# GEOMETRIC PROPERTIES
# OF CRYSTAL LATTICES
# in Spaces of Arbitrary Dimension

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## SUMMARY.

The main theme of this thesis (excepting Chapter 5) is to investigate properties of crystal lattices which are of particular significance in higher dimensions i.e. $> 3$, but which barely show up in low dimensions. We study lattices T and pairs (H,T), where H is a finite subgroup of the orthogonal group acting on T.

In Chapter 1 we present some basic properties of lattices which are used throughout. In Chapter 2 we discuss crystal families and prove that the Face Theorem of [12] can be extended to these.

In Chapter 3 we investigate the decomposability properties of the RH-module V and the QH-module QT and the relationship between them. We introduce the ideas of typically orthogonal decompositions and inclined point groups. We prove some general criteria for determining these.

In Chapter 4 we extend the decomposability study to families and show how our work can be used to describe some higher dimensional families which we consider to be of particular significance. Specific results are given. In particular, we reduce the problem of describing the descendants of one, two and three dimensional families to a problem involving only the partition function.

In Chapter 5 we formulate and study an approach to the problem of the stability of symmetry in lattice hyperplanes. The full solution corresponding to this formulation is given in 3 dimensions. We venture to hope that this solution might be of some interest to practising crystallographers, possibly in the study of twinned crystals with rational twinning planes.

# NOTATION.

## Crystallographic.

We use the following symbols which are standard in crystallography. The reader is referred to [2] or [10; pp.24-29] for a full explanation of these.

Two Dimensional Geometric Crystal Classes.

$\underline{1}$, $\underline{2}$, $\underline{3}$, $\underline{4}$, $\underline{6}$, $\underline{m}$, $\underline{2mm}$, $\underline{3m}$, $\underline{4mm}$, $\underline{6mm}$.

Three Dimensional Geometric Crystal Classes.

$\underline{1}$, $\underline{\bar{1}}$;

$\underline{2}$, $\underline{m}$, $\underline{\frac{2}{m}}$;

$\underline{222}$, $\underline{2mm}$, $\underline{mmm}$;

$\underline{4}$, $\underline{422}$, $\underline{\bar{4}}$, $\underline{\frac{4}{m}}$, $\underline{4mm}$, $\underline{\bar{4}2m}$, $\underline{\frac{4}{m}mm}$;

$\underline{3}$, $\underline{\bar{3}}$, $\underline{3m}$, $\underline{\bar{3}m}$, $\underline{32}$, $\underline{6}$, $\underline{\bar{6}}$, $\underline{622}$, $\underline{\frac{6}{m}}$, $\underline{6mm}$, $\underline{\bar{6}m2}$, $\underline{\frac{6}{m}mm}$;

$\underline{23}$, $\underline{432}$, $\underline{m3}$, $\underline{\bar{4}3m}$, $\underline{m3m}$.

Two Dimensional Bravais Classes.

$\underline{P}$ = Parallelogram;

$\underline{R}$ = Rectangle;

$\underline{D}$ = Diamond;

$\underline{S}$ = Square;

$\underline{H}$ = Hexagon.

## Other Notation.

If the symbol $\bar{x}$ appears as a matrix entry, it means $-x$. We never use $\bar{x}$ to denote the complex conjugate.

We denote the complex, real and rational numbers by C, R and Q respectively. We denote the integers by Z. Moreover, $R^* = R\setminus\{0\}$ and $R^+ = \{x \in R: x > 0\}$. We denote the natural numbers by N.

Continued

By GL(n,Z) we mean the set of n x n integral matrices with determinant +1 or -1.

We denote the adjoint of a linear map $\varphi$ by $\varphi'$.

We denote the identity map by $\iota$.

The symbol $\subset$ means strict inclusion, but when we wish to emphasize this we write $\subsetneqq$. The symbol $\subseteq$ implies 'possibly equal to.'

The symbols DT and ODT used in Chapters 3 and 4 mean 'decomposition type' and 'typically orthogonal decomposition type' respectively. These are fully explained on pages 27 and 44 respectively.

## DECLARATION OF ORIGINALITY.

With a few exceptions, any definition, lemma, proposition or theorem which is not directly attributed to another source ( either in the text or in the introduction), or stated to be standard, is claimed as original.

The exceptions are: Proposition1.4, Proposition 1.6, and all of Section 2.1. These results are well known, but not stated in a convenient form elsewhere which suits our point of view. Proposition 1.6 does not appear to be proved anywhere in the literature, although it is sometimes used in a matrix form.

The idea for the definition of decomposition type comes from [3], although we use the term in a wider context than in [3].

## INTRODUCTION.

If U is an n-dimensional Euclidean space, then an n-dimensional space group is a discrete group of isometries of U containing n linearly independent translations. Space groups (in three dimensions) were first studied by Fedorov and Schoenflies in the 1880's. They discovered (working independently) all 230 classes of three dimensional space groups, under an equivalence relation which we would now call conjugation by an orientation preserving affine map. Hilbert asked if the number of space groups in any given dimension is finite and Bieberbach proved this in the early 1900's. It is worth noting that the theoretical description of three dimensional space groups came well before the realization that these actually corresponded to the physical structure of crystals.

Lattices arise in crystallography as the sets of translations in n-dimensional space groups. Given a choice of origin of U, a lattice T may be regarded as a subgroup of an n-dimensional vector space V. A space group G determines a short exact sequence

$$0 \longrightarrow T \longrightarrow G \longrightarrow H \longrightarrow 1$$

where T is the lattice and H, the point group, is a finite subgroup of the orthogonal group O(V) acting on T. Most methods of deriving space groups begin with pairs of the form (H,T) and these are essentiallywhat we study in this thesis. Lattices themselves are classified according to their symmetry groups $G(T) = \{\theta \in O(V) : \theta T = T\}$, and we consequently show particular interest in pairs (G(T),T).

Space groups and pairs have been classified for $n \leq 4$ (see [2], [3], [4]) but few general results are known. Interest in n-dimensional crystallography for $n > 3$ has recently been revived by Bülow, Neubüser and Wondratschek in [3], and by other authors (e.g. [12], [13]). One of the main themes of this thesis is to formulate and investigate properties of lattices and pairs which we feel are of particular importance in studying their behaviour in higher dimensions, but are not very significant in low dimensions. Subordinate to this theme is the use of crystal families of lattices, introduced by Bülow et al. in [3], which are of particular value in looking at lattices in higher dimensions, particularly with regard to decomposition properties. Chapters One to Four essentially deal with this main theme. Chapter Five, dealing with lattice hyperplanes, is almost a separate unit, although it does rely on some concepts and results from the others.

Chapter One presents some basic properties of crystal lattices which are particularly relevant in all later work. It is immediately clear that our point of view in considering pairs (H,T) is <u>geometric</u>, as in [13], rather than <u>arithmetic</u>, as in [3] and much of the rest of the literature. This means that we consider the representation $H \longrightarrow GL(T)$ explicitly and, if forced to convert to a matrix representation, rely on the scalar product on V to choose an orthonormal basis. An arithmetic approach uses a matrix representation relative to a basis of the lattice T, thus dealing with only integral matrices.

Chapter Two introduces the idea of a crystal family, giving a more general description than in the only other works where it is mentioned (i.e. [3] and [13]). We then place families in the topological context of [12], proving that the Face Theorem for systems in [12] can be extended to families and showing that a family is a manifold of the same dimension as all of the systems which it contains. This is significant because it shows that in some sense families are not all that much bigger than systems. In this chapter we reprove two results of Schwarzenberger, namely our Propositions 2.6 and 2.7 (appearing in [13] and [12] respectively). We do this for two reasons. First, we feel our proof of Proposition 2.7 clears up a certain difficulty in the proof in [12], which is pointed out. Secondly, we use different techniques to Schwarzenberger, relying on positive definite symmetric transformations, some useful properties of which are presented in Section 2.1. We feel that these techniques are more suited to a geometric point of view, and since they are used extensively in the rest of the thesis, it is hoped that their use here makes later work easier to understand. In the course of this chapter we also prove two results stated but not proved by Bülow et al. in [3]. These are pointed out. Also we link our dimension of a family to what they call the 'number of free parameters'.

Chapter Three studies properties of the decomposability of crystallographic point groups which are of particular importance in higher dimensions but which barely show up, if at all, in the first three dimensions. An example of this is the relationship between the decomposability of V over H and that of the rational lattice QT over H, discussed in Section 3.2. In two and three dimensions, V is decomposable if and only if QT is, but we see that this is not true for n even, $n \geq 4$. We prove it is true for $n = 5$, however. Chapter Four relates the work in Chapter Three to the decomposition of families. We discover that crucial to a description of decomposable families in higher dimensions are the notions of what we call 'typically orthogonal decompositions' and 'inclined point groups'. We give some general criteria for determining these. We include rather a large number of specific higher dimensional results in order to assess how useful the properties we have isolated are. There are general results also. In particular, we reduce the problem of determining the descendants of one, two and three dimensional families to a problem involving only the partition function.

In Chapters Three and Four, as in the rest of the thesis, a knowledge of all crystallographic groups and lattice types in one, two and three dimensions is assumed. Nevertheless, results for these are found in some of the tables in Chapter Four for reasons of completeness. We make a specific point of not using the four dimensional results of Bülow et al. in [3], in order to demonstrate how our results work. We do use the names for four dimensional families coined in [3], solely to show how our results relate to the lists in [3] of four dimensional families. Also the table at the end of Section 3.1, which is for illustration only, uses their results. We should point out, however, that many of the ideas in Chapters Three and Four were inspired by studying the list of results in [3].

Chapter Five deals with the problem of the stability of symmetry in lattice hyperplanes. It appears that there has been a recent revival of interest in problems concerning lattice planes in three dimensions, and we venture to hope that our work here might be of some physical relevance. Possible three dimensional applications were mentioned in the original paper on this subject ( [11] ).

For a given lattice T of rank three and rational plane W in three dimensions, several papers have presented methods of finding a basis or reduced basis of $T \cap W$ e.g. [6], [11] . These methods involve a great deal of computation and require either the lattice or the plane, or both, to be fixed. They give no real insight into possible general patterns in the behaviour of lattice hyperplanes. Our aim is to discover some general relationship between the Bravais classes of T and $T \cap W$. It is immediately clear that there is no simple direct relationship, as it is not difficult to establish, by considering simple examples, that any three dimensional Bravais class produces all five two dimensional Bravais classes by means of its lattice planes. Gruber gives some interesting examples relevant to this in [6].

Given an n-dimensional Bravais class $B_n$ and an (n-1)-dimensional Bravais class $B_{n-1}$, any attempt to describe those lattice planes in $B_n$ for which $B_{n-1}$ occurs, seems bound to lead us back to an algorithmic approach as in [6] , and hence to specialized situations. Instead we consider here a related problem which has some chance of a general solution. Given that $B_{n-1}$ occurs on a rational plane for W, to what extent is it accidental ? In other words, is there a relationship between $B_n$, $B_{n-1}$ and the size of the set of small symmetry preserving perturbations of T which also preserve the symmetry of $T \cap W$ ? We show particular interest in the planes W for which the symmetry of $T \cap W$ is always preserved, since this corresponds to a structurally stable situation.

We formulate an approach to this problem in n dimensions, and present the corresponding solution in three dimensions, where we show there is a definite dimensional relationship between $B_n$, $B_{n-1}$ and the symmetry preserving set. We consider the results for the tetragonal, hexagonal and rhombohedral systems to be the most significant.

# CHAPTER ONE. BASIC PROPERTIES OF CRYSTAL LATTICES.

Throughout this thesis, V denotes an n-dimensional real vector space with scalar product, with $n \geq 1$.

In this chapter, we consider some properties of crystal lattices which are of particular importance in the rest of the thesis.

We begin with a standard definition.

Definition. Let $r \in Z$, $0 \leq r \leq n$. Then T is a lattice of rank r in V if and only if it is a subgroup of V generated additively by r linearly independent vectors.

For $r = 0$, $T = 0$. For $r > 0$, $T = \left\{\sum_{i=1}^{r} p_i t_i \; : \; p_i \in Z\right\}$, where $\{t_1, \ldots, t_r\} \subset V$ is a linearly independent set, called a basis of T. For $r > 0$, T has more than one basis, but each basis has exactly r vectors.

A lattice is a discrete subgroup of V, by the following:

Proposition 1.1. [14; Theorem 3,p.275]. Any non-empty subset of a lattice T has a vector of minimum length.

The next proposition is essentially part of a theorem of Bieberbach ( see [15; Theorem 3.2.1., p.100]) but it is felt that our elementary proof is an advantage.

Proposition 1.2. Any discrete subgroup of V spanning a subspace of dimension r is a lattice of rank r. In particular, the set of translations in an n-dimensional space group is a lattice of rank n.

To prove this, we need:

Lemma 1.3. Let D be a discrete subgroup of V and suppose

$\{d_1,\ldots,d_k\} \subset D$. If there exist $s_1,\ldots,s_k \in R$, not all zero, such that $\sum_{i=1}^{k} s_i d_i = 0$, then there exist $p_1,\ldots,p_k \in Z$, not all zero, such that $\sum_{i=1}^{k} p_i d_i = 0$.

