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Disvections: mismatches, dislocations, and non-Abelian properties of quasicrystals

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Abstract. *Complete* dislocations in quasicrystals are intersections of dislocations in a high-dimensional lattice with an irrational cut that represents the physical space. We study the properties which proceed from that definition, either by methods relevant to the Volterra process, or by topological methods. *The Volterra process applies in the high-dimensional lattice* in a rather trivial way, but its restriction to the quasicrystal introduces very unusual geometrical properties, described in terms of *phason* deformations and of their singularities (mismatches). For example, the motion of a defect is generically non-commutative: the 'landscape' of mismatches carried by complete dislocations or disclinations in motion depends on the path which is followed by the defect between two positions, when two such paths surround a defect. The same type of argument applies, *mutatis mutandis*, to the question of the intersection of two defects. Other properties, of a more metallurgical nature, ensue from that use of the Volterra process, like the existence of stacking faults in QCs, bound by incomplete dislocations, and the relationship between mismatches and the reshuffling of atoms. Now, if one wishes to describe these remarkable properties with the sole use of physical observables (i.e. without mentioning the high-dimensional lattice), it appears that the natural language is the language of the *topological theory of defects in the quasilattice*. In particular it is shown that the group which classifies the dislocations is non-Abelian, a property in a direct relationship with the above-mentioned non-commutativity. We give the name of *disvections* to complete dislocations, because of their relationship with Cartan's transvections, which are translations with non-Abelian characters in a hyperbolic space.

1. Introduction

The question of the nature of topological defects in quasicrystals (QCs) has already been addressed by several authors: in particular it has been shown that the concept of dislocation (Levine *et al* 1985, Kléman *et al* 1986) still makes sense (as does the concept of disclination; Bohsung and Trebin 1989), although there are no repeat lattice vectors in a QC. And indeed their existence is not in any doubt, since dislocations have been observed in QCs by electron microscopy techniques, and their Burgers vectors measured with the help of diffraction contrast theory (Wollgarten *et al* 1991, Wang and Dai 1993). However, their true nature is somewhat more involved than in standard crystals. As the theory shows, 'perfect' dislocations in QCs are indeed always attended by other types of defect, usually called phason defects, or phason singularities—in the sense that they are the outcome of the *phase* shifts of the atomic configurations when the physical space $\mathbf{P}_{\parallel}$ is moved parallel to itself through the high-dimensional space $\mathbf{R}^d$—or mismatches. These mismatches continue

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to be mysterious, in spite of the effort devoted to understanding their nature. However, dislocations and their accompanying sets of mismatches have been classified, making use of the topological theory of defects (Kléman 1990, 1992). The same approach is reconsidered in the second section of this paper, in a presentation which is more straightforward than in our former publications. But the main purpose of this paper is different: we want to tackle the classification problem keeping as close as possible to another approach, the standard Volterra process and its implications (e.g. the concepts of stacking fault, and of glide plane—in brief, all of those concepts that have led to the richness of materials science); this methodology not only has the advantage of providing a physical interpretation for the abstractions of the topological theory—this is why its presentation has gained in clarity—but also it is complementary to it, since those concepts would not appear naturally, were the topological theory our only guide.

Hence, section 2 is a description in terms of Volterra concepts of the unusual characteristics of the dislocations of the quasicrystalline lattice in the physical space $\mathbf{P}_\parallel$, conceived as intersections of the (hyper-) dislocations of a high-dimensional crystalline lattice $\mathbf{E}^d$ in $\mathbf{R}^d$ with the physical space. The concepts that we introduce in this section are those of the stacking fault, reshuffling of atoms, and the non-commutativity of dislocation movement, this latter being precisely the effect of the presence of fields of mismatches. Some of these results have already been published in the *Professor Kroupa Festschrift* (Kléman 1995). Section 3 expresses the same subject in terms of the topological theory of defects, which helps to nicely classify defects and in particular gives a firm setting for the concept of non-commutativity. This section of the paper, although less original, contains new views arising from the analysis that precedes it.

We shall assume in the following that the reader has some familiarity with the two approaches to the classification of defects—on one hand the Volterra classification of dislocations (Friedel 1964), and on the other hand the topological theory of defects, to which many reviews have been devoted (Mermin 1979, Michel 1980), and which is indispensable when defects other than dislocations are present. We shall also assume some familiarity with the essentials of the high-dimensional description of quasicrystals (for a bibliography and a selection of articles on quasicrystals, see Steinhardt and Ostlund (1987), DiVincenzo and Steinhardt (1991)); we shall use the definition of a QC as a set of vertices determined by the intersections of the so-called ‘atomic surfaces’ $\mathbf{S}$ with the physical space $\mathbf{P}_\parallel$ (Bak 1985). The deformations of the physical space will be defined as resulting from deformations in the high-dimensional space, that have the effect of modifying the intersections of the atomic surfaces with $\mathbf{P}_\parallel$, which is assumed fixed in the laboratory frame†.

Generically, the $d_\perp$-dimensional atomic surfaces which we consider are manifolds carried by the vertices of a d-dimensional hypercubic lattice $\mathbf{E}^d$, for which they play the same role as atoms play in a 3D crystal; as such, the atomic surfaces are undeformable entities. $\mathbf{P}_\parallel$ is a $d_\parallel$-dimensional linear subset of the euclidean space $\mathbf{R}^d$ where the hyperlattice ‘lives’, and cuts $\mathbf{R}^d$ along an irrational direction in $\mathbf{E}^d$. Therefore $\mathbf{P}_\parallel$ contains at most one vertex of $\mathbf{E}^d$. The $d_\perp$-dimensional complementary space $\mathbf{P}_\perp$ is such that we have $\mathbf{R}^d = \mathbf{P}_\parallel \oplus \mathbf{P}_\perp$, the direct sum; there is therefore a copy of $\mathbf{P}_\perp$ perpendicular to $\mathbf{P}_\parallel$ at any of its points. We also introduce the so-called acceptance domain $\mathbf{A}_\perp$, which is the projection on $\mathbf{P}_\perp$ of a unit hypercube having the size and the orientation of a hypercube belonging to $\mathbf{E}^d$ (see figure 1).

† Another method for deforming the QC consists in keeping the high-dimensional space undeformed, and deforming $\mathbf{P}_\parallel$ accordingly, to get the same result. In that case one has to make a distinction between the deformed $d_\parallel$-dimensional space (call it $\mathbf{P}'_\parallel$), which obviously can no longer play the role of a ‘physical space’, and the physical space *sensu stricto*, the undeformed $\mathbf{P}_\parallel$. This latter method lacks generality, but might help one to visualize the deformation in physical space.

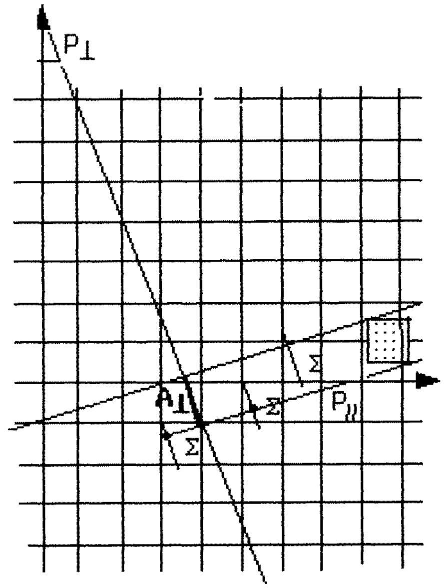

Figure 1. The QC is the intersection of the atomic surfaces carried by the vertices of the hyperlattice with a $d_\parallel$-dimensional irrational cut $\mathsf{P}_\parallel$ of E^d (here $d_\parallel = 1, d = 2, \tan\alpha = \tau^{-1}$; $\tau = (1+\sqrt{5})/2$ is the Golden Ratio). In this picture, the atomic surfaces are supposed to be segments of line congruent to the acceptance domain $\mathsf{A}_\perp$. The lattice is globally invariant under a shift of the cut plane along $\mathsf{P}_\perp$; this is the phase invariance.

