynamic). Its shortcoming (the opposite face of the generality) is a general complexity as it is not based on a higher-dimensional description. For many aperiodic systems, the higher-dimensional description is a very convenient and useful tool. However, its results are perfectly compatible with ours (Steurer & Haibach, 1999*b*; Steurer, 1999, 2000; Steurer & Cervellino, 2001; Cervellino *et al.*, 2002). The formalism used in the latter works is explicitly higher-dimensional, with all the advantages of interpretation that follow. However, it is based on a complex geometrical procedure in direct space.

This contribution is meant to illustrate a new simple method to construct any arbitrary possible PAS of a d-QC. The

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method is based on an arbitrary choice of a base set of reflections in the QC diffraction pattern. The PAS will be generated by the QC structure factors corresponding to the periodic subset of reflections generated by them. This allows one to choose reflections so that this periodic sublattice approximates that of a known periodic phase, whose structure we wish to compare with the QC. The method (as in Wolny, 1998) is actually independent of the higher-dimensional embedding. We develop it in that frame, however, because this allows one to get some new insight into the meaning of PAS of QCs.

2. Embedding of decagonal quasicrystals

A d-QC can be geometrically represented as a periodic stacking of parallel atomic planes along an axis orthogonal to them. Each plane shows pentagonal or decagonal symmetry with respect to the periodic axis. For our purposes, the periodic direction is unimportant and we will consider only one atomic plane as a 2D d-QC. Physically, a QC is represented by a probability density (for atoms and/or electrons) $P(\mathbf{r}^{\parallel})$ on $E^{\parallel}$, a 2D vector space representing one atomic plane (*physical space*). We will henceforth assume that $P(\mathbf{r}^{\parallel})$ is also the scattering density. Denote by $E^{\perp}$ a complementary orthogonal 2D space (*perpendicular space*). Their direct sum $E = E^{\parallel} \oplus E^{\perp}$ is the *embedding space*. We will denote $\Pi^{\parallel}$, $\Pi^{\perp}$ the projectors from E onto $E^{\parallel}$, $E^{\perp}$, respectively. Take also orthonormal bases $\mathbf{v}_1, \mathbf{v}_2$ of $E^{\parallel}$ and $\mathbf{v}_3, \mathbf{v}_4$ of $E^{\perp}$; then $E = \mathrm{span}\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4\}$ (V-basis). The quasiperiodic structure $P(\mathbf{r}^{\parallel})$ on $E^{\parallel}$ can be thought of as a section of a periodic structure in E, represented by a periodic probability density $\hat{P}(\mathbf{r})_{\mathbf{r}=\mathbf{r}^{\parallel}\oplus\mathbf{r}^{\perp}}$. The sectioning acts as

$$P(\mathbf{r}^{\parallel}) = \hat{P}(\Pi^{\parallel}\mathbf{r} + \mathbf{t}_0), \tag{1}$$

where $\mathbf{t}_0$ is a fixed vector of $E^{\perp}$. The 4D lattice is

$$\Lambda_{\mathrm{QC}} = \left\{ \mathbf{R} = \sum_{i=1}^{4} n_i \mathbf{d}_i \middle| n_i \in \mathbb{Z}, \quad i = 1, \ldots, 4 \right\}. \tag{2}$$

It is defined by its fundamental vectors $\mathbf{d}_i$, $i = 1, \ldots, 4$ (D-basis); these are appropriately chosen so that Λ_{QC} is invariant with respect to fivefold rotations and $E^{\parallel}$, $E^{\perp}$ are its irreducible invariant subspaces. The standard 4D embedding (see Steurer & Haibach, 1999*a*, 2001) is the simplest way to ensure these properties. The embedding matrix DV, which transforms vector components from the D-basis to the V-basis, can be written as

$$DV = \frac{a_{\mathrm{QC}}}{5} \begin{vmatrix} -\chi^2 & -\tau^2\chi^2 & -\tau^2\chi^2 & -\chi^2 \\ \tau\chi & \chi & -\chi & -\tau\chi \\ -\tau^2\chi^2 & -\chi^2 & -\chi^2 & -\tau^2\chi^2 \\ -\chi & \tau\chi & -\tau\chi & \chi \end{vmatrix}. \tag{3}$$