Proof. By a well known result in Number Theory (see [8; Theorem 201, p.170]), for any $\delta > 0$ there exist $q \in Z$, $q \neq 0$, and $p_1,\ldots,p_k \in Z$, not all zero, such that $|qs_i - p_i| < \delta$, $1 \leq i \leq k$. Let $d_\delta = q(\sum_{i=1}^{k} s_i d_i) - \sum_{i=1}^{k} p_i d_i$. Then $d_\delta \in D$ and $\|d_\delta\| < \delta(\sum_{i=1}^{k}\|d_i\|)$. Since D is discrete, for sufficiently small $\delta$, $d_\delta = 0$, giving $\sum_{i=1}^{k} p_i d_i = 0$.

Proof of Proposition 1.2. Let D be a discrete subgroup of V spanning a subspace of dimension r. If $\{x_1,\ldots,x_r\}$ is an independent set in D, then the set $A = \{y : y = \sum_{i=1}^{r} s_i x_i,\ |s_i| \leq 1\}$ is bounded and it is easily seen that $A \cap D$ generates D as an additive group. Therefore D is finitely generated, since A is compact.

Let $\{d_1,\ldots,d_k\}$ be a minimal set of generators for D. Clearly $k \geq r$. Suppose $k > r$. Then by Lemma 1.3 there exist $p_1,\ldots,p_k \in Z$, not all zero, with $\sum_{i=1}^{k} p_i d_i = 0$. Write this as $q_k d_k = \sum_{i=1}^{k-1} q_i d_i$ assuming without loss of generality that $q_k \neq 0$ and $q_1$ is the smallest positive $q_i$ for $i = 1,\ldots,k-1$. Choose $m_2,\ldots,m_{k-1}$ such that $0 \leq q_i + m_i q_1 < q_1$, $2 \leq i \leq k-1$. Write $q_k d_k = q_1 d_1 - m_2 q_1 d_2 - m_3 q_1 d_3 - \ldots - m_{k-1} q_1 d_{k-1} + (q_2 + m_2 q_1) d_2 + \ldots + (q_{k-1} + m_{k-1} q_1) d_{k-1}$ i.e. $q_k d_k = q_1 d_1^* + q_2' d_2 + \ldots + q_{k-1}' d_{k-1}$. For $i = 2,\ldots,k-1$ each $q_i'$ is nonnegative and less than $q_1$. Repeat the procedure to get a new set of generators, $d_1^*, d_2^*, \ldots, d_{k-1}^*, d_k$, where $q_k d_k = z d_1^*$; $q_k, z \in Z \backslash \{0\}$ and without loss of generality $HCF(q_k, z) = 1$. It follows that $(\frac{1}{z}) d_k \in D$

and hence that $\{d_1,\dots,d_k\}$ is not a minimal set of generators, which is a contradiction. Therefore $k = r$ and the result follows.

Proposition 1.4. Let $W$ be a vector subspace of $V$. If $T$ is a lattice of rank $r$, then $T \cap W$ is a lattice of rank not greater than $r$.

Proof. Clearly $T \cap W$ is a discrete subgroup of $V$ spanning a subspace of dimension not greater than $r$. Apply Proposition 1.2.

Definition. [14;p.271]. A set $\{t_1,\dots,t_k\}$ in a lattice $T$ is primitive if it forms a basis for the lattice $T \cap W$, where $W$ is the vector subspace spanned by $\{t_1,\dots,t_k\}$.

Proposition 1.5. [14; Theorem 2,p.272]. A primitive set $\{t_1,\dots,t_k\}$ in $T$ can always be extended to a basis $\{t_1,\dots,t_k,t_{k+1},\dots,t_r\}$ of $T$.

We make the following standard definitions.

Definition. A linear transformation $\theta: V \rightarrow V$ is orthogonal if and only if, for all $x,y \in V$, $\langle \theta x, \theta y\rangle = \langle x,y\rangle$ .

We denote the group of orthogonal transformations by $O(V)$.

Definition. If $T$ is a lattice of rank $n$ in $V$, the symmetry group of $T$, denoted $G(T)$, is $\{\theta \in O(V) : \theta T = T\}$.

The group $G(T)$ is a discrete, and hence finite, subgroup of $O(V)$.

As discussed in the introduction to this thesis, we are interested in pairs $(H,T)$, where $T$ is a lattice of rank $n$ in $V$ and $H$ is a finite subgroup of $O(V)$ acting on T. Clearly $H \subseteq G(T)$. We use the following equivalence relations, which appear in [13].

Definition. The pairs $(H_1,T_1)$ and $(H_2,T_2)$ are:
(i) arithmetically equivalent if and only if there exists a linear transformation $\varphi \in GL(V)$ such that $\varphi T_1 = T_2$ and $\varphi H_1 \varphi^{-1} = H_2$ ;
(ii) geometrically equivalent if and only if there exists a linear transformation $\varphi \in GL(V)$ such that $\varphi H_1 \varphi^{-1} = H_2$.

An equivalence class under (i) is an arithmetic crystal class. The set of them is denoted by $\mathcal{A}$.

An equivalence class under (ii) is a geometric crystal class. The set of them is denoted by $\mathcal{G}$.

Definition. The lattices $T_1$ and $T_2$ are arithmetically (respectively geometrically) equivalent if and only if the pairs $(G(T_1),T_1)$ and $(G(T_2),T_2)$ are arithmetically (respectively geometrically) equivalent.

The arithmetic equivalence classes of lattices are called Bravais classes. The set of them is denoted by $\mathcal{B}$.

The geometric equivalence classes of lattices are called crystal systems. The set of them is denoted by $\mathcal{C}$.

For any n, the sets $\mathcal{A}, \mathcal{G}, \mathcal{B}, \mathcal{C}$ are finite (since the number of n-dimensional space groups is finite). They have been fully described for $n \leq 4$ (see [2], [3], [4] ).

Proposition 1.6. Suppose $(H_1,T_1)$ and $(H_2,T_2)$ are geometrically equivalent pairs. Let $QT_j = \{\sum_{i=1}^{m} q_i t_i : q_i \in Q, t_i \in T_j, m \in N\}$ for $j = 1,2$. Then there exists $\varphi \in GL(V)$ such that $\varphi(QT_1) = QT_2$ and $\varphi H_1 \varphi^{-1} = H_2$ .

Proof. Choose a basis $\{t_{11},\ldots,t_{1n}\}$ of $T_1$ and a basis $\{t_{21},\ldots,t_{2n}\}$ of $T_2$. We represent $H_1$ and $H_2$ as groups $\mathcal{H}_1$ and $\mathcal{H}_2$ of integral matrices relative to these bases. Take $\Psi \in GL(V)$ such that $\Psi H_1 \Psi^{-1} = H_2$. Suppose $\Psi$ has matrix F relative to $\{t_{11},\ldots,t_{1n}\}$ and that E is the matrix of $\{t_{21},\ldots,t_{2n}\}$ relative to $\{t_{11},\ldots,t_{1n}\}$. Then $H_2$ has matrix representation $E\mathcal{H}_2E^{-1}$ relative to $\{t_{1j}\}_{j=1}^{n}$. The equation $\Psi H_1 \Psi^{-1} = H_2$ gives the following matrix equation, relative to the basis $\{t_{1j}\}_{j=1}^{n}$:

$$F\mathcal{H}_1F^{-1} = E\mathcal{H}_2E^{-1}.$$

Now suppose $\mathcal{H}_1 = \{A_1,\ldots,A_m\}$, $\mathcal{H}_2 = \{B_1,\ldots,B_m\}$ where $FA_iF^{-1} = EB_iE^{-1}$, $1 \leq i \leq m$. The equation $X\mathcal{H}_1X^{-1} = \mathcal{H}_2$, for which $X = E^{-1}F$ is a solution, yields a system of equations given by:

$$\begin{aligned} XA_1 - B_1X &= 0 \\ XA_2 - B_2X &= 0 \qquad (*) \\ &\vdots \\ XA_m - B_mX &= 0. \end{aligned}$$

There are $mn^2$ equations in $n^2$ variables, $x_{ik}$, $1 \leq i, k \leq n$ (where $X = (x_{ik})$ ). We denote by C the $(mn^2) \times n^2$ matrix of coefficients. The matrix C has all integral entries and has rank less than $n^2$, since $X = E^{-1}F$ provides a non-trivial solution. By elementary column operations, whose product we denote by an invertible matrix U with rational entries, we may reduce C to the form:

$$D = CU = \left( (mn^2) \times r \;\middle|\; 0 \right)$$

where $r = \text{rank } C < n^2$.

The entries of $E^{-1}F$ form a vector in $R^{n^2}$, say $\underline{s}$, where $C\underline{s} = 0$. Therefore $D(U^{-1}\underline{s}) = 0$. The first r coordinates of $U^{-1}\underline{s}$ must be zero, as the rank of C is r. We choose a new vector $\underline{s}'$ in $R^{n^2}$, with the first r coordinates zero and the remaining $n^2 - r$ coordinates in Q and arbitrarily close to the corresponding coordinates in $\underline{s}$. Then $D\underline{s}' = 0$ and $C(U\underline{s}') = 0$. The vector $U\underline{s}'$ has coordinates in Q and is arbitrarily close to $\underline{s}$. Its corresponding matrix S' satisfies (*), where det $S' \neq 0$ since S' is close to $E^{-1}F$. We conclude that det $(ES') \neq 0$ and

$$(ES')\mathcal{H}_1(ES')^{-1} = E\mathcal{H}_2E^{-1}.$$

Let $\varphi$ in GL(V) have matrix ES' relative to $\{t_{11},\ldots,t_{1n}\}$. Then $\varphi H_1\varphi^{-1} = H_2$ and it is clear that for all $t_1 \in T_1$, $\varphi t_1 \in QT_2$. It is easily verified that $\varphi$ maps $QT_1$ onto $QT_2$. This completes the proof.

If T is a lattice of rank n in V and $\varphi \in GL(V)$, then it is clear that $\varphi T$ is another lattice of rank n. If $g \in G(T)$, then $\varphi g\varphi^{-1}$ acts on $\varphi T$ but it may happen that $\varphi g\varphi^{-1} \notin O(V)$, in which case $\varphi g\varphi^{-1} \notin G(\varphi T)$. For example, if n = 2 and T is of class $\underline{S}$, whereas $\varphi T$ is of class $\underline{R}$, then the rotation through $\frac{\pi}{2}$ in G(T) becomes non-orthogonal under conjugation by $\varphi$.

Conversely, there may be elements $\theta$ in $G(\varphi T)$ which are not of the form $\varphi g\varphi^{-1}$ for $g \in G(T)$. However, if $\varphi$ is close to $\iota$, this is not so, as we now show.

<u>Theorem 1.7</u>. Let T be a lattice of rank n in V. Then there exists $\delta > 0$, depending on T, such that for all $\varphi \in GL(V)$ with $\|\varphi - \iota\| < \delta$, $G(\varphi T) = \varphi G(T)\varphi^{-1} \cap O(V)$.

To prove this we need two lemmas, the second dependent on the first.

Lemma 1.8. For any lattice T of rank n in V, there exists $C_T > 0$ with the following property: if $\varphi \in GL(V)$ and $\|\varphi t\| = \|t\|$ for all $t \in T$ with $\|t\| \leq C_T$, then $\varphi \in O(V)$.

Proof. Let $\{t_1,\ldots,t_n\}$ be a basis of T. Put $C_T = \text{maximum}\ \{\|t\| : t = s_i t_i + s_j t_j\ ;\ s_i, s_j \in \{0,1\},\ 1 \leq i,j \leq n\}$. We show that this $C_T$ works. Take $\varphi \in GL(V)$ such that $\|\varphi t\| = \|t\|$ for all $t \in T$ with $\|t\| \leq C_T$. Then for all i, j ,

$$\begin{aligned} 2\langle \varphi t_i, \varphi t_j\rangle &= \langle \varphi(t_i + t_j), \varphi(t_i + t_j)\rangle - \langle \varphi t_i, \varphi t_i\rangle \\ &\qquad - \langle \varphi t_j, \varphi t_j\rangle \\ &= \langle t_i + t_j, t_i + t_j\rangle - \langle t_i, t_i\rangle - \langle t_j, t_j\rangle \\ &= 2\langle t_i, t_j\rangle . \end{aligned}$$

Since $t_1,\ldots,t_n$ span V, the result follows.

Lemma 1.9. Let $H(T) = \{\varphi \in GL(V) : \varphi T = T\}$. Then there exists $D_T > 0$ such that for all $h \in H(T)\backslash G(T)$, $B(h,D_T) \cap O(V)$ is the empty set , where $B(h,D_T) = \{\varphi \in GL(V) : \|\varphi - h\| < D_T\}$.

Proof. Since T is discrete, $T \cap \bar{B}(0,2C_T)$ is finite. Therefore we may define $m_T = \text{minimum}\ \{\,|\,\|t_1\| - \|t_2\|\,| : t_1, t_2 \in T \cap \bar{B}(0,2C_T),\ \|t_1\| \neq \|t_2\|\}$. Let $M_T = \text{minimum}\{\frac{m_T}{2}, C_T\}$ and put $D_T = \frac{M_T}{C_T}$. We show that this $D_T$ works.