It will play the role of an extended parameter space in the second section of this paper, and will under no circumstances be given the meaning that it has in the well-known alternative definition of a QC, the cut-and-project method (Duneau and Katz 1985, Katz and Duneau 1985).

2. Dislocations in R^d and their intersections with $\mathsf{P}_\parallel$

We recall that the definition of a dislocation in a three-dimensional crystal (Friedel 1964) requires two ingredients, the line L along which the symmetry is broken, and the broken symmetry, namely a translation $\boldsymbol{b}$ or a rotation $\boldsymbol{\omega}$, or both. The Volterra process is a *gedanken* experiment aimed at creating such an object starting from the perfect ordered medium, and consists in introducing a 'cut surface' $\boldsymbol{\Sigma}$ bound by the line L, displacing the two lips $\boldsymbol{\Sigma}_1$ and $\boldsymbol{\Sigma}_2$ of the cut surface with respect to each other by a relative displacement (a translation $\boldsymbol{b}$—the so-called Burgers vector—and a rotation $\boldsymbol{\omega}$), filling the void thus created with perfect matter, or removing extra matter, then reintroducing the bonds between the atoms or molecules across $\boldsymbol{\Sigma}_1$ and $\boldsymbol{\Sigma}_2$, and letting the system relax elastically. The result is a singularity along the line L; there is no singularity along the cuts if $\boldsymbol{b}$ and $\boldsymbol{\omega}$ are operations of symmetry of the perfect crystal. Dislocations of rotation are called disclinations, while the term of dislocation is usually reserved to dislocations of translation; we follow this use.

A dislocation line $\mathsf{L}_\parallel$ in a quasicrystal is a $(d_\parallel - 2)$-dimensional manifold which is the intersection of $\mathsf{P}_\parallel$ with a $(d-2)$-dimensional dislocation hyperline L of the hyperlattice (Kléman 1988, Kléman and Sommers 1991); the Burgers vector of the hyperdislocation L is a hyperlattice vector $\boldsymbol{b}$, which splits naturally into two components $\boldsymbol{b}_\parallel$ and $\boldsymbol{b}_\perp$: $\boldsymbol{b} = \boldsymbol{b}_\parallel + \boldsymbol{b}_\perp$,

($\boldsymbol{b}_\parallel \subset \mathbf{P}_\parallel$; $\boldsymbol{b}_\perp \subset \mathbf{P}_\perp$). The cut surface $\boldsymbol{\Sigma}$ is $(d-1)$-dimensional; its $(d_\parallel - 1)$-dimensional intersection with $\mathbf{P}_\parallel$ will be denoted $\boldsymbol{\Sigma}_\parallel$. This is obviously a possible cut surface for a dislocation line $\mathbf{L}_\parallel$ in physical space, since it is bound by $\mathbf{L}_\parallel$.

Physically, it is $\mathbf{L}_\parallel$ which is given, as well as $\boldsymbol{b}$, but we expect that some of the properties of the dislocation in real space, in particular the phason field which it carries, will depend on the entire hyperdislocation ($\mathbf{L}$, $\boldsymbol{b}$). We investigate now possible shapes of $\mathbf{L}$. This question is indeed essential when employing the first method of deforming the QC†.

2.1. *A specialized Volterra process:* ($\mathbf{L}$, $\boldsymbol{b}$) *in* $\mathbf{E}^d$

2.1.1. The shape of $\mathbf{L}$. It is usually assumed that the hyperline $\mathbf{L}$ is a $(d-2)$-dimensional manifold which has the form of the following direct sum of manifolds:

$$\mathbf{L} = \mathbf{L}_\parallel \oplus \mathbf{P}_\perp \tag{1}$$

i.e. $\mathbf{L}$ is a $(d-2)$-dimensional cylinder with generatrices parallel to $\mathbf{P}_\parallel$ and the cross-section along $\mathbf{L}_\parallel$. There is no restriction on the choice of $\mathbf{L}_\parallel$, except that it must be a closed loop or extend to infinity. But the specific choice made as regards $\mathbf{L}$ confers to the dislocation ($\mathbf{L}_\parallel$, $\boldsymbol{b}$) some very special properties.

(i) Property α. The intersection of $\mathbf{L}$ with $\mathbf{P}_\parallel$ does not depend on the relative positions of $\mathbf{E}^d$ and $\mathbf{P}_\parallel$, so $\mathbf{L}_\parallel$ is *invariable in shape and in position* when the hyperlattice $\mathbf{E}^d$ is globally translated in d-space for fixed $\mathbf{P}_\parallel$.

(ii) Property β. The *core* region of $\mathbf{L}_\parallel$ is *isotropic* in shape, an important property from an energetical point of view—see below for a discussion of this property and Kléman and Sommers (1991).

(iii) Property γ. The notion of *glide* of the dislocation makes sense. The $(d-1)$-dimensional 'glide manifold' $\mathbf{G}$ defined by $\mathbf{L}$ and the line $\mathbf{B}$ spanned by $\boldsymbol{b}$, namely

$$\mathbf{G} = \mathbf{L} \oplus \mathbf{B} \equiv (\mathbf{L}_\parallel \oplus \mathbf{P}_\perp) \oplus \mathbf{B} \equiv \mathbf{L}_\parallel \oplus (\mathbf{P}_\perp \oplus \mathbf{B}) \equiv \mathbf{L}_\parallel \oplus (\mathbf{P}_\perp \oplus \mathbf{B}_\parallel) \equiv \mathbf{L} \oplus \mathbf{B}_\parallel \tag{2}$$

does indeed intersect the physical space $\mathbf{P}_\parallel$ along a $(d_\parallel - 1)$-dimensional plane:

$$\mathbf{G}_\parallel = \mathbf{L}_\parallel \oplus \mathbf{B}_\parallel \tag{3}$$

($\dim \mathbf{G}_\parallel = \dim \mathbf{P}_\parallel + \dim \mathbf{G} - d = d_\parallel - 1$) which contains $\mathbf{L}_\parallel$ and $\boldsymbol{b}_\parallel$; $\mathbf{B}_\parallel$ is the infinite line spanned by $\boldsymbol{b}_\parallel$. The third identity in equation (2), namely $\mathbf{P}_\perp \oplus \mathbf{B} \equiv \mathbf{P}_\perp \oplus \mathbf{B}_\parallel$, is obtained easily from the property of associativity of the direct sum, plus the fact that $\mathbf{P}_\perp$ contains $\mathbf{B}_\perp$, the infinite line spanned by $\boldsymbol{b}_\perp$; hence $\mathbf{P}_\perp \oplus \mathbf{B}$ is factorized by the 2-plane containing $\mathbf{B}_\parallel$ and $\mathbf{B}_\perp$. The physical glide manifold (called a glide 'plane' in the usual terminology) $\mathbf{G}_\parallel$ of $\mathbf{L}_\parallel$ is precisely $\mathbf{L}_\parallel \oplus \mathbf{B}_\parallel$, by definition.

Such a quasicrystallographic dislocation shows many similarities with a dislocation in standard crystallography, because of its translational invariance along $\mathbf{P}_\perp$. We make this point precise now.

2.1.2. Construction of ($\mathbf{L}_\parallel$, $\boldsymbol{b}$) *in two steps.* The dislocation ($\mathbf{L}$, $\boldsymbol{b}$) is translationally invariant along $\mathbf{P}_\perp$, because of equation (1). Therefore, neglecting any effect of anisotropy in $\mathbf{E}^d$, the deformation field restricted to $\mathbf{P}_\parallel$ is the same in any realization of the physical space (when $\mathbf{P}_\parallel$ moves parallel to itself).

