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QUASI SYMMETRIES OF SPACE GROUP ORBITS

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In Crystallographic Groups of Four-dimensional Space [1] a *symmetry operation* of an object in space is defined as a mapping of the space onto itself satisfying two conditions:

(a) It is a rigid motion.

(b) It maps the object as a whole onto itself; that is, the object after the mapping is not distinguishable from the original object.

In giving this definition, the authors are careful to point out the significance of considering the symmetry operation as a mapping of the full euclidean space onto itself. The set of all such symmetry operations of a crystal structure is called the *space group* of the crystal structure [1].

Now let G be an n-dimensional space group and let P be a point in E^n. If G is allowed to act on P, it will produce an orbit G(P) where $G(P) = \{X: X = g(P), \quad g \in G\}$. The orbit thus produced will depend greatly on the choice of P within the fundamental cell of the translation lattice associated with G. For instance, it is always possible to choose P so that its stabilizer $G_P = \{g \in G : g(P) = P\}$ consists of the identity only [2].

The set G(P) is discrete, countable, and homogeneous. By *homogeneous* we mean that each point is 'similarly surrounded' by other points of the orbit. Because of their structure, space group orbits can be appropriately called *Discrete Euclidean Universes* (DEU's).

Here we attempt to look at these universes in relief; that is, we concentrate on the points of the orbit and prescind as much as possible from the space in which the orbit is embedded. We will define *quasi* symmetry operations on these universes which will be different, in several respects, from those genuine crystallographic symmetry operations defined in [1].

To define these new operations, we will introduce a neighborhood relation between the points of a DEU. We do this using the concept of Dirichlet region. Let P, Q ε DEU; Q $\neq$ P. Let S(P,Q) be the (n-1)-dimensional subspace of E^n such that X ε S(P,Q) $\Leftrightarrow$ d(P,X)=d(X,Q) where d represents the ordinary euclidean distance. For each point Q ε DEU, Q $\neq$ P, S(P,Q) determines two half-spaces in E^n, one of which contains P. Let H(P,Q) be the closure of this half-space and let V(P) = $\bigcap\{$H(P,Q): Q ε DEU, Q $\neq$ P$\}$. It is easy to show that V(P) is a convex polytope with a finite number of (n-1)-dimensional bounding faces. The interior of V(P) is the *Dirichlet region* of P and V(P) will be called the *Dirichlet cell* associated with P. The set of Dirichlet cells forms a cell *complex* ℓ of congruent cells which fill the space without overlapping and without gaps. Figures 1 to 4 illustrate 2-dimensional complexes. For a thoroughly informative treatment of Dirichlet domains see Fischer [4] and Koch [5].

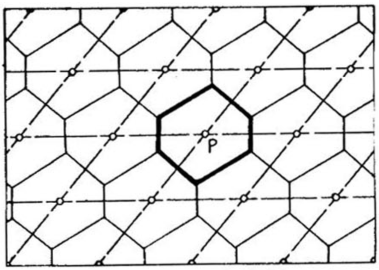


Figure 1

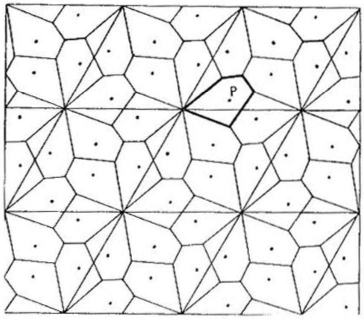


Figure 3

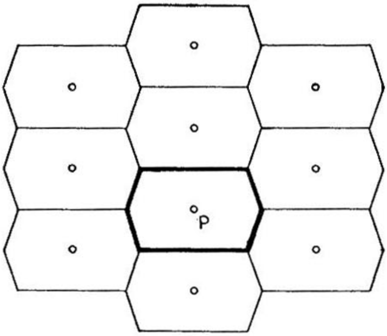


Figure 2

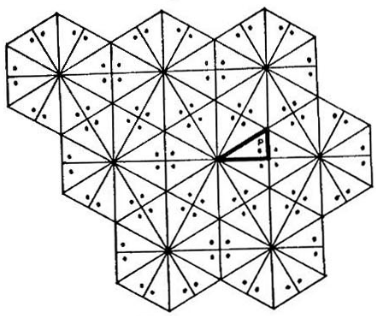


Figure 4

Definition: A neighborhood of $P \varepsilon$ DEU is the finite set
$N(P) = \{Q \varepsilon \text{DEU} \setminus P: V(P) \cap V(Q)$ is an $(n-1)$-dimensional face of $V(P)\}$