Take any $h \in H(T)\backslash G(T)$. By Lemma 1.8, there exists $t_h \in T \cap \bar{B}(0,C_T)$ such that $\|ht_h\| \neq \|t_h\|$ . Either $\|ht_h\| > 2C_T$ or $\|ht_h\| \leq 2C_T$, so $|\,\|ht_h\| - \|t_h\|\,| > M_T$.

For any $\theta \in O(V)$,

$$\begin{aligned} \|h - \theta\| &\geq \left(\frac{1}{\|t_h\|}\right) \|ht_h - \theta t_h\| \\ &\geq \left(\frac{1}{\|t_h\|}\right) |\,\|ht_h\| - \|\theta t_h\|\,| \\ &= \left(\frac{1}{\|t_h\|}\right) |\,\|ht_h\| - \|t_h\|\,| \\ &> \frac{M_T}{\|t_h\|} \\ &\geq D_T \end{aligned}$$

Proof of Theorem 1.7. Choose $\delta > 0$ such that if $\varphi \in GL(V)$ and $\|\varphi - \iota\| < \delta$, then $\|\varphi^{-1}\theta\varphi - \theta\| < D_T$ for all $\theta \in O(V)$. This is possible because for all $\theta \in O(V)$,

$$\begin{aligned}\|\varphi^{-1}\theta\varphi - \theta\| &\leq \|\varphi^{-1} - \iota\|\|\theta\varphi\| + \|\theta\|\|\varphi - \iota\| \\ &\leq \|\varphi^{-1} - \iota\|\|\varphi\| + \|\varphi - \iota\|.\end{aligned}$$

We show that this $\delta$ works in the theorem. Suppose $\|\varphi - \iota\| < \delta$. Take $g \in G(\varphi T)$. Then $\|\varphi^{-1}g\varphi - g\| < D_T$, since $g \in O(V)$. But $\varphi^{-1}g\varphi \in H(T)$, so $\varphi^{-1}g\varphi \in G(T)$, by Lemma 1.9. This proves that $G(\varphi T) \subseteq \varphi G(T)\varphi^{-1} \cap O(V)$. The reverse inclusion is clear.

Corollary. There exists $\delta > 0$, depending on T, such that:

$\varphi \in GL(V)$, $\|\varphi - \iota\| < \delta$ and $G(\varphi T) = \psi G(T)\psi^{-1}$ for some $\psi \in GL(V)$ $\Rightarrow G(\varphi T) = \varphi G(T)\varphi^{-1}$.

Proof. Choose $\delta$ as in the theorem. Comparing group orders gives the result.

# CHAPTER TWO. CRYSTAL FAMILIES.

## 2.1. Functions of Positive Definite Symmetric Transformations.

We make the following standard definitions.

Definition. A linear transformation $\varphi: V \longrightarrow V$ is symmetric if and only if $\langle \varphi v, w\rangle = \langle v, \varphi w\rangle$ for all $v, w \in V$.

Definition. A symmetric linear transformation $p: V \longrightarrow V$ is positive definite if and only if $\langle pv, v\rangle > 0$ for all $v \neq 0$.

We denote the set of symmetric transformations by Sym(V) and the set of positive definite symmetric transformations by Pos(V), where Pos(V) $\subset$ GL(V), but is not a subgroup.

It is well known that for $p \in$ Pos(V) all the eigenvalues of p are real and strictly positive. Also there is an orthonormal basis of V consisting of eigenvectors of p (by the Spectral Theorem). Suppose the eigenvalues $\lambda_1, \ldots, \lambda_n$ of p are contained in some interval $[a,b]$ and that $f \in C^+[a,b]$, the space of continuous, strictly positive, real valued functions on $[a,b]$. If we choose a basis of V relative to which p has the diagonal matrix $D(\lambda_i)$, then we may define f(p) in Pos(V) to have matrix $D(f(\lambda_i))$. This definition of f(p) is independent of the basis chosen, since f(p) equals $P_{(f,p)}(p)$, where $P_{(f,p)}(x)$ is a polynomial in R[x] chosen so that $P_{(f,p)}(\lambda_i) = f(\lambda_i)$, $1 \leq i \leq n$. If p has k distinct eigenvalues (without loss of generality $\lambda_1, \ldots, \lambda_k$) then $P_{(f,p)}(x)$ has degree k - 1 and is defined by:

$$P_{(f,p)}(x) = \sum_{i=1}^{k} \frac{(f(\lambda_i))(x-\lambda_1)(x-\lambda_2)\ldots\widehat{(x-\lambda_i)}\ldots(x-\lambda_k)}{(\lambda_i-\lambda_1)(\lambda_i-\lambda_2)\ldots\widehat{(\lambda_i-\lambda_i)}\ldots(\lambda_i-\lambda_k)}$$

where $\wedge$ denotes omission.

Proposition 2.1. (i) For fixed p, the map from $C^+[a,b]$ to Pos(V) taking f to f(p) is continuous.

(ii) For fixed $f \in C^+(0,\infty)$, the map from Pos(V) to Pos(V) taking p to f(p) is continuous.

Proof. (i) The polynomial $P_{(f,p)}(x)$ clearly depends continuously on f.

(ii) The polynomial $P_{(f,p)}(x)$ depends continuously on the eigenvalues of p. If p and q are close in Pos(V), so are their eigenvalues.

Definition. Let H be a subgroup of O(V). The centralizer of H in GL(V), denoted C(H,GL(V)), is $\{\varphi \in GL(V) : \varphi h = h\varphi$ for all $h \in H\}$.

The centralizers C(H,O(V)) and C(H,Pos(V)) are defined similarly. Note that C(H,GL(V)) and C(H,O(V)) are groups, but C(H,Pos(V)) is not.

Proposition 2.2. Suppose $p \in Pos(V)$ and $f \in C^+[a,b]$, where $\{$eigenvalues of p$\} \subset [a,b]$. If $p \in C(H,Pos(V))$, then $f(p) \in C(H,Pos(V))$.

Proof. Follows directly from the facts that $f(p) = P_{(f,p)}(p)$ and that if $ph = hp$ then $p^m h = hp^m$, any $m \in N$.

For a proof of the following standard result, see [7; Theorem 1, p.169].

Proposition 2.3. (The Polar Decomposition).

There is a homeomorphism $\rho$ from the product space O(V) x Pos(V) onto the space GL(V) defined by $\rho(\theta,p) = \theta p$. The inverse is given by $\rho^{-1}(\varphi) = (\varphi(\varphi'\varphi)^{-\frac{1}{2}}, (\varphi'\varphi)^{\frac{1}{2}})$.

Remark. The continuity of $\rho$ and $\rho^{-1}$ is not included in the proof in [7]. That of $\rho$ is obvious. That of $\rho^{-1}$

follows from Proposition 2.1 (ii).

<u>Proposition 2.4</u>. Let $H_1$ and $H_2$ be subgroups of $O(V)$ such that $\varphi H_1 \varphi^{-1} = H_2$ for some $\varphi \in GL(V)$. If the polar decomposition of $\varphi$ is $\Theta p$, then $p \in C(H_1, Pos(V))$ and $\Theta H_1 \Theta^{-1} = H_2$ .

<u>Proof</u>. Take $h_1 \in H_1$. Then $\varphi h_1 \varphi^{-1} \in O(V)$ so $(\varphi h_1 \varphi^{-1})' = (\varphi h_1 \varphi^{-1})^{-1}$. This gives $(\varphi^{-1})' h_1' \varphi' \varphi h_1 \varphi^{-1} = \iota$ and hence $\varphi' \varphi h_1 = h_1 \varphi' \varphi$. However, $p = (\varphi' \varphi)^{\frac{1}{2}}$ by Proposition 2.3 and by Proposition 2.2 we get $p \in C(H_1, Pos(V))$. It is immediate that $\Theta H_1 \Theta^{-1} = H_2$.

## <u>2.2. Crystal Families</u>.

Before defining a crystal family, we need to establish the existence of a lattice of minimal symmetry in each arithmetic crystal class. This is assumed without full proof in [3] but proved in [13; Theorem 2.1, p. 26]. A different proof is given here, which is more in keeping with our geometric viewpoint. Throughout the remainder of this chapter, we deal with lattices of rank n in V.

<u>Definition</u>. Let A be an arithmetic crystal class in $\mathcal{A}$ and suppose the pairs $(H_1, T_1)$ and $(H_2, T_2)$ belong to it. We write $T_1 \geq T_2$ if and only if there exists $\varphi \in GL(V)$ such that $\varphi T_1 = T_2$, $\varphi H_1 \varphi^{-1} = H_2$ ,$\varphi G(T_1) \varphi^{-1} \supseteq G(T_2)$.

It is clear that this defines a partial ordering on the set of lattices occurring in the pairs of A.

<u>Lemma 2.5</u>. The lattices $T_1$ and $T_2$ are in the same Bravais class if and only if $T_1 \geq T_2$ and $T_2 \geq T_1$.

<u>Proof</u>. This is clear from the definition of $\geq$ .

Proposition 2.6. Each arithmetic crystal class contains a pair $(H_o,T_o)$, where $T_o$ is minimal for the partial ordering i.e. $T_o \leq T$ for all $T$ occurring in pairs $(H,T)$ of the class.

Proof. Since $\mathcal{B}$ is finite, it is enough to show, by Lemma 2.5, that if $(H_1,T_1)$ and $(H_2,T_2)$ are in an arithmetic class, then there exists a pair $(H_3,T_3)$ in the class such that $T_3 \leq T_1$ and $T_3 \leq T_2$. We know there exists $\varphi \in GL(V)$ such that $\varphi T_1 = T_2$, $\varphi H_1 \varphi^{-1} = H_2$. Suppose $\varphi$ has polar decomposition $\Theta p$. For $k \in N$, we may form $p^{\frac{1}{k}}$ and $p^{-\frac{1}{k}} \in Pos(V)$ by the method of Section 2.1. Now $p \in C(H_1,Pos(V))$ by Proposition 2.4 and therefore $p^{\frac{1}{k}}$, $p^{-\frac{1}{k}} \in C(H_1,Pos(V))$ by Proposition 2.2. Consequently $H_1 = (p^{\frac{1}{k}})H_1(p^{-\frac{1}{k}})$ and $H_1$ acts on $(p^{\frac{1}{k}})T_1$. It follows that $(H_1,p^{\frac{1}{k}}T_1)$ is arithmetically equivalent to $(H_1,T_1)$. However, by choosing $k$ sufficiently large, we can make $p^{\frac{1}{k}}$ arbitrarily close to $\iota$ by Proposition 2.1 (i). So for some $k_o$, $G(p^{\frac{1}{k_o}}T_1) = (p^{\frac{1}{k_o}})G(T_1)(p^{-\frac{1}{k_o}}) \cap O(V)$ by Theorem 1.7. Putting $T_3 = (p^{\frac{1}{k_o}})T_1$, we have $T_3 \leq T_1$. It remains to show $T_3 \leq T_2$. Let $H_1' = \{g \in G(T_1) : (p^{\frac{1}{k_o}})g(p^{-\frac{1}{k_o}}) \in O(V)\}$.

Then $p^{\frac{1}{k_o}} \in C(H_1',Pos(V))$ and $G(T_3) = H_1'$ by Proposition 2.4. It follows that $p = (p^{\frac{1}{k_o}})^{k_o} \in C(H_1',Pos(V))$. We now have : $(\varphi p^{-\frac{1}{k_o}})T_3 = \varphi T_1 = T_2$ ; $(\varphi p^{-\frac{1}{k_o}})H_1(\varphi p^{-\frac{1}{k_o}})^{-1} = \varphi H_1 \varphi^{-1} = H_2$;
$(\varphi p^{-\frac{1}{k_o}})G(T_3)(\varphi p^{-\frac{1}{k_o}})^{-1} = \varphi G(T_3)\varphi^{-1} = \Theta H_1'\Theta^{-1} \subseteq O(V)$ and hence $(\varphi p^{-\frac{1}{k_o}})G(T_3)(\varphi p^{-\frac{1}{k_o}})^{-1} \subseteq G(T_2)$. This proves $T_3 \leq T_2$.

<u>Remark</u>. There is a small error in the proof of this result in [13], which, however, does not invalidate it. In the statement of Lemma 2.2(A), if H and G are groups of integral matrices, then "$\Omega(H) \supseteq \Omega(G)$ imples $H \subseteq G$" is true <u>only if G represents the symmetry group of some lattice</u>.

By Lemma 2.5 and Proposition 2.6, there is a well-defined map $\mu: \mathcal{A} \to \mathcal{B}$, taking an arithmetic class A to the Bravais class of a minimal lattice occurring in A.

Let $\nu: \mathcal{A} \to \mathcal{G}$ be the natural surjection. Confusion has arisen in crystallography because of the lack of a natural choice for a set X of crystallographic objects and maps $\mu': \mathcal{G} \to X$ and $\nu': \mathcal{B} \to X$ which make the following diagram commutative:

$$\begin{array}{ccc} \mathcal{A} & \xrightarrow{\nu} & \mathcal{G} \\ \mu\downarrow & & \downarrow\mu' \\ \mathcal{B} & \xrightarrow{\nu'} & X \end{array}$$

Such a set X and maps $\mu'$, $\nu'$ would induce equivalence relations on $\mathcal{A}$, $\mathcal{G}$ and $\mathcal{B}$, the equivalence classes being in bijective correspondence with X.