† In the method in which the deformation carried by $\mathbf{L}$ is restricted to $\mathbf{P}_\parallel$, which is thus transformed to a 'space' $\mathbf{P}'_\parallel$ endowed with torsion due to the presence of dislocations, and with curvature due to the presence of disclinations. It is not necessary to stress the awkwardness of this process.

(i) *Step 1.* We first build a dislocation in physical space, with elements ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$), using a classical Volterra process along $\boldsymbol{\Sigma}_\parallel$. As a dislocation, ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$) is *imperfect* (since $\boldsymbol{b}_\parallel$ is not a repeat vector in $\mathsf{P}_\parallel$) and carries a stacking fault along the cut surface $\boldsymbol{\Sigma}_\parallel$; its orbit ($\mathsf{L}$, $\boldsymbol{b}_\parallel$) under the action of the $\mathsf{P}_\perp$ translation is a $(d-1)$-dimensional *imperfect* dislocation with a stacking fault along $\boldsymbol{\Sigma}$ in E^d.

Now, consider the state of strain in $\mathsf{P}_\parallel$ due to the presence of ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$). One can obviously perform the Volterra process for ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$) while keeping $u_\alpha = 0$ ($\boldsymbol{u}$ is the d-dimensional displacement vector, u_i its components along $\mathsf{P}_\parallel$ ($i, j = 1, 2, \ldots, d_\parallel$), u_α its components along $\mathsf{P}_\perp$ ($\alpha, \beta = 1, 2, \ldots, d_\perp$). Transposing to the language of the elasticity of plates, one can say that the $\mathsf{P}_\parallel$-plate, which is infinitely thin along the directions α, β, etc, and whose $d_\perp$-dimensional normals span $\mathsf{P}_\perp$, is in a state of plane strain. Therefore the deformation carried by ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$) is phasonless. The stacking fault in physical space, alluded to above, is a quite standard stacking fault with no relationship whatsoever to a phason field.

(ii) *Step 2.* Let us concentrate for a while on the hyperdislocation (L, $\boldsymbol{b}$); the $\boldsymbol{\Sigma}$ stacking fault does not persist in (L, $\boldsymbol{b}$); it is dispersed away by a second Volterra process (L, $\boldsymbol{b}_\perp$) which is of a pure screw dislocation type. It is easy to visualize how the transition $(\mathsf{L}, \boldsymbol{b}_\parallel) \to (\mathsf{L}, \boldsymbol{b})$ occurs in E^d: the $\boldsymbol{\Sigma}$ stacking fault divides *the set of hyperlattice points in* E^d, and in its vicinity, into two populations, on either side of the cut surface $\boldsymbol{\Sigma}$; let us call them ω_1 and ω_2, and assume that the Volterra process consists in displacements $\boldsymbol{b}_\parallel$ (step 1) and $\boldsymbol{b}_\perp$ (step 2) of ω_1, for fixed ω_2†. After the completion of step 1, those of the lattice points which are neighbours across $\boldsymbol{\Sigma}$ form two sets, $\omega_{\Sigma 1}$ and $\omega_{\Sigma 2}$ translated one with respect to the other by a vector $\boldsymbol{b}_\parallel$ which is not a repeat vector of the lattice; the screw dislocation adds a complementary translation $\boldsymbol{b}_\perp$ which brings back the two populations into period-matching relative positions. The stacking fault disappears (the cut surface loses any physical reality): the hyperdislocation (L, $\boldsymbol{b}$) is perfect. This analysis is very similar to that used for standard 3D crystals.

(iii) The same sequence of steps involved in the construction of (L, $\boldsymbol{b}$) and now applied to the construction of $(\mathsf{L}_\parallel, \boldsymbol{b})$ does not tell us how the extension from $(\mathsf{L}_\parallel, \boldsymbol{b}_\parallel)$ to ($\mathsf{L}_\parallel$, $\boldsymbol{b}$) proceeds. The question is indeed more involved, as we now describe.

The *quasilattice points* $\omega_{\parallel 1}$ (i.e. the restriction of ω_1 to $\mathsf{P}_\parallel$) and $\omega_{\parallel 2}$ (the restriction of ω_2 to $\mathsf{P}_\parallel$) are intersections of the atomic surfaces with $\mathsf{P}_\parallel$. Choose $\boldsymbol{\Sigma}_\parallel$ such that it does not contain any of those quasilattice points. Consider the quasilattice points which are neighbours across $\boldsymbol{\Sigma}_\parallel$. The atomic surfaces carried by $\omega_{\parallel 1}$ are moved along $\mathsf{P}_\perp$ by an amount $\boldsymbol{b}_\perp$; this process brings some lattice points into 'good' positions with respect to $\omega_{\parallel 2}$, while some others disappear, since the corresponding atomic surfaces do not intersect $\mathsf{P}_\parallel$ any longer, and are replaced by another neighbouring atomic surface which intersects $\mathsf{P}_\parallel$ at a site which corresponds precisely to a phason shift (figure 2). *Phason shifts are not topological objects*; they can easily annihilate—this is visible figure 2—and are made up of two nearest-neighbouring *mismatches* of opposite signs; now two adjoining phason shifts which have a common edge (figure 2(c)) also amount to two mismatches of opposite signs, in positions of next-nearest neighbours, since the common edge carries two mismatches of opposite signs which annihilate. *Mismatches are topological objects*, in the sense that

† One might argue over whether one may divide the set of all atomic surfaces into two populations only, above and below $\boldsymbol{\Sigma}$ (no atomic surfaces in $\boldsymbol{\Sigma}$). In fact the same problem arises in 3D crystals; it is always possible, in this latter case, at the cost of some distortion of the dislocation line and of its cut surface whose amplitude is not larger than the lattice parameter, to make the cut surface before completion of the Volterra process avoid any vertex of the Bravais lattice. The same is true here, although the intersection of an atomic surface S with $\boldsymbol{\Sigma}$ is generically of dimensionality $(d_\perp - 1)$, because the size of the atomic surfaces is of the order of the repeat distance in E^d.

one given mismatch can get isolated, far from another mismatch of opposite sign, if ever a large number of phason shifts separate them. Note also that the sites in shifted positions are intersections of sets of neighbouring atomic surfaces attached to neighbouring vertices in $\mathbf{E}^d$ which can be partitioned into $(d_\parallel - 1)$-dimensional hyperplanar pieces; but it is only the boundaries of these sets which constitute a mismatch, of dimensionality $d_\parallel - 2$, i.e. of the same dimensionality as the dislocation.

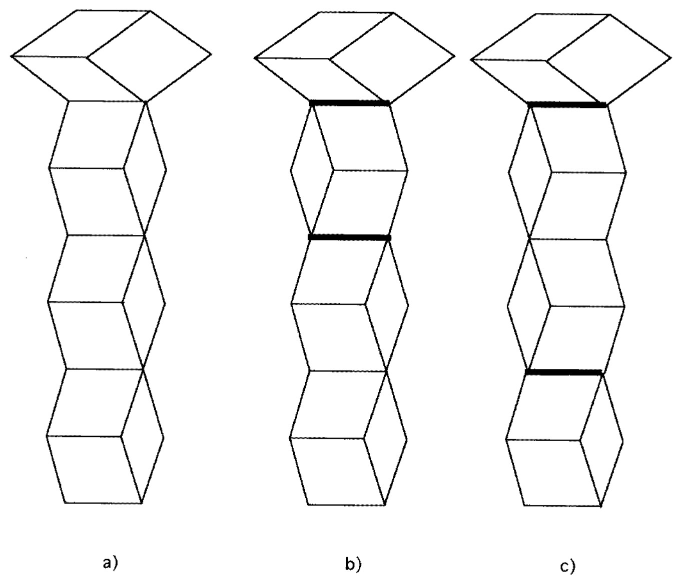

Figure 2. Phason shifts and mismatches illustrated in the Penrose–De Bruijn case: (a) a perfect sequence of hexagonal patterns, obeying matching rules; (b) a single phason shift and the two opposite mismatches which it carries; by mutual annihilation of the mismatches, the phason shift disappears; (c) two neighbouring phason shifts and the two mismatches at the boundaries of the domain affected by the phason shifts.