The form given here uses the Pisot number $\tau = (1 + 5^{1/2})/2 = 2\cos(\pi/5)$, the positive root of $x^2 - x - 1 = 0$, and the algebraic number $\chi = (3 - \tau)^{1/2} = 2\sin(\pi/5)$. Their properties (see Appendix *A*) allow for great compactness in calculations. a_{QC} is the direct-space QC metric constant (Steurer & Haibach, 1999*a*, 2001); typically for known decagonal phases $a_{\mathrm{QC}} \approx 0.38$ nm. We will put $a_{\mathrm{QC}} = 1$ in the following. The reciprocal lattice is

$$\Lambda^*_{\mathrm{QC}} = \left\{ \mathbf{H} = \sum_{i=1}^{4} h_i \mathbf{d}^*_i \middle| h_i \in \mathbb{Z}, \ i = 1, \ldots, 4 \right\}, \tag{4}$$

where $\mathbf{d}^*_i \cdot \mathbf{d}_j = \delta_{ij}$ holds. Therefore, the reciprocal-space embedding matrix can be written as

$$DV^* = \left(\widetilde{DV}\right)^{-1} = \frac{a^*_{\mathrm{QC}}}{2} \begin{vmatrix} 1/\tau & -\tau & -\tau & 1/\tau \\ \tau\chi & \chi & -\chi & -\tau\chi \\ -\tau & 1/\tau & 1/\tau & -\tau \\ -\chi & \tau\chi & -\tau\chi & \chi \end{vmatrix}, \tag{5}$$

where $a^*_{\mathrm{QC}} = 1/a_{\mathrm{QC}}$ (1 in this work).

The concept of *local isomorphism* (LI) is the extension to the embedding space E of the translational invariance of physical laws (Levine & Steinhardt, 1986; Socolar & Steinhardt, 1986). The physical QC is a section of E parallel to $E^{\parallel}$, *cf.* (1). $\mathbf{t}_0$ is an arbitrary origin shift. The case $\mathbf{t}_0 \in E^{\parallel}$ is trivial. When $\mathbf{t}_0 \in E^{\perp}$, we will have a *different* QC (meaning not geometrically congruent) for every different vector $\mathbf{t}_0$. However, these will be *physically indistinguishable* (Steurer & Haibach, 2001), meaning that their Fourier transform will coincide apart from a phase factor and their N-body correlations will be the same. We say that the different QCs are locally isomorphic, or belong to the same LI class. Given the periodicity in E, any arbitrary origin shift can be confined to one 4D unit cell, *e.g.* the Voronoi unit cell; neglecting the $E^{\parallel}$ component, we can limit to the $E^{\perp}$-projected Voronoi unit cell.

3. Construction of an arbitrary average structure

3.1. Reciprocal space

Choose now two reflections $\mathbf{h}_1 = (h_{11}, h_{12}, h_{13}, h_{14})_D \in \mathbb{Z}^4$ and $\mathbf{h}_2 = (h_{21}, h_{22}, h_{23}, h_{24})_D \in \mathbb{Z}^4$ from Λ^*_{QC}, such that:

[*A*] $\mathbf{h}_1$ and $\mathbf{h}_2$ are linearly independent;

[*B*] $\Pi^{\parallel}\mathbf{h}_1$ and $\Pi^{\parallel}\mathbf{h}_2$ are linearly independent;

[*C*] $\mathrm{MCD}\{h_{1i}\}_{i=1,\ldots,4} = \mathrm{MCD}\{h_{2i}\}_{i=1,\ldots,4} = 1$.