Accordingly, Bülow, Neubüser and Wondratschek in [3; p.519] define an equivalence relation $\sim_1$ on $\mathcal{A}$ ($\pi_1 : \mathcal{A} \to \mathcal{A}/\sim_1$) which in our terminology can be described as the weakest for which the maps $\mu' = \pi_1 \cdot \mu^{-1} : \mathcal{B} \to \mathcal{A}/\sim_1$ and $\nu' = \pi_1 \cdot \nu^{-1} : \mathcal{G} \to \mathcal{A}/\sim_1$ are well-defined. This clearly gives a commutative diagram. An equivalence class of $\sim_1$ is a <u>crystal family</u>.

In view of our remarks, we can also define crystal families by using the weakest equivalence relation $\sim_2$ on $\mathcal{G}$ for which $\pi_2 \cdot \nu \cdot \mu^{-1}$ is well-defined or by using the weakest equivalence relation $\sim_3$ on $\mathcal{B}$ for which $\pi_3 \circ \mu \circ \nu^{-1}$ is well-defined. It is easily seen that the equivalence relation induced on $\mathcal{A}$ in either case is the same as that defined by Bülow et al.

We are interested in the relation $\sim_3$ on $\mathcal{B}$. Again we call an equivalence class a crystal family and we denote the set of them by $\mathcal{F}$. We can readily describe the equivalence relation on lattices induced by $\sim_3$ to be that generated by $\sim$, where:

Definition. $T_1 \sim T_2$ if and only if there exist geometrically equivalent pairs $(H_1,T_1)$ and $(H_2,T_2)$ such that:

$T_1$ is minimal in the arithmetic class of $(H_1,T_1)$;

$T_2$ is minimal in the arithmetic class of $(H_2,T_2)$.

This is the characterization of a family which we use subsequently. It is immediate from this definition that each family of lattices contains whole crystal systems. In general $\mathcal{F}$ and $\mathcal{C}$ do not coincide and this is why confusion has sometimes arisen, since an arithmetic crystal class does not always belong to a crystal system. Clearly any arithmetic class (and its associated space groups) belong to a unique family. For n = 2, $\mathcal{F} = \mathcal{C}$ but for n = 3, if $\pi_{\mathcal{B}} : \mathcal{B} \to \mathcal{C}$ is the natural surjection, there are two possible answers for $\pi_{\mathcal{B}} \cdot \mu \cdot \nu^{-1}$ ($\underline{3}$), namely the hexagonal or the rhombohedral system. In [3], it is shown that, for n=4, $|\mathcal{F}| = 23$, $|\mathcal{C}| = 33$.

In [13], Schwarzenberger approaches the problem from the point of view of systems, using the natural surjection $\mathcal{B} \to \mathcal{C}$ and a map from $\mathcal{G}$ to $\mathcal{C}$ which is defined by the existence of a lattice of minimal symmetry in each geometric crystal class. Families are then defined by the weakest equivalence relation on $\mathcal{C}$ which makes the diagram:

$$\begin{tikzcd}
\mathcal{A} \arrow[r, "\nu"] \arrow[d, "\mu"'] & \mathcal{G} \arrow[d] \\
\mathcal{B} \arrow[r, "\pi_{\mathcal{B}}"] & \mathcal{C}
\end{tikzcd}$$

commutative. This does have the advantage of producing a more natural map from $\mathcal{G}$ to $\mathcal{F}$ than our $\pi_3 . \mu . \nu^{-1}$, but there is some doubt about the proof in [13] that this map exists. This proof contains several mistakes and gaps. Some explicit problems are the following.

(1) p.27, line 12. The statement "only a finite number of choices of integer $n_{ij}$ are possible" is false.

(2) Lines 18-19. The statement " $\Lambda(G_1) \supseteq \Lambda(G_2)$ only if $G_1 \subseteq G_2$" is false.

(3) Lines 24-27. There are two gaps here. First, it is not clear that the union $\bigcup \varphi\Lambda(G_0)$ can be taken over the normalizer of H. Secondly, even if this can be done, what special properties of the normalizer are being used to justify $V = \bigcup \varphi\Lambda(G_0)$ ? Other problems in this proof could be mentioned and this is why our approach to families avoids the need for this result.

<u>Problem</u>. Prove or disprove the statement that each geometric crystal class contains a lattice of minimal symmetry.

We shall see in Chapters 3 and 4 that families are very useful for investigating lattices in higher dimensions.

## <u>2.3. The Dimension of a Family.</u>

<u>Definition</u>. [12; p.328]. Let $\{e_1,\ldots,e_n\}$ be a basis of V. The <u>unimodular group</u> relative to $\{e_1,\ldots,e_n\}$ is the

subgroup of GL(V) consisting of those maps whose matrix relative to $\{e_1,\dots,e_n\}$ is in GL(n, Z ).

<u>Definition</u>. [12; p.328]. Two bases $\{e_1,\dots,e_n\}$ and $\{f_1,\dots,f_n\}$ are <u>unimodularly equivalent</u> if and only if there exist a linear map $\varphi$ belonging to the unimodular group relative to $\{e_1,\dots,e_n\}$ and $c > 0$ such that $\varphi e_i = cf_i$, $1 \leq i \leq n$.

We denote the set of equivalence classes by $\mathcal{L}_n'$. This is clearly in bijective correspondence with the set of all lattices of rank n in V, given that we make no distinction between a lattice T and multiples cT, $c > 0$. Since every lattice possesses a reduced basis ([12; Proposition 2] ), our definition of $\mathcal{L}_n'$ is equivalent to that in [12], where $\mathcal{L}_n'$ is regarded as the unimodular equivalence classes of reduced bases.

<u>Definition</u>. ([12; p.330]). Two points x' and y' in $\mathcal{L}_n'$ are <u>orthogonally equivalent</u> if and only if there exist bases $\{e_1,\dots,e_n\}$ in x' and $\{f_1,\dots,f_n\}$ in y' such that, for some $\Theta \in O(V)$, $\Theta e_i = f_i$, $1 \leq i \leq n$.

We denote the set of equivalence classes by $\mathcal{L}_n$. There is a natural surjection $\lambda_n\colon \mathcal{L}_n' \longrightarrow \mathcal{L}_n$. Choosing any basis $\{e_1,\dots,e_n\}$ in V determines a map $\alpha : GL(V) \xrightarrow{\text{onto}} \mathcal{L}_n$, taking $\varphi$ to the class of $\{\varphi e_1,\dots,\varphi e_n\}$. The space ($\mathcal{L}_n$, quotient topology of $\alpha$) is then homeomorphic to $GL(V)/\sim$, where $\sim$ is the equivalence relation induced by $\alpha$. The quotient topology on $\mathcal{L}_n$ is independent of $\{e_1,\dots,e_n\}$, for suppose we take a basis $\{\beta e_1,\dots,\beta e_n\}$, with corresponding map

$\gamma : GL(V) \xrightarrow{onto} \mathcal{L}_n$. Then $\gamma = \alpha r_\beta$ where $r_\beta$ is the homeomorphism of GL(V) onto itself given by right translation through $\beta$. Consequently, the quotient topologies of $\alpha$ and $\gamma$ coincide. For this reason, we can choose the most convenient basis for any particular situation, since we are interested in the topology on $\mathcal{L}_n$, not the exact nature of $\alpha$.

The map $\pi$: GL(V) $\longrightarrow$ GL(V)/$\sim$ is open since $\pi^{-1}(\pi(W)) = O(V).W.U$, where U is generated by $(R^+)\iota$ and the unimodular group relative to $\{e_1,\ldots,e_n\}$. Since GL(V) is a topological group, O(V).W.U. is open if W is open, Consequently, $\alpha$: GL(V) $\longrightarrow (\mathcal{L}_n, \tau_\alpha)$ is open, where $\tau_\alpha$ is the quotient topology induced by $\alpha$.

If we now restrict $\alpha$ to Pos(V) we still have an onto map $\alpha|$: Pos(V) $\longrightarrow \mathcal{L}_n$, since if $\varphi \in GL(V)$ has polar decomposition $\Theta p$, then $\alpha(\varphi) = \alpha(p)$. Moreover, $(\mathcal{L}_n, \tau_{\alpha|})$ is homeomorphic to Pos(V)/$\sim$, where $\sim$ is the equivalence relation induced by $\alpha|$. The map $\alpha|$: Pos(V) $\longrightarrow (\mathcal{L}_n, \tau_\alpha)$ is open, since if $\rho_2$: GL(V) $\longrightarrow$ Pos(V) takes $\varphi$ to its positive definite symmetric part $(\varphi'\varphi)^{\frac{1}{2}}$, we have $(\alpha|)(W) = (\alpha(\rho_2)^{-1})(W)$, for any $W \subseteq$ Pos(V). Since $\alpha$ is open and $\rho_2$ is continuous, $\alpha|$ is open. It follows that $\tau_\alpha = \tau_{\alpha|}$. We shall regard $\mathcal{L}_n$ as a quotient space of Pos(V), whereas in [12] it is regarded as a quotient space of GL(V).

<u>Notation</u>. Let G be a finite subgroup of O(V). We denote by $\mathcal{L}_n(G)$ the subset of $\mathcal{L}_n$ consisting of those classes which contain a basis determining a lattice with symmetry group G. By Proposition 2.4, $\mathcal{L}_n(G)$ consists of the classes of lattices in the system determined by G.

We give $\mathcal{L}_n(G)$ the subspace topology from $\mathcal{L}_n$.

The following is essentially the same as Proposition 6 in [12; p.331], but a different proof is given here. Also, a difficulty in the proof in [12] is indicated.

Proposition 2.7. Each point x in $\mathcal{L}_n(G)$ has a neighbourhood homeomorphic to a neighbourhood of $\iota$ in $C(G, Pos(V) \cap SL(V))$. In particular, $\mathcal{L}_n(G)$ is a smooth manifold.

Proof. We assume that $x = (\alpha|)\iota$. Suppose $p_1$ and $p_2$ belong to Pos(V), with $\| p_1 - \iota \|$ and $\| p_2 - \iota \|$ arbitrarily small, such that $(\alpha|)(p_1) \in \mathcal{L}_n(G)$ and $(\alpha|)(p_2) \in \mathcal{L}_n(G)$. By the Corollary to Theorem 1.7 and by Proposition 2.4, $p_1$ and $p_2 \in C(G, Pos(V))$. Suppose moreover $(\alpha|)(p_1) = (\alpha|)(p_2)$. Then there exist $\Theta \in O(V)$, $c > 0$ and $u \in GL(V)$, where u is unimodular relative to a fixed basis in x, such that $cp_1u = \Theta p_2$. Since $\| u - \Theta \| = \|(\frac{1}{c})p_1^{-1}\Theta p_2 - \Theta \|$, which is small, we know, by Lemma 1.9, that $u \in O(V)$ and hence $u \in G$. Thus $p_1u = up_1$ and $cp_1 = \Theta' p_2$, $\Theta' \in O(V)$, giving $cp_1 = p_2$, since $p_1, p_2 \in Pos(V)$.

Consequently, there is a neighbourhood W of $\iota$ in Pos(V) such that $\alpha|$ maps $W \cap C(G, Pos(V))$ onto $(\alpha|)(W) \cap \mathcal{L}_n(G)$ and for $p_1, p_2 \in W \cap C(G, Pos(V))$, $(\alpha|)(p_1) = (\alpha|)(p_2)$ if and only if $cp_1 = p_2$, $c > 0$. We know $\alpha|$ is open. It is easily checked that its restriction to $W \cap C(G, Pos(V))$ is open. We can then deduce that $(\alpha|)(W) \cap \mathcal{L}_n(G)$ is homeomorphic to the quotient space $(W \cap C(G, Pos(V))) / (R^+)\iota$, which in turn is clearly homeomorphic to a neighbourhood of $\iota$ in $C(G, Pos(V) \cap SL(V))$. This completes the proof.

Remarks. In the proof of this result in [12], some result like our Theorem 1.7 is needed several times but is not quoted. This omission seems to occur directly because of the error in lines 9-10 on p.329 which read: "If $\alpha \in GL(V)$ then the lattice $\alpha T$ ... has symmetry group consisting of all orthogonal maps of the form $\alpha\gamma\alpha^{-1}$ for some $\gamma$ in the symmetry group of T." Clearly "consisting of" should be replaced by "containing."

Notation. If $B \in \mathcal{B}$, we denote by $\mathcal{L}_n^B$ the space of all points in $\mathcal{L}_n$ whose lattices belong to B.

If $F \in \mathcal{F}$, we denote by $\mathcal{L}_n^F$ the space of all points in $\mathcal{L}_n$ whose lattices belong to F.

By the Corollary to Theorem 1.7, if $B \in \mathcal{B}$ is in the crystal system determined by $G \subset O(V)$, then $\mathcal{L}_n^B$ is open in $\mathcal{L}_n(G)$. We may write

$$\mathcal{L}_n(G) = \bigsqcup_{i=1}^{k} \mathcal{L}_n^{B_i} ,$$

where $k \in N$, each $B_i \in \mathcal{B}$ and each $\mathcal{L}_n^{B_i}$ is open and closed in $\mathcal{L}_n(G)$ ( $\bigsqcup$ denotes disjoint union).

Similarly for $F \in \mathcal{F}$ we may write

$$\mathcal{L}_n^F = \bigsqcup_{i=1}^{k} \mathcal{L}_n(G_i) ,$$

where $k \in N$.