2.1.3. The landscape of mismatches. The mismatches result from a special reshuffling (the phason shifts) of the atoms in the physical space $\mathbf{P}_\parallel$, by a cooperative movement varying from one point to another in a complex way which remains to be analysed; a possible analogy is with the 'synchro-shear' dislocation loops of Kronberg (see, for instance, Amelinckx 1979), which sweep the surface of the stacking fault coherently in standard crystals with complex structures, in order to relocate some atoms *too badly* displaced by the imperfect Burgers glide. In order to illustrate what we have in mind, remember as an example that in corundum (Amelinckx 1979), the stacking fault, which affects the fcc lattice of the oxygen atoms, brings the small Al atoms into 'bad' tetrahedral sites, while the synchro-shear loops transform those local 'bad' tetrahedral sites into 'good' octahedral sites, by a process which is clearly analogous to a phason shift—which transforms a 'bad' empty site (or a bad analytical continuation of the intersection of the atomic surface with $\mathbf{P}_\parallel$) into a 'good' site. As a consequence, this suggests studying in more detail the nature of those sites which have suffered shifts in QCs, before and after the introduction of the $(\mathbf{L}, \boldsymbol{b}_\perp)$ dislocation.

We shall refer to the set of mismatches as a 'landscape' seen by the dislocation (see Kléman and Sommers (1991) for a 2D illustration). The perpendicular component $\boldsymbol{b}_\perp$

of the complete Burgers vector $\boldsymbol{b}$ therefore measures the phason singularity content (the mismatches) carried by the dislocation; but it is clear that the detailed structure of the landscape depends in an intrinsic way on the phase of $\mathbf{P}_{\parallel}$, i.e. its relative position in $\mathbf{E}^d$.

2.1.4. Relative movement of two dislocations. We consider now the problem of two dislocation lines $\mathbf{L}_1$ and $\mathbf{L}_2$ of complete Burgers vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$, crossing in $\mathbf{P}_{\parallel}$ or circumnavigating one another.

When *crossing* occurs, the manifold common to the lines $\mathbf{L}_1$ and $\mathbf{L}_2$ is $\mathbf{P}_{\perp}$ itself. In the physical space $\mathbf{P}_{\parallel}$, the result is a 'jog' very similar to the jogs analysed in standard crystals (see Kléman and Sommers 1991). The jog on $\mathbf{L}_{1\parallel}$ is $\boldsymbol{b}_{2\parallel}$; that on $\mathbf{L}_{2\parallel}$ is $\boldsymbol{b}_{1\parallel}$. This modification of the shape of the line modifies the elastic (phonon) field accordingly. By the same process of crossing, the jog on $\mathbf{L}_1$ (in $\mathbf{E}^d$) is $\boldsymbol{b}_2$, i.e. it has a component $\boldsymbol{b}_{2\perp}$ which pushes a part of the line $\mathbf{L}_1$ on one side of the jog relative to that on the other side by this quantity; but since $\boldsymbol{b}_{2\perp} \in \mathbf{P}_{\perp}$, which itself belongs to $\mathbf{L}_1$, this has no effect on the 'phason' field carried by the dislocation, except along a strip contour of width $\boldsymbol{b}_{2\parallel}$, since the cut surface has been translated by the quantity $\boldsymbol{b}_{2\parallel}$: the landscape is not modified after the crossing has occurred.

The analysis for *circumnavigation* is very similar. We start first with a remark regarding standard crystals, which is of some importance below. The natural definition of the path traversed by a dislocation line $\mathbf{L}_2$ of Burgers vector $\boldsymbol{b}_2$ circumnavigating a fixed dislocation line $\mathbf{L}_1$ and of Burgers vector $\boldsymbol{b}_1$ is as follows: during its motion, $\mathbf{L}_2$ experiences glide and climb; *glide*, which is conservative, does not affect the positioning of the atoms, which stay in place; but in contrast, *climb* is not conservative and the atoms diffuse away from or towards the dislocation: the net amount of diffusion is zero when $\mathbf{L}_2$ has moved by a quantity $\pm\boldsymbol{b}_1$ in the reference frame of $\mathbf{L}_1$, because each direction is then traversed by equal amounts back and forth, independently of the Burgers vector $\boldsymbol{b}_2$ of the moving dislocation. The sign depends on whether the motion is clockwise or anticlockwise. In other words, a complete circumnavigation does not imply a closed traversed path in the real crystal, but does imply a closed path in the mapping of the path in a perfect reference crystal.

Similarly, in the $\mathbf{E}^d$ lattice, after circumnavigation, the two dislocation lines are in different relative positions, $\pm\boldsymbol{b}_2$ for the line $\mathbf{L}_1$, $\pm\boldsymbol{b}_1$ for the line $\mathbf{L}_2$. As above, this displacement of the lines does not change their landscape, except on a contour strip of width $\pm|\boldsymbol{b}_2|$ along the line $\mathbf{L}_1$, $\pm|\boldsymbol{b}_1|$ along the line $\mathbf{L}_2$.

2.2. A more generic Volterra process: $(\mathbf{L}, \boldsymbol{b})$ *in* $\mathbf{E}^d$

The generic case, i.e. when $\mathbf{L}$ does not contain $\mathbf{P}_{\perp}$ as a factor in the direct sum of equation (1), yields new properties. We first consider in some detail an intermediary case.

Let us drop property α but not properties β and γ, which are of more physical significance than property α. Start with property γ alone: a glide plane still exists if $\mathbf{G}_{\parallel}$ contains $\mathbf{B}_{\parallel}$. By definition, we have $\mathbf{G}_{\parallel} = \mathbf{L}_{\parallel} \oplus \mathbf{B}_{\parallel}$. It can be shown that this is satisfied if $\mathbf{L}$ contains the infinite line $\mathbf{B}_{\perp}$ as a factor in the cartesian product, i.e. if $\mathbf{L}$ has the form

$$\mathbf{L} = \mathbf{L}_{\parallel} \oplus \mathbf{B}_{\perp} \oplus \boldsymbol{\sigma} \tag{4}$$

where $\boldsymbol{\sigma}$ is a $(d_{\perp} - 1)$-dimensional manifold living in $\mathbf{P}_{\perp}$ in a hyperplane perpendicular to $\mathbf{B}_{\perp}$. In effect, we have by definition

$$\mathbf{G} = \mathbf{L}_{\parallel} \oplus \mathbf{B}_{\perp} \oplus \mathbf{B}_{\parallel} \oplus \boldsymbol{\sigma} \equiv (\mathbf{L}_{\parallel} \oplus \mathbf{B}_{\perp} \oplus \boldsymbol{\sigma}) \oplus \mathbf{B}_{\parallel} \tag{5}$$

and hence $\mathbf{G}_{\parallel} = \mathbf{L}_{\parallel} \oplus \mathbf{B}_{\parallel}$.

Note that, if $\boldsymbol{\sigma}$ is a $(d_\perp - 1)$-plane, one returns to the previous case where $\mathbf{B}_\perp \oplus \boldsymbol{\sigma} = \mathbf{P}_\perp$.