MCD denotes the largest common divisor of a set of integers. For compactness, we will operate the change of variable[1]

$$\begin{cases} M = h_{11} + h_{14} \\ N = h_{12} + h_{13} \\ P = h_{11} - h_{14} \\ Q = h_{12} - h_{13} \end{cases}; \quad \begin{cases} R = h_{21} + h_{24} \\ S = h_{22} + h_{23} \\ T = h_{21} - h_{24} \\ U = h_{22} - h_{23} \end{cases}. \tag{6}$$

By this, we can calculate the V-basis components as

[1] The transformation is always invertible over $\mathbb{Q}$; it is invertible over $\mathbb{Z}$ provided that $M + P$, $N + Q$ (and $R + T$, $S + U$) are even integers.

$$\mathbf{h}_1 = \frac{1}{2}\begin{pmatrix} \tau(M-N)-M \\ \chi(\tau P+Q) \\ \tau(N-M)-N \\ \chi(\tau Q-P) \end{pmatrix}_V ; \tag{7}$$

$$\mathbf{h}_2 = \frac{1}{2}\begin{pmatrix} \tau(R-S)-R \\ \chi(\tau T+U) \\ \tau(S-R)-S \\ \chi(\tau U-T) \end{pmatrix}_V . \tag{8}$$

Now we introduce a shear deformation in E. This means that the V-basis vectors and the structure of E are left invariant, but the point $\mathbf{r}$ of direct space ($\mathbf{q}$ of reciprocal space) shifts to $\mathbf{r}^S = \mathcal{A}_{||}\mathbf{r}$ ($\mathbf{q}^S = \mathcal{A}_{||}^*\mathbf{q}$, respectively; $\mathcal{A}_{||}$, $\mathcal{A}_{||}^*$ denote the shear operators in the two spaces). Therefore, the QC-defining probability density after shearing will be $\hat{P}^S(\mathbf{r}) = \hat{P}(\mathcal{A}_{||}^{-1}\mathbf{r})$. Shear deformations have been proposed (Elser & Henley, 1985; Jarić & Mohanty, 1987; Goldman & Kelton, 1993; Jarić & Qiu, 1993; Gratias *et al.*, 1995; see also Steurer & Haibach, 1999*a*, 2001, and references therein) to obtain periodic approximants from quasicrystals. In this case, the physical QC is thought to be subjected to a linear phason strain and deformed into a periodic approximant. However, that is not our present purpose. In fact, we seek a kind of shear transformation (Steurer & Haibach, 1999*b*; Steurer, 1999, 2000) that leaves invariant all physical properties of the QC. In reciprocal space, this means that the shear must not affect the projection onto $E^{||}$; therefore, the shear will be parallel to $E^{\perp}$. The converse must happen in direct space: there the $E^{||}$ section must remain invariant [*i.e.* $\hat{P}^S(\mathbf{r}^S) = \hat{P}(\mathbf{r}^S)$ for $\mathbf{r}^S \in E^{||}$], therefore we use a linear shear parallel to $E^{||}$. We will work in the V-basis. From a vector $\mathbf{q}$, we obtain the sheared vector $\mathbf{q}^S = \mathcal{A}_{||}^*\mathbf{q}$ with the matrix

$$\mathcal{A}_{||}^* = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ A_{11} & A_{12} & 1 & 0 \\ A_{21} & A_{22} & 0 & 1 \end{vmatrix}. \tag{9}$$

Note that $|\det\mathcal{A}_{||}^*| = 1$ and $(\mathcal{A}_{||}^*)^{-1} = 2\mathbb{I} - \mathcal{A}_{||}^*$, where $\mathbb{I}$ is the 4×4 identity matrix. The $E^{||}$ components of $\mathbf{h}_1^S$, $\mathbf{h}_2^S$ will not change, conserving their values from (7) and (8). We solve for the coefficients $A_{\alpha\beta}$ by imposing that $\mathbf{h}_1^S$, $\mathbf{h}_2^S$ have zero $E^{\perp}$ components:

$$\begin{aligned} \mathbf{h}_1^S &= ([\mathbf{h}_1^S]_1, [\mathbf{h}_1^S]_2, 0, 0)_V; \\ \mathbf{h}_2^S &= ([\mathbf{h}_2^S]_1, [\mathbf{h}_2^S]_2, 0, 0)_V. \end{aligned} \tag{10}$$