Thus each point $X \varepsilon$ DEU has a finite number of neighbors and this neighborhood relation is symmetric but neither reflexive nor transitive. Clearly, this relation is preserved under all crystallographic symmetry operations; however, there are permutations of a DEU which are not rigid symmetries but nevertheless preserve the neighborhood relation. See figures 1 and 2. Here the non-rigid symmetry groups are much larger (C_{6v}).

We proceed now to characterize certain neighborhood-preserving automorphisms on the Dirichlet cell complex associated with a DEU. For this purpose, we introduce a special combinatorial group [6].

Let ℓ be the Dirichlet cell complex for some discrete euclidean universe.

Definition: A tower is an $(n+1)$-tuple $(s_0, s_1, \ldots, s_n)$ where s_0 is a 0-cell (vertex), s_1 a 1-cell (edge), s_2 a 2-cell (face), etc. and $s_0 \subset \bar{s}_1 \subset \bar{s}_2 \subset \ldots \subset \bar{s}_n$.

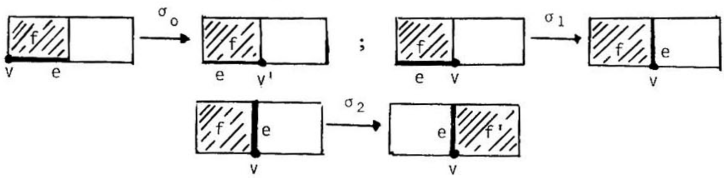
Let $\mathfrak{J}(\ell)$ be the set of all towers in ℓ. We construct the following group Σ generated by n+1 involutions for which $\mathfrak{J}(\ell)$ will form a homogeneous Σ-space, i.e. Σ will act transitively on $\mathfrak{J}(\ell)$. We illustrate its construction for a 2-dimensional complex; the extension to high dimensions is simple. We introduce the following operations:

(1) An involution σ_0 which interchanges any two adjacent vertices but leaves face and edge fixed, i.e. $\sigma_0((s_0, s_1, s_2)) = (s_0', s_1, s$ if $\delta\bar{s}_1 = \{s_0, s_0'\}$.

(2) An involution σ_1 which interchanges any pair of edges incide with a vertex and a face but leaves that vertex and face fixed, i.e. $\sigma_0((s_0, s_1, s_2)) = (s_0, s_1', s_2)$, if $s_1, s_1' \subseteq \bar{s}_2, \bar{s}_1 \cap \bar{s}_1' = s$

(3) An involution σ_2 which leaves any vertex and edge fixed but interchanges any two faces with a common edge, i.e., $\sigma_2((s_0, s_1, s_2)) = (s_0, s_1, s_2')$, if $\bar{s}_2 \cap \bar{s}_2' \supseteq s_1$.

The following, where $(v,e,f) = (s_0, s_1, s_2)$, is a pictorial representation of a 2-dimensional example:



The combinatorial group for the 2-dimensional towers is $\Sigma_2 = \langle \sigma_0, \sigma_1, \sigma_2 \rangle$, the group generated by these involutions. For the n-dimensional case we have $\Sigma_n = \langle \sigma_0, \sigma_1, \sigma_2, \ldots, \sigma_n \rangle$. It is easy to show that this group acts transitively on the towers of the Dirichlet cell complex associated with any DEU [2].