The reciprocal theorem is true (see the appendix), i.e. property γ alone (the existence of a glide plane in physical space) yields (a) $\mathbf{G} = \mathbf{L}_\parallel \oplus \mathbf{B}_\perp \oplus \mathbf{B}_\parallel \oplus \boldsymbol{\sigma}(M_\parallel)$, where $\boldsymbol{\sigma}$ is a manifold which lives in $\mathbf{P}_\perp$ in a hyperplane perpendicular to $\mathbf{B}_\perp$ and is allowed to vary along $\mathbf{L}_\parallel$ ($M_\parallel \in \mathbf{L}_\parallel$); it also yields (b) a core that is isotropic in shape (see the appendix). For the sake of simplicity, we take $\boldsymbol{\sigma}$ as a constant manifold in the following.

As a consequence the dislocation line is translationally invariant along $\boldsymbol{b}_\perp$, as above, but not along other directions in $\mathbf{P}_\perp$, generically. This geometry yields new properties when considering *two* dislocations ($\mathbf{L}_1$, $\boldsymbol{b}_1$) and ($\mathbf{L}_2$, $\boldsymbol{b}_2$).

Note first that the $\boldsymbol{b}_{1\perp}$ component of $\boldsymbol{b}_1$ belongs to the dislocation hyperline; hence any motion of the hyperline along $\boldsymbol{b}_{1\perp}$ leaves the geometry of the hyperline invariant as a whole and invariant with respect to $\mathbf{P}_\parallel$. Therefore the effect on a dislocation ($\mathbf{L}_1$, $\boldsymbol{b}_1$) of the complete circumnavigation of a dislocation ($\mathbf{L}_2$, $\boldsymbol{b}_2$) about it amounts to nil if $\boldsymbol{b}_{2\perp} = \boldsymbol{b}_{1\perp}$ (which yields $\boldsymbol{b}_{2\parallel} = \boldsymbol{b}_{1\parallel}$, and therefore $\boldsymbol{b}_2 = \boldsymbol{b}_1$): the translational helical symmetry of ($\mathbf{L}_1$, $\boldsymbol{b}_1$) is not broken by the symmetry of ($\mathbf{L}_2$, $\boldsymbol{b}_1$). Contrariwise, when $\boldsymbol{b}_{2\perp} \neq \boldsymbol{b}_{1\perp}$ (which entails that $\boldsymbol{b}_{2\perp}$ and $\boldsymbol{b}_{1\perp}$ are not parallel), a point A belonging to $\mathbf{L}_1$ is transported after the circumnavigation of $\mathbf{L}_2$ about it to a point $\mathrm{A}' = \mathrm{A} + \boldsymbol{b}_{2\perp}$ which does not belong to $\mathbf{L}_1$, and the entire hyperline is displaced to a new position $\mathbf{L}_1'$. The landscape has been modified in a fundamental manner, because the dislocation hyperline $\mathbf{L}_1$ has been translated in $\mathbf{E}^d$; note that the translation $\boldsymbol{b}_{2\perp}$ does not affect the position of its intersection $\mathbf{L}_{1\parallel}$, but it affects the u_α-components along $\mathbf{P}_\perp$ of the d-dimensional displacement vector $\boldsymbol{b}$, and hence it affects the phason singularity field carried by $\mathbf{L}_{1\parallel}$.

Note that the same property of non-commutativity implies that the intersection of dislocations in relative motion is not so simple as in standard solids: the fact that the hyperlines $\mathbf{L}_1$ and $\mathbf{L}_2$ are not parallel outside $\mathbf{P}_\parallel$ yields intersections in the physical space which cannot be analysed as jogs or kinks. The above arguments, supplemented by the topological analysis below, suggest that the topological obstruction to crossing (i.e. the non-commutativity) results in the formation of a singularity of the phason field joining the points of contact of the two lines after their separation.

2.3. *The generic case*

The above detailed discussion makes easy the formulation of general statements for the generic case. A complete circumnavigation of a dislocation ($\mathbf{L}_{2\parallel}$, $\boldsymbol{b}_2$) in physical space about another one ($\mathbf{L}_{1\parallel}$, $\boldsymbol{b}_1$) has the effect of translating $\mathbf{L}_1$ to $\mathbf{L}_1' = \mathbf{L}_1 + \boldsymbol{b}_2$, and hence modifying the phonon as well as the phason field (including its singularities) carried by $\mathbf{L}_{1\parallel}$. The modification of the phonon field is due to the displacement $\boldsymbol{b}_{2\parallel}$ of the cut surface $\boldsymbol{\Sigma}_\parallel$, and hence of the line $\mathbf{L}_{1\parallel}$. The modification of the phason field is due to the displacement $\boldsymbol{b}_{2\perp}$ of the hyperline $\mathbf{L}_1$.

An obvious generalization of the above statement is when one of the defects (or both) are disclinations: a mixed defect ($\mathbf{L}_2$, $\boldsymbol{\omega}_2$, $\boldsymbol{b}_2$) circumnavigating a mixed defect ($\mathbf{L}_1$, $\boldsymbol{\omega}_1$, $\boldsymbol{b}_1$) displaces $\mathbf{L}_1$ by a rotation $\boldsymbol{\omega}_2$ and a translation $\boldsymbol{b}_2$, and consequently changes the landscape that it carries.

The change of landscape depends on the circumnavigating defect and on the shape of the defect hyperline; this points towards a possible experimental study of the shape of the defect in $\mathbf{E}^d$.

Finally, the same type of arguments apply, *mutatis mutandis*, to the question of the intersection of two defects. In all cases the existence of non-commutativity of the physical space defects in movement boils down to commutative geometrical properties in the high-dimensional space. A description of defects limited to the physical space observables introduces topological concepts in a natural way, as we shall see in section 3.

2.4. Glide with and without the presence of complete or incomplete dislocations

As discussed above, the notion of glide makes sense with the above construction and definition of L. If the creation of a dislocation in physical space does not involve the second part of the Volterra process, for example at low temperature when the reshuffling is not thermally activated, then one expects that dislocations ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$) will glide in planes of high density (twofold, threefold or fivefold planes), in which the stacking fault would lie. Such imperfect dislocations have been observed in AlLiCu icosahedral alloys (Yu DaPeng 1993, Baluc *et al* 1995).

Note finally that, since $\boldsymbol{b}_\parallel$ is an irrational projection of a lattice vector $\boldsymbol{b}$ in E^d, it can be as close as one wishes to any vector $\boldsymbol{b}_\parallel$ fixed in advance, and hence as small as one wishes. From that point of view, the displacement of an incomplete dislocation ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$) on its glide plane in a QC is very much akin to the glide of a dislocation in a metglass, whose Burgers vector is not quantified (Friedel 1995a). On the other hand, the addition of a landscape of mismatches to ($\mathsf{L}_\parallel$, $\boldsymbol{b}_\parallel$), making the dislocation complete—($\mathsf{L}_\parallel$, $\boldsymbol{b}$)—should stabilize the line $\mathsf{L}_\parallel$ in some sense (Friedel 1995b) and therefore probably contribute to a decrease in mobility.

3. Topological classification of defects

The above results can be expressed in the language of the topological theory of defects. For simplicity, we shall have in mind, as an example, the octagonal tiling (Socolar 1990), made up of two types of rhombus, with $d_\parallel = 2, d_\perp = 2$. The acceptance domain $\mathsf{A}_\perp$ is a regular octagon. The octagonal case bears some physical interest, since octagonal QCs do exist in nature (Kuo 1990). It has also been handled in some detail in the important paper of Frenkel *et al* (1986). This example extends without much difficulty to the duodecagonal and the icosahedral tilings; however, some care should be taken with the decagonal (Penrose–De Bruijn) tiling. For more details about this extension, see the remarks at the end of this section.