This condition determines completely the coefficients $A_{\alpha\beta}$. Their expressions are

$$\begin{aligned} A_{11} &= (1/\Delta)[(-2PR + PS - QR + 2TM + MU - TN)\tau \\ &\quad - PR - QR + QS + TM + MU - NU], \\ A_{12} &= \chi(\tau+1)(SM - RN)/\Delta, \\ A_{21} &= \chi(3\tau+1)(PU - QT)/\Delta, \\ A_{22} &= (1/\Delta)[(2NU - MU + QR - 2QS - TN + PS)\tau \\ &\quad + NU - PR - QS - TN + TM + PS], \end{aligned} \tag{11}$$

where

$$\begin{aligned} \Delta &= (2PS - PR + QS - 2TN - NU + TM)\tau \\ &\quad + PS + QS - QR - TN - NU + MU. \end{aligned} \tag{12}$$

The denominator Δ results to zero iff the system[2] of equations

$$\begin{cases} 0 = (MU - QR) - (NU - QS) - (NT - PS) \\ 0 = (MU - QR) - (MT - PR) + (NT - PS) \end{cases} \tag{13}$$

is satisfied. It is easy to see from (7) and (8) that this condition is equivalent to having $\Pi^{||}\mathbf{h}_1$ parallel to $\Pi^{||}\mathbf{h}_2$ (*contra* hypothesis [*B*]). Further simplifications of the $A_{\alpha\beta}$ can be obtained using (22).

The $E^{||}$ periodic lattice

$$\Lambda_{\rm av}^* = \{m\mathbf{h}_1^S + n\mathbf{h}_2^S | m, n \in \mathbb{Z}\} \tag{14}$$

plays the role of main reflections lattice. We have that $\Lambda_{\rm av}^* \subset E^{||}$ because of (10). Denote now by $\Lambda_{{\rm QC}_S}^* = \mathcal{A}_{||}^*\Lambda_{\rm QC}^* = \{\mathcal{A}_{||}^*\mathbf{h} | \mathbf{h} \in \Lambda_{\rm QC}^*\}$ the sheared lattice. We show now that $\Lambda_{{\rm QC}_S}^* \cap E^{||} = \Lambda_{\rm av}^*$. In fact, $E^{||} = {\rm span}(\mathbf{h}_1^S, \mathbf{h}_2^S)$; so all and only the points of $E^{||}$ will be a linear combination of $\mathbf{h}_1^S$, $\mathbf{h}_2^S$. By hypothesis [*C*], linear combinations of $\mathbf{h}_1^S$, $\mathbf{h}_2^S$ belong to $\Lambda_{{\rm QC}_S}^*$ iff they have integer coefficients, and these are all in $\Lambda_{\rm av}^*$: *q.e.d.*

As an example, consider the PAS of Cervellino *et al.* (2002). There, $\mathbf{h}_1 = (1, 0, 0, -1)_D$ (hence $M = N = Q = 0$, $P = 2$) and $\mathbf{h}_2 = (0, -1, -1, -1)_D$ ($R = -1$, $S = -2$, $T = 1$, $U = 0$). In the V-basis,

$$\begin{aligned} \mathbf{h}_1 &= (0, \quad \chi\tau, \quad 0, \quad -\chi)_V; \\ \mathbf{h}_2 &= (\tau^2/2, \quad \chi\tau/2, \quad \tau^{-2}/2, \quad -\chi/2)_V. \end{aligned} \tag{15}$$

So we obtain

$$A_{11} = -\tau^{-4}, \quad A_{12} = A_{21} = 0, \qquad A_{22} = \tau^{-1}. \tag{16}$$

3.2. Direct space

The shear in direct space will be enacted by the matrix

$$\mathcal{A}_{||} = \left(\widetilde{\mathcal{A}_{||}^*}\right)^{-1} = \begin{vmatrix} 1 & 0 & -A_{11} & -A_{21} \\ 0 & 1 & -A_{12} & -A_{22} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix}. \tag{17}$$