Proposition 2.8. Each $\mathcal{L}_n(G_i)$ is open (and hence closed) in $\mathcal{L}_n^F$.

In order to prove this we need two lemmas.

Lemma 2.9. For a pair (H,T), T is a minimal lattice in the arithmetic crystal class determined by (H,T) if and only if $C(H, Pos(V)) = C(G(T), Pos(V))$.

Proof of Lemma. Only if. Let T be minimal in the arithmetic class of (H,T). Since $G(T) \supseteq H$,

$C(H, Pos(V)) \supseteq C(G(T), Pos(V))$. Suppose there exists $p$ in $C(H, Pos(V))$ which is not in $C(G(T), Pos(V))$.

By taking the function $p^{\frac{1}{k}}$ $(k \in N)$ of $p$ for sufficiently large $k$, we can ensure that $G(p^{\frac{1}{k}} T) = (p^{\frac{1}{k}})G(T)(p^{-\frac{1}{k}}) \cap O(V)$, by Theorem 1.7. Let $H' = \left\{ g \in G(T) : (p^{\frac{1}{k}})g(p^{-\frac{1}{k}}) \in O(V) \right\}$. Then $p^{\frac{1}{k}} \in C(H', Pos(V))$ by Proposition 2.4. However, $H' \subsetneqq G(T)$, since $p \notin C(G(T), Pos(V))$ and hence $p^{\frac{1}{k}} \notin C(G(T), Pos(V))$. Therefore $G(p^{\frac{1}{k}} T) \subsetneqq G(T)$. Since $p^{\frac{1}{k}} \in C(H, Pos(V))$ (by Proposition 2.2), we have a pair $(H, p^{\frac{1}{k}} T)$ contradicting the minimality of $T$.

<u>If</u>. Suppose $C(H, Pos(V)) = C(G(T), Pos(V))$ but $T$ is not minimal. Let $T_1$ be minimal with $\varphi T = T_1$, $\varphi H \varphi^{-1} = H_1 \subseteq O(V)$, $\varphi G(T) \varphi^{-1} \supsetneqq G(T_1)$. If $\varphi$ has polar decomposition $\theta p$, then $p \in C(H, Pos(V))$. But $p \in C(G(T), Pos(V))$ would imply $\varphi G(T) \varphi^{-1} \subseteq G(T_1)$. Therefore, $p \notin C(G(T), Pos(V))$ and $C(H, Pos(V)) \subsetneqq C(G(T), Pos(V))$ which is a contradiction.

<u>Remark</u>. If $T$ is minimal in the class of $(H,T)$, it is not true in general that $C(H, O(V)) = C(G(T), O(V))$, and hence not true that $C(H, GL(V)) = C(G(T), GL(V))$. For example consider a pair $(H,T)$ in the class $(\underline{4}, \underline{S})$ for $n = 2$. Then $G(T)=\underline{4mm}$ and $T$ is minimal in the arithmetic class of $(H, T)$. However, $C(H, O(V)) = SO(V)$ $(= O(V) \cap SL(V))$ whereas $C(G(T), O(V)) = \{\iota, -\iota\}$. Nevertheless, $C(H, Pos(V)) = (R^+)\iota = C(G(T), Pos(V))$.

<u>Lemma 2.10</u>. If the lattices $T_1$ and $T_2$ belong to the same family, then there exists $\theta \in O(V)$ such that $\theta(C(G(T_1), Pos(V))\theta^{-1} = C(G(T_2), Pos(V))$.

Proof of Lemma 2.10. For $H_1$, $H_2 \subseteq O(V)$ with $\varphi H_1 \varphi^{-1} = H_2$, we have $\theta(C(H_1, Pos(V))\theta^{-1} = C(H_2, Pos(V))$, by Proposition 2.4 (where $\varphi$ has polar decomposition $\theta p$). The result now follows from the definition of a family and Lemma 2.9.

Proof of Proposition 2.8. Take $x_i \in \mathcal{L}_n(G_i)$ and any lattice $T_i$ determined by $x_i$. Then there is a neighbourhood $U(T_i)$ of $\iota$ in Pos(V) such that for $p \in U(T_i)$,

$G(pT_i) = pG(T_i)p^{-1} \cap O(V)$, by Theorem 1.7. Suppose $pT_i$ is in the family F. Put $H_i = \{ g \in G(T_i) : pgp^{-1} \in O(V)\}$. Then $p \in C(H_i, Pos(V))$ by Proposition 2.4 and $G(pT_i) = H_i$. From Lemma 2.10, $C(G(T_i), Pos(V)) = C(H_i, Pos(V))$ by a dimension argument. Therefore, $p \in C(G(T_i), Pos(V))$ and $G(pT_i) = G(T_i) = H_i$. Consequently,

$$(\alpha|)(U(T_i)) \cap \mathcal{L}_n^F \subseteq \mathcal{L}_n(G_i).$$

However, $(\alpha|)(U(T_i)) \cap \mathcal{L}_n^F$ is a neighbourhood of $x_i$ in $\mathcal{L}_n^F$ since we know $\alpha| : Pos(V) \longrightarrow \mathcal{L}_n$ is open. This completes the proof.

We have now proved:

Theorem 2.11. For any $F \in \mathcal{F}$, $\mathcal{L}_n^F$ is a smooth manifold whose dimension equals that of $C(G(T), Pos(V) \cap SL(V))$, for any lattice T in F.

Notice that this theorem and Proposition 2.8 imply that, topologically speaking, a family is not much "bigger" than a system.

We shall call the dimension of $\mathcal{L}_n^F$ "the dimension of the family F." By Lemma 2.9, it also equals the dimension of $C(H, Pos(V) \cap SL(V))$, for any pair (H,T) determining a geometric crystal class belonging to F.

Remark. Sometimes it is more convenient to consider the space $\Lambda_n$, which is also a space of equivalence classes of bases under unimodular and orthogonal equivalence, but with a weaker definition of unimodular equivalence. For $\Lambda_n$, we distinguish between a lattice T and multiples cT, $c > 0$. All the results of this section follow through for $\Lambda_n$ in a similar way. The manifolds $\Lambda_n{}^B$, $\Lambda_n(G)$ and $\Lambda_n{}^F$ are, however, modelled on C(G(T), Pos(V)) and hence have dimensions which are one larger than those of their counterparts $\mathcal{L}_n{}^B$, $\mathcal{L}_n(G)$ and $\mathcal{L}_n{}^F$.

We now establish the connection between the dimension of a family as we have defined it and what Bülow et al. in [3] define as "the number of free parameters of a family."

The arithmetic approach in [3] uses, instead of a pair (H,T), an integral matrix group $\mathcal{H}$ representing H relative to some fixed basis $\{t_1,\ldots,t_n\}$ of T. The space $\Omega(\mathcal{H})$ of all symmetric matrices S such that $\mathfrak{z}'S\mathfrak{z} = S$, for all $\mathfrak{z} \in \mathcal{H}$, is then a subspace of the vector space of all symmetric matrices. Bülow et al. state in [3] without proof that the dimension of $\Omega(\mathcal{H})$ is the same for all arithmetic classes in a family, and they call this dimension "the number of free parameters of the family." The following proposition shows the connection between this number of free parameters and our dimension of a family and also, in view of the results in this section, establishes that dim $\Omega(\mathcal{H})$ is an invariant of a family.

<u>Proposition 2.12</u>. Let $(H,T)$, $\{t_1,\dots,t_n\}$ and $\Omega(\mathcal{H})$ be as above. Then $\Omega(\mathcal{H}) \cap \mathrm{Pos}(n, R)$ is homeomorphic to $C(H, \mathrm{Pos}(V))$, where $\mathrm{Pos}(n, R)$ is the set of positive definite symmetric matrices over R.

<u>Proof</u>. Define $\beta : C(H, \mathrm{Pos}(V)) \longrightarrow \mathrm{Pos}(n, R)$ by $(\beta(p))_{ij} = \langle pt_i, pt_j\rangle$. For $p \in C(H, \mathrm{Pos}(V))$ the group H equals $pHp^{-1}$ and so has matrix representation $\mathcal{H}$ relative to $\{pt_1,\dots,pt_n\}$. Since $H \subseteq O(V)$, $\xi'(\beta(p))\xi = \beta(p)$ for all $\xi \in \mathcal{H}$, so $\beta(p) \in \Omega(\mathcal{H})$. Hence $\beta$ maps into $\Omega(\mathcal{H}) \cap \mathrm{Pos}(n, R)$.

<u>$\beta$ is one-to-one</u>. Suppose $\beta(p_1) = \beta(p_2)$. Then $\langle p_1t_i, p_1t_j\rangle = \langle p_2t_i, p_2t_j\rangle$ all $i,j \in \{1,\dots,n\}$ and therefore $\langle p_1x, p_1y\rangle = \langle p_2x, p_2y\rangle$ all $x, y \in V$, giving $\langle x, y\rangle = \langle p_2p_1^{-1}x, p_2p_1^{-1}y\rangle$ all $x, y \in V$. Therefore $p_2p_1^{-1} \in O(V)$ and $p_2 = p_1$ by the uniqueness of the polar decomposition.

<u>$\beta$ is onto</u>. Take $S \in \Omega(\mathcal{H}) \cap \mathrm{Pos}(n, R)$. Choose n independent vectors $v_1,\dots,v_n$ in V such that $S_{ij} = \langle v_i, v_j\rangle$, $1 \leq i, j \leq n$. Define $\varphi \in GL(V)$ by $\varphi t_i = v_i$, $1 \leq i \leq n$. Suppose $\varphi$ has polar decomposition $\Theta p$. Then $S_{ij} = \langle \varphi t_i, \varphi t_j\rangle = \langle pt_i, pt_j\rangle$. The group $pHp^{-1}$ has matrix representation $\mathcal{H}$ relative to $\{pt_1,\dots,pt_n\}$ and since $S \in \Omega(\mathcal{H})$, $pHp^{-1}$ is contained in $O(V)$. Therefore, $p \in C(H, \mathrm{Pos}(V))$ by Proposition 2.4 and $S = \beta(p)$.

The maps $\beta$ and $\beta^{-1}$ are clearly continuous.

# CHAPTER THREE. THE DECOMPOSITION OF CRYSTALLOGRAPHIC POINT GROUPS.

## 3.1. The Decomposition of Three Representations Associated with a Pair (H,T).

We use the following standard definitions in relation to a left module M over a ring S with unit, $M \neq 0$.

M is reducible if it has a proper non-zero submodule. Otherwise, M is irreducible.

M is completely reducible if every submodule K of M is complemented i.e. there exists a submodule K' such that $M = K \oplus K'$.

M is decomposable if there exist submodules $M_1$, $M_2$, both non-zero, such that $M = M_1 \oplus M_2$. Note that henceforth whenever we write $M = M_1 \oplus \dots \oplus M_k$, we assume that each $M_i$ is non-zero, unless specifically stated otherwise.

The decomposition $M = M_1 \oplus \dots \oplus M_k$ is a complete decomposition if each $M_i$ is indecomposable.

We use the following standard term.

Finite groups $H \subseteq O(V)$ occurring in pairs (H,T) (i.e. subgroups which can act on lattices of rank n) are called crystallographic point groups.

For a pair (H,T) the lattice T is a free Z-module of rank n and corresponding to the left linear action of H on T we have a faithful representation of degree n:

(i) $\pi_Z : H \longrightarrow GL(T)$, where GL(T) is the group of Z-automorphisms of T.

By choosing a basis for T we obtain a matrix representation $P_Z: H \longrightarrow GL(n, Z)$. We can replace Z by R or Q to get:

$$P_Q: H \longrightarrow GL(n, Q);$$

$$P_R: H \longrightarrow GL(n, R).$$

The representations $P_Q$, $P_R$ may be regarded as the matrix representations derived from:

(ii) $\pi_Q: H \longrightarrow GL(QT)$;

(iii) $\pi_R: H \longrightarrow GL(V)$;

where QT is isomorphic to $Q \otimes_Z T$ and is defined in the statement of Proposition 1.6 - it is a vector space of dimension n over Q, by Lemma 1.3.

Associated with the representations (i), (ii), (iii) we have: (i) the left ZH-module T, of Z-rank n;

(ii) the left QH-module QT, of Q-dimension n;

(iii) the left RH-module V, of R-dimension n;

where ZH, QH and RH are group algebras.

We denote these modules by ${}_HT$, ${}_HQT$, ${}_HV$. In general, the decomposition properties of these three modules are different. It is true, however, that

${}_HT$ decomposable $\Rightarrow {}_HQT$ decomposable $\Rightarrow {}_HV$ decomposable,

since if ${}_HT = T_1 \oplus \dots \oplus T_k$ then ${}_HQT = QT_1 \oplus \dots \oplus QT_k$,

and if ${}_HQT = M_1 \oplus \dots \oplus M_k$ then ${}_HV = RM_1 \oplus \dots \oplus RM_k$.

Let (SH, M) be either (ZH, T), (QH, QT) or (RH, V). Take any matrix representation $P_S: H \longrightarrow GL(n, S)$. If ${}_HM$ is decomposable then $P_S(H)$ is conjugate in GL(n, S) to a matrix group $\mathcal{H}$ whose elements are all of the form:

$$\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$$

where $A_1$ is m x m ($m \neq 0$), $A_2$ is (n - m) x (n - m) and m is the same for each element. Conversely, if $P_S(H)$ is conjugate to a group of this form then ${}_HM$ is decomposable.