Consider a deformed QC, with defects. Let Γ be an oriented loop, entirely drawn in the 'good' quasicrystal—good in the sense that it is possible to recognize the lift M^d in E^d of any vertex M belonging to the QC. Therefore Γ lifts in E^d along a path Γ^d, such that each vertex encountered inside the QC goes to the vertex which carries the corresponding atomic surface in E^d and, by extrapolating between vertices, each point inside a 2-face goes to the corresponding point in some 2-face in E^d, and each point inside a rhombohedron goes to the corresponding point inside some 3-face in E^d. Note that this mapping does not require that the matching rules be obeyed along Γ. If Γ^d is an open path, its closure failure $\boldsymbol{b}$ necessarily joins two equivalent points in the hyperlattice, and Γ, considered as a oriented circuit embedded in E^d, is simply a Burgers circuit which encloses a dislocation line L of the Burgers vector $\boldsymbol{b}$ in the hyperlattice; L intersects the $d_\parallel$-dimensional physical space $\mathsf{P}_\parallel$ along some line $\mathsf{L}_\parallel$. Such defects are therefore classified by the Abelian group of translational symmetries of the hyperlattice, or equivalently by the fundamental group $\pi_1(\mathsf{T}^d)$ of the d-dimensional torus (i.e. the unit hypercell with $(d-1)$-dimensional faces identified point by point).

T^d is the order parameter space of the hypercrystal (restricted to the translational part of the order parameter), but the order parameter space of the QC itself is certainly smaller,

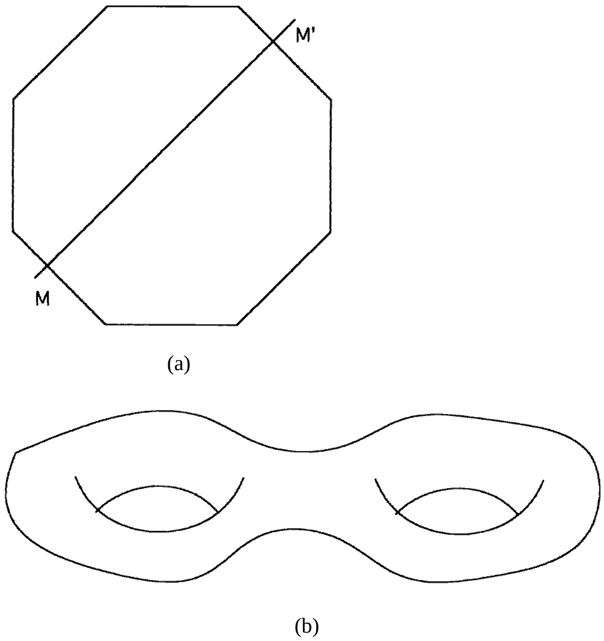

Figure 3. The order parameter space for an octagonal QC: (a) its planar development $\mathbf{A}_\perp$ as an octagon with opposite sides identified; the octagon is the projection of the 4-cube onto $\mathbf{P}_\perp$; (b) its representation $\mathbf{U}$ as a closed manifold (a pretzel with two handles; see Hilbert and Cohn-Vossen 1952).

and embeddable in $\mathbf{T}^d$. Since any point $M_\perp \in \mathbf{P}_\perp$ yields a unique realization of the QC in a $d_\parallel$-plane, $\mathbf{P}_\parallel$ ($M_\perp$ is the intersection of $\mathbf{P}_\parallel$ with $\mathbf{P}_\perp$), nothing (but see below for an important caveat) is lost by replacing $\mathbf{T}^d$ by the projection of the hypercell $\mathbf{C}^d$ onto $\mathbf{P}_\perp$—this projection is precisely $\mathbf{A}_\perp$—with $(d_\perp - 1)$-dimensional faces identified according to the identification of the hypercell $\mathbf{C}^d$. Call the manifold obtained by performing this identification $\mathbf{U}$. In the octagonal case $\mathbf{U}$ is a 2D torus with two handles (figure 3). Any two points in $\mathbf{A}_\perp$ (the octagon) equivalent in this identification are separated by a vector $\boldsymbol{A}_{i\perp}$ which is the projection of a vector $\boldsymbol{A}_i$ in $\mathbf{E}^d$ which joins two points on the hypercell equivalent in a 'silhouetting' translation (in the language of Frenkel *et al*). The $\boldsymbol{A}_{i\perp}$ generate a group which has the following structure, discussed in Coxeter and Moser's classic book (Coxeter and Moser 1972). We follow their notation (except for the introduction of the subscript '$\perp$'.)

The four-dimensional hypercube $\mathbf{C}^4$ (this is the octagonal case) projects onto $\mathbf{P}_\perp$ along a regular octagon, whose directed edges $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ and $\boldsymbol{a}_4$ are the projections of the hypercube edges $\boldsymbol{e}_i$ ($i = 1, 2, 3, 4$). The translation $\boldsymbol{A}_5 = -\boldsymbol{A}_1$ in $\mathbf{T}^d$ brings $\boldsymbol{e}_1$ onto $\boldsymbol{e}_1$, on the opposite silhouetting edge of the hypercube, etc. Consequently, $\boldsymbol{A}_{5\perp} = -\boldsymbol{A}_{1\perp}$ in $\mathbf{P}_\perp$ brings $\boldsymbol{a}_1$ onto $\boldsymbol{a}_1$ on the opposite edge of the octagon, etc. The group of translations represented by the $\boldsymbol{e}_i$ yield a group represented by the $\boldsymbol{a}_i$; clearly, this group generates the Burgers vectors $\boldsymbol{b}$ alluded to in section 2 of this article: $\boldsymbol{b} = \sum_i n_i \boldsymbol{e}_i$. We can equally well consider the group represented by the $\boldsymbol{A}_i$, since these vectors form a complete basis: $\boldsymbol{b} = \sum_i m_i \boldsymbol{A}_i$. Now, call the generators of the 'projected' abstract group $A_{i\perp}$; as shown by Coxeter and Moser, the group generated by the four generators $A_{i\perp}$ is no longer Abelian and obeys the relation

$$r \equiv A_{1\perp}A_{2\perp}A_{3\perp}A_{4\perp}A_{1\perp}^{-1}A_{2\perp}^{-1}A_{3\perp}^{-1}A_{4\perp}^{-1} = 1. \tag{6}$$

Define new generators

$$a_1 = A_{2\perp}A_{3\perp}A_{4\perp} \qquad a_2 = A_{5\perp}A_{6\perp}A_{7\perp}$$
$$a_3 = A_{8\perp}A_{1\perp}A_{2\perp} \qquad a_4 = A_{3\perp}A_{4\perp}A_{5\perp}. \tag{7}$$

Their effect is clearly a translation along $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ and $\boldsymbol{a}_4$. Note that there is not just one choice (e.g. $a_1 = A_{3\perp}A_{2\perp}A_{4\perp}$, etc, would fit equally), but ours has the advantage of putting in place of equation (6) another one which has a very symmetric form, and corresponds to a natural order on the octagon:

$$r \equiv a_1a_2a_3a_4a_1^{-1}a_2^{-1}a_3^{-1}a_4^{-1} = 1. \tag{8}$$

The important issue as regards the choice of $\mathbf{U}$ as the order parameter space of the QC is that now the fundamental group $\pi_1(\mathbf{U})$ generated by the $A_{i\perp}$ (or equivalently by a_1, a_2, a_3 and a_4), and whose elements are oriented closed loops in $\mathbf{U}$, is no longer Abelian. Hence $\pi_1(\mathbf{U})$ is the group generated by the a_i defined above, obeying the relation of equation (7); it is also the group of hyperbolic translations of the hyperbolic plane tiled with octagons (cf. Coxeter and Moser 1972), the $\{8, 8\}$ tessellation in the Schläfli–Coxeter notation. The complete symmetry group of this tessellation, denoted [8, 8], is generated by reflections in the edges of the fundamental triangle ONZ of the octagon. $\pi_1(\mathbf{U})$ is an invariant subgroup (of index 16) of [8, 8]. In crystallographic terms, it is useful to consider [8, 8] as a *curved crystal*; it carries all of the symmetries of the quasicrystal—not only the octagonal symmetries, but also its hidden translational symmetries. As an object of algebraic topology, it is the *universal cover* $\tilde{\mathbf{U}}$ of $\mathbf{U}$; it has the same relationship with $\mathbf{U}$ that the simple cubic Bravais lattice has with the 3-torus $\mathbf{T}^3$ opened out under the shape of a cube; the simple cubic lattice is the universal cover of the 3-torus.