This preserves the values of the Euclidean scalar products between vectors of direct space and reciprocal space: if $\mathbf{q}^S = \mathcal{A}_{||}^*\mathbf{q}$ and $\mathbf{r}^S = \mathcal{A}_{||}\mathbf{r}$, then $\mathbf{r}\cdot\mathbf{q} = \mathbf{r}^S\cdot\mathbf{q}^S$. Therefore, the Fourier transform connecting the two spaces will conserve its

[2] By the principle of rational independence, see Appendix *A*.

form after shearing. We want now to determine the average structure direct lattice

$$\Lambda_{\rm av} = \{m\Pi^{||}\mathbf{r}_1^S + n\Pi^{||}\mathbf{r}_2^S \big| m, n \in \mathbb{Z}\}, \tag{18}$$

which is the reciprocal of $\Lambda_{\rm av}^*$ in $E^{||}$. This means determining the fundamental vectors[3] $\Pi^{||}\mathbf{r}_1^S$, $\Pi^{||}\mathbf{r}_2^S$, by the conjugation relations $\mathbf{r}_i^S \cdot \mathbf{h}_j^S = \delta_{ij}$. We obtain

$$\begin{aligned} [\mathbf{r}_i^S]_1 &= (\boldsymbol{\alpha}_{i1}\tau + \boldsymbol{\beta}_{i1})/\mathcal{D}; \\ [\mathbf{r}_i^S]_2 &= \chi(\boldsymbol{\alpha}_{i2}\tau + \boldsymbol{\beta}_{i2})/\mathcal{D}; \\ \boldsymbol{\alpha}_{ij}, \boldsymbol{\beta}_{ij} &\in \mathbb{Z}\ \forall\, i, j = 1, 2, \mathcal{D} \in \mathbb{Z}. \end{aligned} \tag{19}$$

Explicit expressions are given in Appendix *B*. For the example at the end of §3.1, we get

$$\begin{aligned} \mathbf{r}_1^S &= (-\tau^{-2}, \chi^3\tau/5)_V; \\ \mathbf{r}_2^S &= (2\tau^{-2}, 0)_V. \end{aligned} \tag{20}$$

By transforming this primitive monoclinic lattice into a centred orthorhombic lattice [defined by $2\mathbf{r}_1^S + \mathbf{r}_2^S = (0, 2\chi^3\tau/5)_V$ and $\mathbf{r}_2^S$], we obtain the PAS of Cervellino *et al.* (2002).

4. On the meaning of periodic average structure

We have now determined a periodic lattice $\Lambda_{\rm av} \subset \Lambda_{\rm QC}$ ($\Lambda_{\rm av}^* \subset \Lambda_{\rm QC}^*$). What is the relation of the QC structure to this lattice? Selecting from the QC diffraction pattern only the reflections in $\Lambda_{\rm av}^*$ means taking an $E^{||}$ parallel section of reciprocal space. In fact, we have shown in §3.2 that $\Lambda_{\rm av}^* = \Lambda_{\rm QC}^* \cap E^{||}$. By a known property of the Fourier transform, in direct space this corresponds to a projection of the structure onto $E^{||}$ (Steurer & Haibach, 1999*b*; Steurer, 2000). Note that it is possible to bound the projection to the $E^{\perp}$-projected Voronoi cell $\mathcal{V}$ of $\Lambda_{\rm QC}$ instead of the whole $E^{\perp}$. This inverts the cut-and-project scheme. The projection in direct space is an integration (*i.e.* an averaging) on $\Pi^{\perp}\mathcal{V}$, so that the average structure probability density results as

$$P^{\rm av}(\mathbf{r}^{||}) = \int_{\Pi^{\perp}\mathcal{V}} \mathrm{d}^2\mathbf{r}^{\perp}\, \hat{P}^S(\mathbf{r}^{||} \oplus \mathbf{r}^{\perp}). \tag{21}$$

It appears clear now that *the PAS of a QC is a particular average over all possible different QCs of the same LI class*.