Part (ii) of Proposition 3.1 (see below) establishes that in the case S = Q, M = QT, $\mathcal{H}$ may be taken to be a subgroup of $GL(n, Z) \subset GL(n, Q)$. It is now easy to see that the "matrix group" definition of decomposability in [3; p.526] corresponds to the decomposability of ${}_HQT$.

Proposition 3.1. (i) If $T_1$ is a direct summand of ${}_HT$ and $W = RT_1$ then W is a submodule of ${}_HV$, $T_1 = T \cap W$ and $\mathrm{rank}_Z(T \cap W) = \dim_R W$.

(ii) If M is a submodule of ${}_HQT$ and W = RM, then W is a submodule of ${}_HV$, $M = QT \cap W = Q(T \cap W)$ and $\dim_Q M = \dim_R W = \mathrm{rank}_Z(T \cap W)$.

Proof. (i) Since $T_1$ is a submodule of T as a Z-module, $T_1$ is free with rank $r \leq n$, as Z is a principal ideal domain. Let $\{t_1,\ldots,t_r\}$ be a basis. Then $W = R\{t_1,\ldots,t_r\}$ and W is clearly a submodule of ${}_HV$ of dimension r, by Lemma 1.3. Clearly, $T_1 \subseteq T \cap W$. Also, since $\{t_1,\ldots,t_r\}$ may be extended to a basis of T as a Z-module, $T_1 \supseteq T \cap W$.

(ii) Let $\dim_Q M = k$, with $\{x_1,\ldots,x_k\}$ a basis. Then $W = R\{x_1,\ldots,x_k\}$ and is clearly a submodule of ${}_HV$. There exist integers $m_1,\ldots,m_k$ such that $\{m_1x_1,\ldots,m_kx_k\} \subset T \cap W$. By Lemma 1.3, $\{m_1x_1,\ldots,m_kx_k\}$ is a basis for W. It follows that $M = Q(T \cap W)$ and $\dim_Q M = \dim_R W = \mathrm{rank}_Z(T \cap W)$. Clearly, $Q(T \cap W) \subseteq QT \cap W$. If $x \in QT \cap W$, there exists $m \in Z$ such that $mx \in T \cap W$, giving $x \in Q(T \cap W)$.

<u>Proposition 3.2.</u> (i) The modules ${}_HQT$ and ${}_HV$ are completely reducible.

(ii) A complete decomposition of ${}_HQT$ (respectively ${}_HV$) is unique up to order and QH- (respectively RH- ) isomorphism of the summands.

<u>Proof</u>. (i) The modules both satisfy the conditions of Maschke's Theorem (see [5; p.88]).

(ii) The modules both satisfy the conditions of the Krull-Schmidt Theorem (see [5; p.83]), since their submodules, being vector subspaces, must satisfy both chain conditions.

By (ii), any complete decomposition of ${}_HQT$ (respectively ${}_HV$) has the same set of associated Q- (respectively R-) dimensions for the summands. If the k-tupleof dimensions is $(n_1,\ldots,n_k)$, where we specify $n_1 \geq n_2 \geq \ldots \geq n_k$ to get uniqueness, then we call $(n_1,\ldots,n_k)$ the <u>decomposition type</u> of ${}_HQT$ (respectively ${}_HV$). We abbreviate this to DT in the sequel.

In general, ${}_HT$ is not completely reducible. For example, let n = 2 and let T be of class <u>D</u>, with H = G(T) - this is of class <u>2mm</u>. The lattice of rank 1 lying in a mirror line is a non-zero proper submodule, but is not complemented.

Also, ${}_HT$ does not satisfy the conditions of the Krull-Schmidt Theorem, since $T \supset 2T \supset 3T \supset \ldots$ is an infinite descending chain of submodules, for any H.
As we might expect, there are cases when different complete decompositions of ${}_HT$ have different rank types, and we cannot define a decomposition type for ${}_HT$ in general.
Bülow et al. in [3; p.527] note this fact, but produce

no examples when the rank type is not well-defined. The following, for $n = 5$, seems to be one of the simplest.

T is generated by $e_1, e_2, e_3, e_4, e_5, f_1, f_2$, where $\{e_1, \ldots, e_5\}$ is a basis of V, $f_1 = \frac{1}{2}(e_1) + \frac{1}{2}(e_3)$, $f_2 = \frac{1}{3}(e_2) + \frac{2}{3}(e_4) + \frac{1}{3}(e_5)$ and the quadratic form A ( $A_{ij} = \langle e_i, e_j \rangle$ ) of $\{e_1, \ldots, e_5\}$ is :

$$A = \begin{pmatrix} a & e & 0 & 0 & 0 \\ e & b & 0 & 0 & 0 \\ 0 & 0 & c & 0 & 0 \\ 0 & 0 & 0 & d & -\frac{d}{2} \\ 0 & 0 & 0 & -\frac{d}{2} & d \end{pmatrix}, \text{ where}$$

a, b, c, d are arbitrary strictly positive real numbers, $e \neq \sqrt{ab}$ .

We denote $e_1, e_2, e_3, e_4, e_5$ by (1 0 0 0 0), (0 1 0 0 0), (0 0 1 0 0), (0 0 0 1 0), (0 0 0 0 1) respectively. They form a unit cell $\left\{ \sum_{i=1}^{5} s_i e_i : 0 \leq s_i \leq 1 \right\}$ whose interior (or "centring") points are $(\frac{1}{2}\ 0\ \frac{1}{2}\ 0\ 0)$, $(0\ \frac{1}{3}\ 0\ \frac{2}{3}\ \frac{1}{3})$, $(0\ \frac{2}{3}\ 0\ \frac{1}{3}\ \frac{2}{3})$, $(\frac{1}{2}\ \frac{1}{3}\ \frac{1}{2}\ \frac{2}{3}\ \frac{1}{3})$, $(\frac{1}{2}\ \frac{2}{3}\ \frac{1}{2}\ \frac{1}{3}\ \frac{2}{3})$. This verifies that T is in fact a lattice, since it is discrete (see Proposition 1.2). We can choose $H \subset O(V)$ acting on T to be the product of: $\{\iota\}$ on $R\{e_1, e_2\}$ ; $\{\iota, -\iota\}$ on $R\{e_3\}$ ; $\underline{\bar{3}m}$ on $R\{e_4, e_5\}$ . Let $T_1$ denote the rhombohedral lattice of rank 3 generated by $e_2, e_4, e_5, f_2$ and let $T_2$ denote the diamond lattice of rank 2 generated by $e_1, e_3, f_1$. Then ${}_HT = T_1 \oplus T_2$ is complete with ranks (3, 2).

Now put $e_1' = (1\ 1\ 0\ 0\ 0)$, $e_2' = (3\ 2\ 0\ 0\ 0)$.
Since $\det\begin{pmatrix}1 & 3\\ 1 & 2\end{pmatrix} = -1$, $T$ is generated by $e_1'$, $e_2'$, $e_3$, $e_4$, $e_5$, $f_1$, $f_2$. Let $e_1' = (1\ 0\ 0\ 0\ 0)'$, $e_2' = (0\ 1\ 0\ 0\ 0)'$, $e_3 = (0\ 0\ 1\ 0\ 0)'$, $e_4 = (0\ 0\ 0\ 1\ 0)'$, $e_5 = (0\ 0\ 0\ 0\ 1)'$.
The unit cell formed by $e_1'$, $e_2'$, $e_3$, $e_4$, $e_5$ has centring points $(0\ \frac{1}{2}\ \frac{1}{2}\ 0\ 0)'$, $(0\ \frac{2}{3}\ 0\ \frac{2}{3}\ \frac{1}{3})'$, $(0\ \frac{1}{3}\ 0\ \frac{1}{3}\ \frac{2}{3})'$, $(0\ \frac{1}{6}\ \frac{1}{2}\ \frac{2}{3}\ \frac{1}{3})'$, $(0\ \frac{5}{6}\ \frac{1}{2}\ \frac{1}{3}\ \frac{2}{3})'$. Let $T_1'$ denote the lattice of rank 4 generated by $e_2'$, $e_3$, $e_4$, $e_5$, $f_1$, $f_2$ and $T_2'$ the lattice of rank 1 generated by $e_1'$. Then ${}_HT = T_1' \oplus T_2'$ is complete with ranks $(4, 1) \neq (3, 2)$.

We omit the proof of the following straightforward result:

<u>Proposition 3.3</u>. (i) If $(H_1, T_1)$ and $(H_2, T_2)$ are arithmetically equivalent pairs, then any $\varphi$ in $GL(V)$ satisfying $\varphi T_1 = T_2$ and $\varphi H_1 \varphi^{-1} = H_2$ takes a complete decomposition of ${}_{H_1}T_1$ to a complete decomposition of ${}_{H_2}T_2$.

(ii) If $(H_1, T_1)$ and $(H_2, T_2)$ are geometrically equivalent pairs, then any $\varphi$ in $GL(V)$ satisfying $\varphi(QT_1) = QT_2$ and $\varphi H_1 \varphi^{-1} = H_2$ takes a complete decomposition of ${}_{H_1}QT_1$ to a complete decomposition of ${}_{H_2}QT_2$. Any $\varphi$ in $GL(V)$ satisfying $\varphi H_1 \varphi^{-1} = H_2$ takes a complete decomposition of ${}_{H_1}V$ to a complete decomposition of ${}_{H_2}V$.

<u>Proposition 3.4</u>. Let $(SH, M)$ be either $(ZH, T)$, $(QH, QT)$ or $(RH, V)$. Let $T$ be minimal in the arithmetic crystal class of $(H, T)$. Then ${}_HM = M_1 \oplus \ldots \oplus M_k$ is complete if and only if ${}_{G(T)}M = M_1 \oplus \ldots \oplus M_k$ is complete.

<u>Proof</u>. It suffices to show that if ${}_HM = M_1 \oplus \cdots \oplus M_l$, then ${}_{G(T)}M = M_1 \oplus \cdots \oplus M_l$. Suppose ${}_HM = M_1 \oplus \cdots \oplus M_l$ is a decomposition contradicting this. Then without loss of generality, we may assume there exists $g_1 \in G(T)$ and $m_1 \in M_1$ such that $g_1(m_1) \notin M_1$. For $\delta > 0$ define $\varphi_\delta$ in $GL(V)$ by $\varphi_\delta = \delta(\iota_{M_1}) \oplus \iota_{(M_2 \oplus \cdots \oplus M_l)}$. Then $(\varphi_\delta)H(\varphi_\delta)^{-1} = H$ and $(H, \varphi_\delta T)$ is arithmetically equivalent to $(H, T)$. Also, by Theorem 1.7, if $\delta$ is chosen sufficiently close to 1, $G(\varphi_\delta T) = (\varphi_\delta)G(T)(\varphi_\delta)^{-1} \cap O(V)$. Let $g_1(m_1) = x_1 + y_1$, where $x_1 \in M_1$, $y_1 \in M_2 \oplus \cdots \oplus M_l$, $y_1 \neq 0$. Then $(\varphi_\delta)g_1(\varphi_\delta)^{-1}(m_1) = (\varphi_\delta)g_1(\frac{1}{\delta}m_1) =$

$= \varphi_\delta(\frac{1}{\delta}x_1 + \frac{1}{\delta}y_1) = x_1 + (\frac{1}{\delta})y_1$. Now

$$\|(\varphi_\delta)g_1(\varphi_\delta)^{-1}(m_1)\|^2 - \|m_1\|^2$$

$$= \|(\varphi_\delta)g_1(\varphi_\delta)^{-1}(m_1)\|^2 - \|g_1(m_1)\|^2$$

$$= \|x_1 + (\tfrac{1}{\delta})y_1\|^2 - \|x_1 + y_1\|^2$$

$$= (\frac{1-\delta^2}{\delta^2})\|y_1\|^2 + (\frac{2-2\delta}{\delta})\langle x_1, y_1\rangle.$$

This is 0 only if $\dfrac{\langle x_1, y_1\rangle}{\|y_1\|^2} = \dfrac{-1-\delta}{2\delta}$, but we can choose $\delta$ avoiding this and still arbitrary close to 1. Consequently, for appropriate $\delta > 0$, $(\varphi_\delta)g_1(\varphi_\delta)^{-1} \notin O(V)$, giving $G(\varphi_\delta T) \subsetneqq \varphi_\delta G(T)(\varphi_\delta)^{-1}$, which contradicts the fact that T is minimal.

<u>Corollary</u>. (Also uses Proposition 3.3(ii)). The DT of ${}_HV$ and ${}_HQT$ is the same for all geometric crystal classes in the same family.

We are mainly interested in the decomposability of ${}_HQT$, although we shall also use that of ${}_HV$. The decomposability of ${}_HT$ is much harder to analyse as ${}_HT$ lacks complete reducibility and the unique decomposition property. Also, ${}_HT$ has a lower occurrence of decomposability e.g. for n = 3, ${}_HQT$ is decomposable for 27 of the 32 geometric crystal classes. Of the 58 arithmetic crystal classes belonging to these 27, ${}_HT$ is decomposable for 39.