The elements of $\pi_1(\mathbf{U})$ classify the defects in the QC; according to the way in which we have constructed them—by projection of the $\boldsymbol{A}_i$—these defects are akin to dislocations, but non-Abelian, a property reminiscent of what we have obtained by the naive Volterra construction. We can go further in the comparison between the two approaches; in the Volterra process approach, we showed that the landscape carried by a moving defect was dependent on the path followed, and in particular was modified in a fundamental way if the defect performs a complete circumnavigation about another one. On the other hand it is a result of the topological theory of defects that a defect of class $g \in \pi_1(\mathbf{U})$ is turned into a defect of the homotopy class hgh^{-1} ($h \in \pi_1(\mathbf{U})$) after it has achieved a complete turn about h (Kléman 1977, Trebin 1984); in other words, one gets in this way *a different realization of the same defect*, represented in $\pi_1(\mathbf{U})$ by a different element but belonging to the same conjugacy class as g, if the classes h and g do not commute. This is exactly what we got above, which makes it natural to interpret the non-commutativity of $\pi_1(\mathbf{U})$ in terms of mismatches. More precisely, let $c_{ij} = a_ia_ja_i^{-1}a_j^{-1}$ be a commutator of the fundamental group $\pi_1(\mathbf{U})$, and let $N(c_{ij})$ be the commutator subgroup generated by the c_{ij}; all of the elements of $N(c_{ij})$ are of the form $\ldots a_i^{l_i}a_j^{l_j}a_k^{l_k}\ldots a_i^{m_i}a_j^{m_j}a_k^{m_k}\ldots a_i^{n_i}a_j^{n_j}a_k^{n_k}\ldots$ such that $\ldots + l_i + m_i + n_i + \ldots = 0$. It is easy to show that $N(c_{ij})$ is an invariant subgroup of $\pi_1(\mathbf{U})$; the quotient group

$$H_1(\mathbf{U}) = \pi_1(\mathbf{U})/N(c_{ij}) \tag{9}$$

is the largest Abelian subgroup of $\pi_1(\mathbf{U})$; it has the representation

$$H_1(\mathbf{U}) = \langle a_{1,}a_{2,}a_{3,}a_4; a_ia_ja_i^{-1}a_j^{-1} = 1\rangle \tag{10}$$

that is

$$H_1(\mathbf{U}) = \mathrm{Z}^4 \tag{11}$$

as expected for the group of dislocations, which we retrieve with their ordinary significance. Any element of $H_1(\mathbf{U})$ is in one-to-one correspondence with a conjugacy class in $\pi_1(\mathbf{U})$. Take for example the conjugacy class of a_k; its elements are of the form

$$a_i a_k a_i^{-1} = a_i a_k a_i^{-1} a_k^{-1} a_k = c_{ik} a_k \tag{12}$$

and are homomorphic with the same element a_k in $H_1(\mathbf{U})$: they all represent the same complete dislocation. We also understand this in the light of our former discussion of the Volterra process. We can therefore interpret the commutator c_{ik} as the class of a defect which has been added to $\mathbf{L}$ by a rotation about a defect of homotopy class a_i; were the group Abelian, the class of this defect would be the null class. In fact, c_{ik} is precisely the class of the defect which joins two dislocations after they have crossed. Such commutators are therefore related to the set of mismatches (the landscape) surrounding a complete dislocation. For the sake of completeness, note that the classification of *individual* mismatches has also been considered (Misirpashaev 1995).

The elements of $H_1(\mathbf{U})$ are isomorphic with the elements of $\pi_1(\mathbf{T}^d)$, i.e. with the whole set of dislocations of the high-dimensional lattice $\mathbf{E}^d$. This comes from the fact that the vector basis $\boldsymbol{a}_i$ is complete, so any lattice vector, however small its projection in $\mathbf{A}_\perp$, is a linear combination of the $\boldsymbol{a}_i$.

Caveat: in fact, the situation is somewhat more complicated, because $\mathbf{U}$ is an *extended* order parameter space, in the sense that infinitely many points represent the same realization of the QC, but with the exception of some global translation along $\mathbf{P}_\parallel$. It is indeed possible to find a projection $\boldsymbol{b}_\perp$ in $\mathbf{P}_\perp$ of some d-dimensional vector $\boldsymbol{b}$ whose modulus $|\boldsymbol{b}_\perp|$ is as close as one wishes to any value (and in particular as small as one wishes; think of a very long $\boldsymbol{b}$-vector nearly parallel to $\mathbf{P}_\parallel$), and whose extremities can therefore both be in $\mathbf{A}_\perp$. A Burgers circuit surrounding the corresponding dislocation would map onto an open circuit in $\mathbf{E}^d$; its closure failure would correctly measure a Burgers vector $\boldsymbol{b} = \sum_{i=1,\ldots,d} n_i \boldsymbol{e}_i$, but its projection $\boldsymbol{b}_\perp = \sum_{i=1,\ldots,d} n_i \boldsymbol{a}_i$ in $\mathbf{A}_\perp$ would not be recognized as joining equivalent points in $\mathbf{U}$. In fact, because of the way in which we have constructed the order parameter space, these two points are not equivalent in $\mathbf{U}$. We call those dislocations which are not visible as loops in $\mathbf{U}$ *inner defects*, because for each of them the value of $|\boldsymbol{b}_\perp|$ is smaller than the span of the acceptance domain, and, correlating with this, the physical Burgers vector modulus $|\boldsymbol{b}_\parallel|$ is large. The way to resolve this difficulty is as follows.

Consider the case where the quasicrystal is invariant under inflation. Then such inner vectors belong to some superquasicrystal of the quasicrystal lattice, which can be defined in a precise way, as follows. Introduce the star of all of the vectors $\boldsymbol{b}_{\perp\iota}$ which form the orbit of $\boldsymbol{b}_\perp$ under the action of the quasicrystalline point group in $\mathbf{P}_\perp$; after the manner of Olami and Alexander (1988), introduce the intersection $\mathbf{A}_{\perp\iota} = \mathbf{A}_\perp(\mathbf{0}) \cap \mathbf{A}_\perp(\boldsymbol{b}_{\perp\iota})$, which is the set of the vertices which have a neighbouring vertex at a distance equal to or larger than $\boldsymbol{b}_{\parallel\iota}$. The intersection

$$\mathcal{A}_\perp(\boldsymbol{b}_\perp) = \bigcap_\iota \mathbf{A}_{\perp\iota}$$

of all of the sets forming the orbit of $\mathbf{A}_{\perp\iota}$ defines an acceptance domain which is deflated with respect to $\mathbf{A}_\perp$ by some factor, and such that $\boldsymbol{b}_\perp$ joins identifiable points on $\mathcal{A}_\perp$, on opposite boundaries. Identifying these boundaries yields an order parameter space $\mathcal{U}_\perp$, whose (non-Abelian) fundamental group $\pi_1(\mathbf{U}_\perp)$ classifies the dislocations (and disvections) of a 'quasisuperstructure', for which all of the above arguments can be repeated.