In order to obtain all towers attached to a given vertex v_0 in a 2-dimensional world we take the subgroup $\Sigma_0 = \langle \sigma_1, \sigma_2 \rangle$ of Σ and allow it to act on the triple (v_0, e, f). The orbit of (v_0, e, f) under Σ_0 is the set of all such towers. See figure (5). Similarly we allow $\Sigma_1 = \langle \sigma_0, \sigma_2 \rangle$ to act on (v, e_0, f) to get all towers associated with e_0 and $\Sigma_2 = \langle \sigma_0, \sigma_1 \rangle$ acts on (v, e, f_0) to yield all towers attached to f_0. The towers with a common 2-cell form an equivalence class. The quadruple $(\mathcal{J}(\ell), \sigma_0, \sigma_1, \sigma_2)$ describes in abstract combinatorial manner the Dirichlet cell complex of a DEU.

Let $C_i(\ell)$ denote the i-cells of a DEU complex, then we have the following one-to-one correspondences in the n-dimensional case:

$$
\begin{array}{lcl}
C_0(\ell) & \longleftrightarrow & \text{orbits of } \Sigma_0 = \langle \sigma_1, \sigma_2, \ldots, \sigma_n \rangle \\
C_1(\ell) & \longleftrightarrow & \text{orbits of } \Sigma_1 = \langle \sigma_0, \sigma_2, \ldots, \sigma_n \rangle \\
\vdots & & \vdots \\
C_i(\ell) & \longleftrightarrow & \text{orbits of } \Sigma_i = \langle \sigma_0, \ldots, \sigma_{i-1}, \sigma_{i+1}, \ldots, \sigma_n \rangle \\
\vdots & & \vdots \\
C_n(\ell) & \longleftrightarrow & \text{orbits of } \Sigma_n = \langle \sigma_0, \sigma_1, \ldots, \sigma_{n-1} \rangle
\end{array}
$$

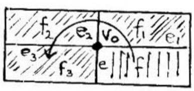


Figure 5

We now characterize the quasi symmetry operations by defining admissible automorphisms as follows:

Definition: An automorphism of a DEU complex ℓ is a permutation π of the set of towers $\mathcal{J}(\ell)$ which commutes with each element of the group Σ, i.e. with words formed from the generators, $\sigma_0,\sigma_1,\ldots,\sigma_n$.

We shall elaborate on this definition. Since π commutes with $\Sigma_0 = \langle\sigma_1,\sigma_2,\ldots,\sigma_n\rangle$, $\Sigma_1 = \langle\sigma_0,\sigma_1,\ldots,\sigma_{n-1}\rangle$, ..it defines a permutation on the orbits of $\Sigma_0,\Sigma_1,\ldots,\Sigma_n$, that is, on the sets $C_0(\ell)$, $C_1(\ell),\ldots,$ $C_n(\ell)$. In other words, if $\pi((s_0,s_1,\ldots,s_n)) = (s_0', s_1',\ldots,s_n')$, $\pi((t_0,t_1,\ldots,t_n)) = (t_0',t_1',\ldots,t_n')$ is a permutation on the towers of th complex such that $s_i = t_i$, then $s_i' = t_i'$. Thus π can be reconstructed from the permutations $\pi_0,\pi_1,\ldots,\pi_n$, induced by π on $C_0(\ell)$, $C_1(\ell),\ldots,$ $C_n(\ell)$ and defined by $\pi((s_0,s_1,\ldots,s_n)) = (\pi_0(s_0), \pi_1(s_1),\ldots, \pi_n(s_n))$ This implies, in particular, that π can be viewed through $(\pi_0,\pi_1,\ldots,\pi_{\text{|}}$ as an automorphism of the cell complex ℓ; it preserves incidences in th sense that $s_i \subset \overline{s}_j$ implies $\pi_i(s_i) \subset \overline{\pi_j(s_j)}$. As a consequence, the abo defined neighborhood relation on the points of DEU is preserved, since by the association $P \to V(P)$, these may be identified with $C_n(\ell)$. Thus A can be identified with its action on $C_n(\ell)$ or equivalently the points in DEU. We have considered the possibility of even larger groups of permutations preserving the neighborhood relation but this possibility seems remote since it would appear that they would disconnect the neigh borhood graph (network).