Owing to the shearing, the integrated origin shifts in $E^{\perp}$ are linearly coupled with an $E^{||}$ shift (before shearing). This makes the average structure meaningful (all the more so when $\Lambda_{\rm av}^*$ contains a significant fraction of the scattered intensity, as we have in Steurer & Cervellino (2001) and Cervellino *et al.* (2002). In fact, with a zero-coupled $E^{||}$ shift, the average structure probability density results in a constant and its Fourier spectrum contains only $\mathbf{h} = 0$. This is what happens when we perform the same average of (21) in the standard embedding, without shear.

It is interesting to notice that the shear breaks the fivefold symmetry of the QC. Therefore, for every possible PAS, there exists a set of five equivalent PAS, related by a rotation of $2\pi/5$. It is straightforward to see that the union of the basis vectors of these five PAS lattices spans the QC 4D lattice (or a proper 4D sublattice of rank four). Otherwise, a complete 4D basis set can be obtained by combining two different PASs, in appropriate orientations.

[3] The projection onto $E^{||}$ is necessary because the $\mathbf{r}_i^S$ vectors will not generally have zero $E^{\perp}$ component.

5. Conclusions and discussion

We have presented a method for obtaining every possible PAS of a d-QC and explained their meaning in terms of structural average. The generalization to other QCs is surely possible; in fact, the extension to icosahedral QCs is straightforward (Steurer, 2000). Less simple – if we want to consider all the algebraic subtleties – is the extension to octagonal and dodecagonal QCs, but it is certainly possible. For other possible (but never discovered in nature) classes – *e.g.* heptagonal – there is a substantial difference, namely that $\dim E^{\perp} > \dim E^{||}$ (Niizeki, 1989). The consequences of this fact have to be theoretically explored.

How do we understand the significance of a PAS? First, we can calculate the density $P^{\rm av}(\mathbf{r}^{||})$ and compare it with the known structure of a periodic phase (based on whose diffraction pattern the fundamental reflections $\mathbf{h}_1$, $\mathbf{h}_2$ have been chosen). The recognition of a substantial similarity, apart from some statistical broadening, is an excellent indication of a strict phase relationship.

Any PAS, to be meaningful, needs to have an atomic like scattering density, with consistently peaked maxima. A necessary condition is that the lattice $\Lambda_{\rm av}^*$ contains some strong reflections; so one does not need to consider infinite PASs because PASs with only a lot of weak reflections will have an almost constant scattering density.

Another important reason to consider significant PASs that have atomic like scattering density is the possibility of using them to understand in a new way the theory of electrons in QCs. In fact, in certain cases (as we will publish elsewhere), it appears that there are possible electron wavefunctions that are substantially similar to Bloch waves of the PAS, allowing for a weak perturbation.

We recall, finally, that the concept of PAS has been thoroughly discussed in relation to the issue of the stability of QCs (Duneau & Oguey, 1990; Steurer & Haibach, 1999*b*; Steurer, 2000; Steurer & Cervellino, 2001; Cervellino *et al.*, 2002). The arguments presented, even if they need to be deepened, are convincing. For comparison, the theory of the stability of IMSs and CSs is well developed (see *e.g.* Janssen, 1986) and it is based on similar principles. It is very likely that, *mutatis mutandis*, some concepts can also be applied to QCs.

APPENDIX *A*
Number-theoretical tricks

We recall here some rules we use to simplify the passage throughout the paper. Integer powers of the golden mean τ can be reduced as $\tau^n = F_n\tau + F_{n-1}$, where F_n are the Fibonacci