The decomposability of ${}_HQT$ and ${}_HV$ for n = 2,3,4, where the geometric classes are known, is summarised in the following table. The last row (n = 4) uses the list of geometric crystal classes in 4 dimensions given in [3] and also some of our later results.

| n | Number of Geometric Crystal Classes in Total. | Number of Geometric Crystal Classes for which ${}_HQT$ is Decomposable. | Number of Geometric Crystal Classes for which ${}_HV$ is Decomposable. |
|---|---|---|---|
| 2 | 10 | 4 | 4 |
| 3 | 32 | 27 | 27 |
| 4 | 227 | 153 | 161 |

In the next section we discuss the implications of the difference between the last two numbers in the table.

## 3.2. Some Results on the Relationship Between the Decomposability of ${}_HQT$ and ${}_HV$.

Whenever ${}_HQT$ is decomposable, we may regard H as a subgroup of the product of lower dimensional crystallographic point groups, by Proposition 3.1(ii) - hence H is, in a sense, not a new crystallographic point group. However, ${}_H QT$ is in general not an absolutely irreducible QH-module and there are crystallographic point groups H for which ${}_H V$ is decomposable but ${}_H QT$ is not. We shall see that the first of these occur for $n = 4$. Although we may regard H in these cases as a subgroup of the product of lower dimensional groups, not all of these are crystallographic point groups, as we now show.

Proposition 3.5. Let H be a crystallographic point group acting on T. Suppose ${}_H V = V_1 \oplus \ldots \oplus V_k$ where for $1 \leq i \leq k$, $\dim V_i = n_i$. If $H|_{V_i}$ is a crystallographic point group in $V_i$ for each i, then ${}_H QT$ has a decomposition with dimensions $(n_1, \ldots, n_k)$.

Proof. For each i, let $T_i$ be a lattice of rank $n_i$ in $V_i$ on which $H|_{V_i}$ acts. Let T' be the lattice generated by $\{T_i : 1 \leq i \leq k\}$. Then T' is of rank n, ${}_H T' = T_1 \oplus \ldots \oplus T_k$ and ${}_H QT' = QT_1 \oplus \ldots \oplus QT_k$. However, (H, T) and (H, T') are geometrically equivalent and Proposition 3.3(ii) gives the result.

Terminology. Suppose $\varphi \in GL(V)$. Then $\varphi$ extends to a map $\varphi^C$ in $GL(V + iV)$, where $\varphi^C(x + iy) = \varphi x + i\,\varphi y$. If $\lambda$ is a non-real eigenvalue of $\varphi^C$ and $x_0 + iy_0$ a corresponding eigenvector, then $x_0$ and $y_0$ span a 2-dimensional subspace of V left invariant by $\varphi$. We call the sum of such subspaces over all eigenvectors of $\lambda$, the eigenspace of $\lambda$ in V. This is the same as the eigenspace of the complex conjugate of $\lambda$. If $\lambda$ is a real eigenvalue then, as usual, the eigenspace of $\lambda$ is $\mathrm{Ker}(\varphi - \lambda\iota)$.

The following lemma is a consequence of the Spectral Theorem for normal operators.

Lemma 3.6. ([7; §81, p.162]). Let $\theta \in O(V)$. Then the eigenspaces of $\theta$ in V are mutually orthogonal and span V.

Proposition 3.7. Let T be a lattice of rank n in V and let $g \in G(T)$. Regard two eigenvalues of g as equivalent if they have the same order. Suppose there are m equivalence classes of eigenvalues, and that the sum of eigenspaces for the $i^{th}$ class is $E_i$. Then rank $(T \cap E_i) = \dim E_i$, $1 \leq i \leq m$.

Proof. By Lemma 3.6, $V = E_1 \oplus \dots \oplus E_m$. Let $\dim E_i = n_i$, $1 \leq i \leq m$. We may assume without loss of generality that $k_1 < k_2 < \dots < k_m$, where $k_i$ is the order of the $i^{th}$ class. Consider $g^{k_1} \in G(T)$. Clearly $(g^{k_1})|_{E_1} = \iota|_{E_1}$ and $(g^{k_1})|_{E_1^\perp}$ fixes no points but 0. There is a set of $n - n_1$ vectors in T whose projections into $E_1^\perp$ form an independent set, otherwise T has rank less than n. Let $\{t_1, \dots, t_{n-n_1}\}$ be such a set. Then $\{(g^{k_1})t_j - t_j :$ $1 \leq j \leq n - n_1\}$ is an independent set in $T \cap E_1^\perp$ since if $\sum_{j=1}^{n-n_1} l_j[(g^{k_1})t_j - t_j] = 0$, then $(g^{k_1})(\sum_{j=1}^{n-n_1} l_j t_j) = \sum_{j=1}^{n-n_1} l_j t_j$, giving $l_j = 0$ all j, since the projection of $\sum_{j=1}^{n-n_1} l_j t_j$ into $E_1^\perp$ must be 0. Consequently, rank $(T \cap E_1^\perp) = \dim E_1^\perp$

There is a set of $n_1$ vectors in T whose projections into $E_1$ are independent. Let $\{s_1,\ldots,s_{n_1}\}$ be such a set. We may write $s_j = f_j + e_j$, where $f_j \in E_1^{\perp}$, $e_j \in E_1$, $1 \leq j \leq n_1$. Choose a basis $v_1,\ldots,v_{n-n_1}$ for $T \cap E_1^{\perp}$ and write $f_j = \sum_{l=1}^{n-n_1} a_{jl}v_l$. Now $(g^{k_1})f_j - f_j = (g^{k_1})s_j - s_j \in T$ and also $(g^{k_1})f_j - f_j = \sum_{l=1}^{n-n_1} a_{jl}[(g^{k_1})v_l - v_l]$. Since each $(g^{k_1})v_l - v_l$ is in T, each $a_{jl}$ is rational. Hence there exist $q_1,\ldots,q_{n_1}$ in $Z \setminus \{0\}$ such that $\{q_1f_1,\ldots,q_{n_1}f_{n_1}\}$ is contained in T, meaning that $\{q_1e_1,\ldots,q_{n_1}e_{n_1}\}$ is an independent set in $T \cap E_1$. Therefore rank$(T \cap E_1)$ = dim $E_1$. Now repeat the argument for $E_2$ and the lattice $T \cap E_1^{\perp}$.

Remarks. (1) If we consider the $E_i$'s to be simply eigenspaces, this result does not hold.

(2) This proposition is the generalization of statements like (in 3 dimensions): "the plane perpendicular to a non-trivial rotation axis contains a lattice of rank 2"; "a mirror plane contains a lattice of rank 2."

Corollary. Suppose ${}_HV = V_1 \oplus V_2$, where (H, T) is a pair. (Recall that in writing ${}_HV = V_1 \oplus V_2$ we assume $V_1, V_2 \neq 0$). If there exists $h \in H$ such that $h|_{V_1}$ has an eigenvalue of order k, whereas $h|_{V_2}$ has no eigenvalue of order k, then ${}_HQT$ is decomposable.

Proof. There exists $t \in T \cap V_1$, $t \neq 0$, by Proposition 3.7. The module $QH\{t\}$ is a non-zero, proper submodule of ${}_HQT$. Hence ${}_HQT$ is reducible and therefore decomposable by complete reducibility (Proposition 3.2(i )).

<u>Theorem 3.8</u>. If (H, T) is a pair and ${}_HV$ has a decomposition with dimensions either

(i) $(n - 1, 1)$, $n \geq 2$

or (ii) $(n - 2, 2)$, <u>n odd</u>, $n \geq 3$,

then ${}_HQT$ is decomposable.

<u>Proof</u>. (i) Let ${}_HV = V_{n-1} \oplus V_1$, $\dim V_{n-1} = n - 1$, $\dim V_1 = 1$.

Let $H_o = \{h \in H : h|_{V_1} = \iota_{V_1}\}$, $H_1 = \{h \in H : h|_{V_1} = -\iota_{V_1}\}$.

Then $H = H_o \cup H_1$. If for all $h \in H_o$, $h|_{V_{n-1}} = \iota_{V_{n-1}}$, and, for all $h \in H_1$, $h|_{V_{n-1}} = -\iota_{V_{n-1}}$, then $H = \{\iota, -\iota\}$ and ${}_HQT$ is clearly decomposable (${}_HQT = Q\{t_1\} \oplus \ldots \oplus Q\{t_n\}$ where $\{t_1, \ldots, t_n\}$ is a basis of T). If this is not true, the Corollary to Proposition 3.7 gives the result.

(ii) Let ${}_HV = V_{n-2} \oplus V_2$, $\dim V_{n-2} = n - 2$, $\dim V_2 = 2$.

Since $n - 2$ is odd, $h|_{V_{n-2}}$ has an eigenvalue 1 or -1 for all $h \in H$. If $H|_{V_2}$ always has real eigenvalues, then $H|_{V_2}$ is of class <u>1</u>, <u>2</u>, <u>m</u> or <u>2mm</u>, ${}_HV_2$ decomposes, and we are in case (i). If, for some $h \in H$, $h|_{V_2}$ has a non-real eigenvalue, use the Corollary to Proposition 3.7.

<u>Remark</u>. It follows immediately that for n = 2, 3 or 5, ${}_HV$ is decomposable $\Leftrightarrow$ ${}_HQT$ is decomposable.

In order to treat the case when ${}_HV$ has a decomposition with dimensions $(n - 2, 2)$, <u>n even</u>, we need to consider a special type of crystallographic point group. Suppose n is even ($n \geq 2$) and $\Theta \in O(V)$ is a transitive symmetry operation, in the sense of Hermann [9; p.140] i.e. the eigenvalues of $\Theta$ are a full set of primitive $k^{th}$ roots of unity, where $\Phi(k) = n$ ( $\Phi(k)$ is the Euler function denoting the number of positive integers less than k but coprime to k). Since $n \geq 2$, all the eigenvalues of $\Theta$ are non-real and we denote them by $e^{i\eta_1}, e^{-i\eta_1}, \ldots, e^{i\eta_{\frac{n}{2}}}, e^{-i\eta_{\frac{n}{2}}}$. The characteristic polynomial of $\Theta$ is $\prod_{j=1}^{\frac{n}{2}} (x - e^{i\eta_j})(x - e^{-i\eta_j})$, the kth cyclotomic polynomial, which has integral coefficients and is irreducible over Q. Choose $t \in V$ such that t has non-zero projection into each of the $\frac{n}{2}$ eigenspaces of $\Theta$ in V. Let W be the linear span of $\{t, \Theta t, \ldots, \Theta^{n-1}t\}$. By Cayley-Hamilton , $\Theta$ satisfies its characteristic equation and hence W is invariant under $\Theta$. It follows that W = V. Therefore $\{t, \Theta t, \ldots, \Theta^{n-1}t\}$ is a basis of V and can be regarded as the basis of a lattice $T_\Theta$ of rank n. Since the characteristic polynomial of $\Theta$ is in $Z[x]$, $\Theta$ acts on $T_\Theta$, as does $H_\Theta = \{\Theta^j : 1 \leq j \leq k\}$. The DT of ${}_{H_\Theta}V$ is (2, 2,...,2) but ${}_{H_\Theta}QT$ is indecomposable, since $\Theta$ cannot act on a lattice of rank less than n, as this would contradict the irreducibility of the $k^{th}$ cyclotomic polynomial over Q.

Let $V_1, \ldots, V_{\frac{n}{2}}$ be the eigenspaces of $\Theta$ and let $x^n + c_{n-1}x^{n-1} + \ldots + c_1 x + 1$ be the $k^{th}$ cyclotomic polynomial. The matrix of $\Theta$ relative to the basis $\{t, \Theta t, \ldots, \Theta^{n-1}t\}$ is

$$A = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 & \overline{1} \\ 1 & 0 & 0 & \ldots & 0 & \overline{c}_1 \\ 0 & 1 & 0 & \ldots & 0 & \overline{c}_2 \\ 0 & 0 & 1 & \ldots & 0 & \overline{c}_3 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 1 & \overline{c}_{n-1} \end{pmatrix} .$$

It is easily shown that:

$$A^{-1} = \begin{pmatrix} \bar{c}_1 & 1 & 0 & \dots & 0 \\ \bar{c}_2 & 0 & 1 & \dots & 0 \\ \bar{c}_3 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ \bar{c}_{n-1} & 0 & 0 & \dots & 1 \\ \bar{1} & 0 & 0 & \dots & 0 \end{pmatrix}.$$

Let $\beta \in GL(V)$ have matrix, relative to the same basis:

$$B = \begin{pmatrix} & & & & 1 \\ & 0 & & 1 & \\ & & \cdot & & \\ & 1 & & 0 & \\ 1 & & & & \end{pmatrix}.$$

Clearly, $\beta$ acts on $T_\Theta$ and $\beta^2 = \iota$. Also,

$$AB = \begin{pmatrix} \bar{1} & 0 & 0 & \dots & 0 \\ \bar{c}_1 & 0 & 0 & \dots & 1 \\ \vdots & \vdots & \vdots & & \vdots \\ \bar{c}_{n-2} & 0 & 1 & \dots & 0 \\ \bar{c}_{n-1} & 1 & 0 & \dots & 0 \end{pmatrix} \quad \text{and}$$

$$BA^{-1} = \begin{pmatrix} \bar{1} & 0 & 0 & \dots & 0 \\ \bar{c}_{n-1} & 0 & 0 & \dots & 1 \\ \vdots & \vdots & \vdots & & \vdots \\ \bar{c}_2 & 0 & 1 & \dots & 0 \\ \bar{c}_1 & 1 & 0 & \dots & 0 \end{pmatrix}.$$

However, the coefficients of the cyclotomic polynomial satisfy $c_{n-m} = c_m$, $m = 1, \dots, \frac{n}{2}$. This is because the product of m primitive $k^{th}$ roots of unity equals the complex conjugate of the product of the complementary n-m primitive $k^{th}$ roots.