If G is any rigid symmetry group of a DEU it will certainly prese incidences and thus each $g \in G$ will commute with each element (word) in It is easy to see that G can be viewed as a permutation subgroup $\overline{G}$ of

If $\pi((s_0,s_1,\ldots,s_n)) = (s_0,s_1,\ldots,s_n)$ then $\pi(s_0) = Id(s_0),\ldots,$ $\pi_n(s_n) = Id(s_n)$. See (2) below.

Let A = Aut (DEU) be the group of all automorphisms defined abov We can associate at least three groups with each orbit of a space grou

(i) The minimal generating group G_0

(ii) The maximal rigid symmetry group G_1 or the eigen symmetry group

(iii) The group of neighborhood-preserving automorphisms A.

We have $\overline{G}_o \subseteq \overline{G}_1 \subseteq A$ where again $\overline{G}_1$, i=o,1, is viewed as a permutation group on $\mathfrak{J}(\ell)$. Note that although Σ acts transitively on $\mathfrak{J}(\ell)$, the same may not be true for A or $\overline{G}_i$; however, both of these groups are transitive on the points of DEU, i.e. on $C_n(\ell)$.

We state the following well-known but important facts:

(1) A is the full group of automorphisms of the homogeneous Σ-space, namely the set of towers, $\mathfrak{J}(\ell)$, of the Dirichlet cell complex.

(2) There exists at most one neighborhood-preserving automorphism π (as defined above) taking a given tower T_1 into any other given tower T_2 [2].

(3) There exists such a π if, and only if, the stabilizer in Σ of T_1 is equal to the stabilizer in Σ of T_2.

(4) Let T be any tower in $\mathfrak{J}(\ell)$ and let Γ be its stabilizer in Σ, then A is isomorphic to $N(\Gamma)/\Gamma$, where $N(\Gamma)$ is the normalizer of Γ in Σ. This automorphism depends on the choice of T.

(5) If $\alpha \in A$ leaves an n-cell V(P) fixed and $\alpha \neq 1$, then it must permute the towers contained on V(P) among themselves since it respects incidences. Thus α is a regular permutation of the finitely many towers of V(P) and the action of α leaves P fixed. Hence, we may say α stabilizes V(P) if and only if α stabilizes P [2].

The following is a simple consequence of our discussion, but we state it as a theorem because of its importance.

Theorem: Let A be the group of automorphisms of a DEU. Let $P \in$ DEU and V(P) its associated Dirichlet cell. Let A_P be the stabilizer of P in A, i.e. $A_P = \{\pi \in A : \pi_n(V(P))=V(P)\}$. Then A_P is a finite group.

Proof: A_P is a set of regular permutations of a finite set and hence finite. Q.E.D.

This theorem is important because it enables us to show that the group A of automorphisms of any DEU, which contains a copy $\overline{G}_o$ of the generating group, G_o, of that orbit, has the property that the index, $[A:\overline{G}_o]$, is finite. This implies that there is a subgroup $H \trianglelefteq \overline{G}_o$, where H is normal and of finite index in A. This can be proved by representing A as a permutation group on the cosets of $\bar{G}_0$. If we consider A as a permutation group on the towers $\mathfrak{J}(\ell)$ and G_0 as a permutation group on the points, then it would be natural to consider the wreath product A w G_0. It is proved in [3] that A modulo a <u>finite</u> normal subgroup is isomorphic to a space group.

One of the results of this investigation is that if a monad (point) in a discrete euclidean universe should wish to make some rough determination of the kind of world in which he lived, his case would n be quite hopeless. He could carry out local permutations of his first, second, and third step neighbors and study those which did not disturb the neighborhood relation. These permutations will form a group and somewhere within that group will be a subgroup which is the eigen symme group G_1 of the universe in which the monad lives. Some examples from Fischer [4] and Koch [5] indicate that the monad's task will frequently not be an easy one!

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