Extension to other quasicrystalline symmetries. We have shown elsewhere (Kléman 1990, 1992) that the universal cover of the acceptance domains of the pentagonal and the icosahedral QCs have properties similar to the above, i.e. infinite groups of translations with remarkable non-commutative properties, and we have interpreted the commutators in terms of mismatches carried by the complete dislocations. First, notice that the discussion of the first section of this paper is general, and applies to any quasicrystalline symmetry; therefore the effects of non-commutativity on the dislocations, displayed by Volterra process considerations, are still true. Second, the acceptance domain of any type of quasicrystal, in the d-dimensional description, does not tile $\mathbf{P}_\perp$; furthermore the projection of the hypercube always provides equivalence relations between opposite edges, faces, etc, since the hypercube has equivalent opposite boundaries, due to the periodicity in $\mathbf{E}^d$; therefore, an interpretation of the acceptance domain as a closed manifold $\mathbf{U}$ playing the role of an extended order parameter space is possible; furthermore, by gluing infinitely many acceptance domains $\mathbf{A}_\perp$ along equivalent faces, one obtains a 'crystal', which is not flat since it does not tile $\mathbf{P}_\perp$; its translational properties are therefore non-Abelian, etc.

A question of terminology. E Cartan (1963) has introduced the term *transvections*—which generalize the concept of translations—for the displacements in a hyperbolic plane which are represented by commutators of the group of displacements which leave the hyperbolic plane invariant—remember that the a_i introduced above for the octagonal QC are translations in a *hyperbolic* crystal, the universal cover $\tilde{\mathbf{U}}$ of $\mathbf{U}$. The complete dislocations $(\mathbf{L}_\parallel, \boldsymbol{b})$ in a QC are very special objects, since, through the presence of mismatches, they break the symmetries of this hyperbolic crystal. In that sense the hyperbolic crystal thus constructed is the true crystalline representative of the QC, one of its advantages being that it has the same dimensionality as the QC. All of these properties point to the necessity of using a specific substantive for the 'dislocations' of the type $(\mathbf{L}_\parallel, \boldsymbol{b})$, which we have up to now called *complete dislocations* in order to differentiate them from the imperfect dislocations $(\mathbf{L}_\parallel, \boldsymbol{b}_\parallel)$; although imperfect, $(\mathbf{L}_\parallel, \boldsymbol{b}_\parallel)$ is a dislocation in the usual meaning of the term, while $(\mathbf{L}_\parallel, \boldsymbol{b})$ is not. In a former paper we suggested calling the complementary $(\mathbf{L}_\parallel, \boldsymbol{b}_\perp)$, i.e. the landscape—an object, made up of many partly independent parts—which transforms the imperfect dislocation into a complete one, a disvection, in honour of Cartan. However, the noun 'mismatches' (for the parts) fits them quite properly; on the other hand complete dislocations $(\mathbf{L}_\parallel, \boldsymbol{b})$ have been observed and their total Burgers vectors measured. Therefore we propose to reserve the name *disvection* for a 'complete dislocation' $(\mathbf{L}_\parallel, \boldsymbol{b})$ in a quasicrystal, an object which after all is not a dislocation in the usual sense of the term.

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Appendix

$\mathbf{G} \equiv \mathbf{L} \oplus \mathbf{B}$ is the glide manifold in $\mathbf{E}^d$; we can write it as a union of manifolds carried by $\mathbf{G}_\parallel$: hence

$$\mathbf{G} = \bigcup_{\boldsymbol{r} \in \mathbf{G}_\parallel} \boldsymbol{g}(\boldsymbol{r})$$

where $\boldsymbol{g}(\boldsymbol{r}) \subset \mathbf{P}_\perp$ is a $d_\perp$-dimensional manifold and $\boldsymbol{r}$ a running point in $\mathbf{G}_\parallel$. Extracting $\mathbf{B}_\parallel$ from $\mathbf{G}_\parallel$, we can alternatively write

$$\mathbf{G} = \bigcup_{\boldsymbol{r} \in \mathbf{L}_\parallel} \{\mathbf{B}_\parallel \oplus \boldsymbol{g}(\boldsymbol{r})\}. \tag{A1}$$

Since

$$\mathbf{L} = \bigcup_{r \in \mathbf{L}_{\parallel}} \boldsymbol{\lambda}(\boldsymbol{r})$$

where $\boldsymbol{\lambda}(\boldsymbol{r}) \subset \mathbf{P}_{\perp}$ is a $d_{\perp}$-dimensional manifold, we also have

$$\mathbf{G} = \bigcup_{r \in \mathbf{L}_{\parallel}} \{\mathbf{B} \oplus \boldsymbol{\lambda}(\boldsymbol{r})\}. \tag{A2}$$

Therefore $\boldsymbol{\Gamma}(r) = \{\mathbf{B}_{\parallel} \oplus \boldsymbol{g}(\boldsymbol{r})\}$ and $\boldsymbol{\Lambda}(\boldsymbol{r}) = \{\mathbf{B} \oplus \boldsymbol{\lambda}(\boldsymbol{r})\}$ generate the same manifold $\mathbf{G}$, when translated along $\mathbf{L}_{\parallel}$. $\boldsymbol{\Gamma}(\boldsymbol{r})$ is a ruled manifold (along $\mathbf{B}_{\parallel}$); hence $\boldsymbol{\Lambda}(\boldsymbol{r})$ itself must be ruled along $\mathbf{B}_{\parallel}$, which is possible only if $\boldsymbol{\lambda}(\boldsymbol{r})$ is ruled along $\mathbf{B}_{\perp}$, because the cartesian product $\mathbf{B} \oplus \mathbf{B}_{\perp}$ (which is also $\mathbf{B}_{\parallel} \oplus \mathbf{B}_{\perp}$) then appears in $\boldsymbol{\Lambda}(\boldsymbol{r})$. Hence,

$$\boldsymbol{\lambda}(\boldsymbol{r}) = \mathbf{B}_{\perp} \oplus \boldsymbol{\sigma}(\boldsymbol{r}) \tag{A3}$$

and

$$\mathbf{L} = \bigcup_{r \in \mathbf{L}_{\parallel}} \{\mathbf{B}_{\perp} \oplus \boldsymbol{\sigma}(\boldsymbol{r})\}. \tag{A4}$$

Let us now assume for a while that $\boldsymbol{\sigma}(\boldsymbol{r})$ is a manifold which has non-zero dimensional components which do not belong to $\mathbf{P}_{\perp}$. Now, take a running point $\boldsymbol{r}$ on $\mathbf{L}_{\parallel}$. Using the same argument as in Kléman and Sommers (1991), the atomic surfaces $\mathbf{S}$ attached to $\boldsymbol{\sigma}(\boldsymbol{r})$ intersect $\mathbf{P}_{\parallel}$ along a singular region $\mathbf{L}'_{\parallel}$ which has the shape of a 2D singular furrow about $\boldsymbol{r}$ and therefore has the disadvantage of extending the core region geometrically. None of the other atomic surfaces attached to the components of $\{\mathbf{B}_{\perp} \oplus \boldsymbol{\sigma}(\boldsymbol{r})\}$ in $\mathbf{P}_{\perp}$ at point $\boldsymbol{r}$ yield any intersection with $\mathbf{P}_{\parallel}$ other than $\boldsymbol{r}$ itself. Hence in the generic case we must take $\boldsymbol{\sigma}(\boldsymbol{r}) \subset \mathbf{P}_{\perp}$ in order to preserve a *small* and locally *isotropic* core. The precise shape of $\boldsymbol{\sigma}(\boldsymbol{r})$ probably depends on $\boldsymbol{b}$, and shows up possibly quasicrystalline symmetries. The intersection of $\mathbf{L}$ with $\mathbf{P}_{\perp}$ must contain $\mathbf{B}_{\perp}$, in order to satisfy conditions β and γ.

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