numbers, defined recursively $\forall n \in \mathbb{Z}$ as $F_{n+1} = F_n + F_{n-1}$, with seeds $F_0 = 0$, $F_1 = 1$. The number χ is the smallest positive root of the equation $x^4 - 5x^2 + 5 = 0$. The latter's four roots $\pm\tau\chi$, $\pm\chi$ are the (doubled) imaginary parts of the roots $\exp(\pm 2\pi i/5)$, $\exp(\pm 4\pi i/5)$ of the cyclotomic polynomial $x^4 + x^3 + x^2 + x + 1 = 0$, which appears in the theory of decagonal embedding (see Niizeki, 1989). As $\chi^2 = 3 - \tau$, by the aforesaid properties of τ, it is possible to derive that $\chi^2\tau^n = L_n\tau + L_{n-1}$. L_n are the Lucas numbers, defined $\forall n \in \mathbb{Z}$ as $L_{n+1} = L_n + L_{n-1}$, with seeds $L_0 = -1$, $L_1 = 2$. For completeness, we give the cross-relation $L_n = F_n + F_{n-2}$. Any rational linear combination of powers of τ and χ can be reduced by these rules to a rational linear combination of 1, τ, χ and $\tau\chi$.

The principle of rational independence (*i.e.* $ax + b = 0$ iff $a = b = 0$ when $a, b \in \mathbb{Q}$ and x irrational) also allows one to simplify quotients. For $a, b, c, d \in \mathbb{Q}$, we have

$$\frac{a\tau + b}{c\tau + d} = \frac{(ad - bc)\tau + cb + bd - ca}{cd - c^2 + d^2}. \qquad (22)$$

APPENDIX *B*
Lengthy expressions

We give here explicitly the quantities in (19):

$$\begin{aligned}\mathcal{D} = 5\{&(T^2 - U^2 - TU)M^2 + (-R^2 - S^2 + 3SR)Q^2 \\ &+ (-3SR + S^2 + R^2)P^2 + [(-3T^2 + 3U^2 + 3TU)N \\ &+ (RU + 3ST - 2RT - 4SU)P \\ &+ (2RU - 3SU + ST + RT)Q]M \\ &+ (T^2 - U^2 - TU)N^2 \\ &+ [(SU - 2ST + 3RT + RU)P \\ &+ (ST + 2SU - 4RT - 3RU)Q]N \\ &+ (-R^2 - S^2 + 3SR)QP\};\end{aligned}$$

$$\begin{aligned}\boldsymbol{\alpha}_{11} &= 10(-SPU + SPT + NTU - NT^2 + NU^2 + RQT \\ &\quad - U^2M + T^2M - RPT + RQU - SQU - TUM); \\ \boldsymbol{\beta}_{11} &= 10(2SPU + SQU - SQT - SPT - NU^2 + RQT \\ &\quad - RPU - NTU + NT^2);\end{aligned}$$

$$\begin{aligned}\boldsymbol{\alpha}_{12} &= 2(2S^2P - S^2Q - 6RSP + 3RNT + RNU + 3RSQ \\ &\quad - 2SNT + SNU + RUM - 4USM + 3TSM - 2RTM \\ &\quad + 2R^2P - R^2Q); \\ \boldsymbol{\beta}_{12} &= 2(-S^2P - 2S^2Q - 2R^2Q + 3RSP - 4RNT - 3RNU \\ &\quad + 6RSQ + SNT + 2SNU + RTM + 2RUM - 3USM \\ &\quad + TSM - R^2P);\end{aligned}$$

$$\begin{aligned}\boldsymbol{\alpha}_{21} &= -10(RQ^2 + SP^2 - SQ^2 + RPQ - RP^2 - NPT \\ &\quad + NQT + NQU - MPU + MPT - MQU - SPQ); \\ \boldsymbol{\beta}_{21} &= -10(-MPU + MQT - SP^2 + SQ^2 + SPQ + NPU \\ &\quad + NPT - 2NQT - NQU);\end{aligned}$$

$$\begin{aligned}\boldsymbol{\alpha}_{22} &= 2(-2MRP + MRQ + 3MSP - 6MNT + 3MNU \\ &\quad + MSQ + 3RNP - 4RNQ - 2NSP + 2N^2T - N^2U \\ &\quad + NSQ + 2M^2T - M^2U); \\ \boldsymbol{\beta}_{22} &= -2(-MRP - 2MRQ + 4MSP - 3MNT - 6MNU \\ &\quad + 3MSQ - RNP + 3RNQ - NSP + N^2T + 2N^2U \\ &\quad - 2NSQ + M^2T + 2M^2U).\end{aligned}$$

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