Therefore $\Theta\beta = \beta\Theta^{-1}$. It follows that $\Theta(\beta V_j) = \beta V_j$, $1 \le j \le \frac{n}{2}$, since $V_1, \ldots, V_{\frac{n}{2}}$ are also the eigenspaces of $\Theta^{-1}$. Also, since $\Theta^{-1} = \beta^{-1}\Theta\beta = \beta\Theta\beta$, the eigenvalues of $\Theta|_{\beta V_j}$ are the same as those of $\Theta|_{V_j}$. Therefore, $\beta V_j = V_j$, $1 \le j \le \frac{n}{2}$. Moreover, $\beta \in O(V)$, since for $0 \le j, l \le n - 1$,

$$\begin{aligned}\langle\beta\Theta^j t, \beta\Theta^l t\rangle &= \langle\Theta^{n-(j+1)}t, \Theta^{n-(l+1)}t\rangle \\ &= \langle\Theta^{-j}t, \Theta^{-l}t\rangle \\ &= \langle\Theta^l t, \Theta^j t\rangle\end{aligned}$$

and $\{t, \Theta t, \ldots, \Theta^{n-1}t\}$ is a basis of V. Consequently, $\beta \in G(T_\Theta)$. The characteristic polynomial of $\beta$ is $(x-1)^{\frac{n}{2}}(x+1)^{\frac{n}{2}}$, so $\beta$ has all real eigenvalues. If $\beta|_{V_j} = \iota_{V_j}$ or $-\iota_{V_j}$ then $\Theta|_{V_j} = (\Theta^{-1})|_{V_j}$, which contradicts $k > 2$. So $\beta|_{V_j}$ is a reflection for all j.

For a given k with $\Phi(k) = n$ we have established the existence of two geometric crystal classes - that of $(H_\Theta, T_\Theta)$ and that of $(H_{(\Theta,\beta)}, T_\Theta)$, where $H_\Theta \cong Z_k$, $H_{(\Theta,\beta)} \cong D_{2k}$ (the dihedral group of order 2k). We call these the <u>cyclic</u> and <u>dihedral</u> <u>transitive</u> classes of k respectively. For n = 2, there are six such classes, given by k = 3, 4, 6. These are <u>3</u>, <u>3m</u>, <u>4</u>, <u>4mm</u>, <u>6</u> and <u>6mm</u>. For n = 4, there are eight such classes, given by k = 5, 8, 10, 12. For cyclic and dihedral transitive classes, the DT of $_HV$ is (2, 2,...,2), but $_HQT$ is indecomposable.

Note that for a given k, the cyclic and dihedral transitive classes of k belong to the same family, since the discussion above shows that a lattice minimal in the arithmetic class of $(H_\theta, T_\theta)$ is also in the arithmetic class of $(H_{(\theta,\beta)}, T_\theta)$.

<u>Theorem 3.9</u>. Suppose n is even $(n \geq 2)$, $(H, T)$ is a pair and ${}_HV$ has a decomposition with dimensions $(n - 2, 2)$. Then either ${}_HQT$ is decomposable, or $(H, T)$ belongs to a cyclic or dihedral transitive geometric crystal class.

<u>Proof</u>. Suppose ${}_HQT$ is not decomposable. We know ${}_HV = V_{n-2} \oplus V_2$, where $\dim V_{n-2} = n - 2$, $\dim V_2 = 2$. Now ${}_HV_2$ is indecomposable, or Theorem 3.8 produces a contradiction. Also $H|_{V_2}$ has an eigenvalue of highest order $k_1 > 2$. Suppose $h_1 \in H$ is such that $h_1|_{V_2}$ has an eigenvalue of order $k_1$. Suppose for $h_2 \in H$, $h_2|_{V_2}$ has a non-real eigenvalue of order $k_2$. Then $H|_{V_2}$ has an eigenvalue of order $\mathrm{LCM}(k_1, k_2)$, which must equal $k_1$. Hence $(h_2|_{V_2}) = (h_1|_{V_2})^m$ for some $m \in N$, and $(h_2h_1^{-m})|_{V_2} = \iota_{V_2}$. Since ${}_HQT$ is indecomposable, the Corollary to Proposition 3.7 gives $h_2h_1^{-m} = \iota$ and $h_2 = h_1^m$. The cyclic subgroup $H_{(h_1)}$ of H, generated by $h_1$, contains all the elements of H with non-real eigenvalues, again by the Corollary to Proposition 3.7. If $\iota$ and $-\iota$ are the only possible elements of H with real eigenvalues, then $H = H_{(h_1)}$. Now $h_1$ is a sum of transitive parts (any $h \in O(V)$ acting on a lattice is such a sum). Also the restriction of H to each part is in a cyclic transitive class. Proposition 3.5 establishes that $h_1$ has only one transitive part and that $(H, T)$ belongs to the cyclic transitive class of $k_1$.

Suppose there exists $\beta \in H$ such that $\beta \neq \iota$ or $-\iota$ but $\beta$ has some real eigenvalues. Then $\beta$ has all real eigenvalues and, by the Corollary to Proposition 3.7, $\beta|V_2$ must be a reflection, giving $(\beta|V_2)(h_1|V_2)(\beta|V_2) = (h_1|V_2)^{-1}$. It follows that $h_1$ and $\beta$ generate H and that $\beta$ leaves invariant the eigenspaces of $h_1|V_{n-2}$. If W is such an eigenspace with eigenvalues $e^{i\eta}$, $e^{-i\eta}$, and $w \in W$, $w \neq 0$, then the linear span of $\{w, h_1w\}$ is invariant under $h_1$, since there exists $x \in V$ such that $w + ix$ is in the complex eigenspace of $e^{i\eta}$. Choose w such that $\beta w = w$ or $-w$. Then $\beta h_1 w = (h_1)^{-1}\beta w = \pm (h_1^{-1}) w$, which is in the span of $\{w, h_1w\}$, since $(h_1)^{-1} = h_1^{(k_1 - 1)}$. Therefore the 2-dimensional span of $\{w, h_1w\}$ is invariant under $\beta$. In this way we can write W as an orthogonal sum of 2-dimensional subspaces invariant under H. The restriction of $\beta$ to each must be a reflection. Now $h_1$ is a sum of transitive parts, to each of which the restriction of H is in a dihedral transitive class. Application of Proposition 3.5 now completes the proof.

<u>Remark</u>. In any even dimension n, the number of families corresponding to cyclic and dihedral transitive classes is equal to the number of <u>even</u> integers k for which $\Phi(k) = n$. This is because for k odd, the corresponding $H_\theta$ or $H_{(\theta,\beta)}$ does not contain $-\iota$, and the classes of k are in the same family as those of 2k (for k odd, $\Phi(k) = \Phi(2k)$). It is easily checked that distinct even integers k with $\Phi(k) = n$ give distinct families, using Proposition 3.4 and properties of the Euler function.

Theorems 3.8 and 3.9 give:

Proposition 3.10. (i) In dimensions 2, 3, and 5,

$_HV$ is decomposable $\Leftrightarrow$ $_HQT$ is decomposable.

(ii) In dimension 4, there are 8 geometric crystal classes for which $_HV$ is decomposable but $_HQT$ is not. These are the cyclic and dihedral transitive classes of 5, 8, 10, 12. They determine 3 families.

(iii) In dimension 6, there are at least 8 geometric crystal classes for which $_HV$ is decomposable but $_HQT$ is not. These are the cyclic and dihedral transitive classes of 7, 9, 14 and 18. They determine 2 families. The only other possibilities are when $_HV$ has DT = (3, 3).

Problem. Are there in fact any crystallographic point groups in dimension 6 for which $_HV$ has DT = (3, 3) but $_HQT$ is indecomposable? Suppose $_HV = V_1 \oplus V_2$ is complete, corresponding to such a situation. Then by Proposition 3.5 and the Corollary to Proposition 3.7, $H|_{V_1}$ and $H|_{V_2}$ are both in the class 53 or are both in the class 53m.

Remark. Similar statements to those in Proposition 3.10 are clearly possible in higher dimensions, but more problem cases such as (3, 3) arise. For n = 7, DT = (4, 3) is the only problem case. For n = 8, there are 10 transitive cyclic and dihedral classes (8 = $\Phi(15)$ = = $\Phi(16)$ = $\Phi(20)$ = $\Phi(24)$ = $\Phi(30)$) belonging to 4 families. The problem cases are DT = (5, 3) and (4, 4). For n = 9, the problem cases are DT = (6, 3), (3, 3, 3) and (5, 4). For n = 10, there are 4 transitive cyclic and dihedral classes ($10 = \Phi(11) = \Phi(22)$) belonging to 1 family. The problem cases are DT = (7, 3), (6, 4), (5, 5) and (4, 3, 3).

Conjecture. There are geometric classes other than cyclic and dihedral transitive ones for which ${}_HV$ is decomposable but ${}_HQT$ is not.

## 3.3. Typically Orthogonal Decompositions.

Proposition 3.11. Let H be a crystallographic point group. If ${}_HV = V_1 \oplus \dots \oplus V_k$ then there exists $\varphi \in C(H, GL(V))$ such that ${}_HV = \varphi V_1 \oplus \dots \oplus \varphi V_k$ is an orthogonal decomposition (i.e. one in which the summands are mutually orthogonal).

Proof. Choose a basis $\{v_1, \dots, v_n\}$ of V adapted to $V_1, \dots, V_k$, such that the included basis of each $V_i$ is orthonormal. Then the matrix of any $h \in H$ relative to this basis is an orthogonal matrix. Let $\varphi$ be any map taking $\{v_1, \dots, v_n\}$ to an orthonormal basis of V. Without loss of generality, we may assume $\varphi \in Pos(V)$. Clearly $\varphi H \varphi^{-1} \subseteq O(V)$, and by Proposition 2.4, $\varphi \in C(H, Pos(V))$.

This illustrates that orthogonality is not in itself a special property for decompositions. The important property is:

Definition. A decomposition ${}_HV = V_1 \oplus \dots \oplus V_k$ is typically orthogonal if for all $\varphi$ in GL(V) with $\varphi H \varphi^{-1} \subseteq O(V)$, the decomposition ${}_{\varphi H \varphi^{-1}}V = \varphi V_1 \oplus \dots \oplus \varphi V_k$ is orthogonal.

In other words, the decomposition is forced to be orthogonal by the geometric nature of H.

Example. Let $n = 3$, T be triclinic, $H = G(T) = \underline{\bar{1}}$. No decomposition of ${}_HV$ is typically orthogonal, but there are orthogonal decompositions. If T is orthorhombic and $H = G(T) = \underline{mmm}$, all decompositions of ${}_HV$ are typically orthogonal.

We say that a decomposition of ${}_HQT$ is typically orthogonal if it produces a typically orthogonal decomposition of ${}_HV$ (by multiplying through the decomposition by R).

Definition. A decomposition of ${}_HV$ (respectively ${}_HQT$) is a complete typically orthogonal decomposition if it is typically orthogonal but cannot be further reduced to a typically orthogonal decomposition of ${}_HV$ (respectively ${}_HQT$).

Using the Krull-Schmidt property (Proposition 3.2(ii)) it is easy to show that any complete decomposition can be "built up" to a complete typically orthogonal decomposition.

Proposition 3.12. The modules ${}_HV$ and ${}_HQT$ each have a unique complete typically orthogonal decomposition (up to the order of the summands).

Proof. We prove the proposition for ${}_HV$ - the proof for ${}_HQT$ is similar.

Let ${}_HV = V_1 \oplus \dots \oplus V_k$ and ${}_HV = W_1 \oplus \dots \oplus W_m$ be two such decompositions. For $1 \leq i \leq k$, define $\varphi_i \in GL(V)$ by $\varphi_i|_{V_i} = 2(\iota_{V_i})$, $\varphi_i|_{V_j} = \iota_{V_j}$, $i \neq j$. Then $\varphi_i \in C(H, Pos(V))$ and ${}_HV = \varphi_i W_1 \oplus \dots \oplus \varphi_i W_m$ is orthogonal. Suppose $w_l \in W_l$, $w_j \in W_j$, $l \neq j$. Then

$\langle w_l, w_j \rangle = 0 = \langle \varphi_i w_l, \varphi_i w_j \rangle$. However, $\varphi_i$ is symmetric, so $\langle w_l, (\varphi_i)^2 w_j \rangle = 0$. This implies that $\varphi_i^2$ leaves each $W_j$ invariant and so does its positive square root $\varphi_i$.

For $w_j \in W_j$, $\varphi_i(w_j) - w_j \in W_j$. But $\varphi_i(w_j) - w_j = \pi_i(w_j)$, where $\pi_i: V \to V_i$ is the projection map. Therefore $\pi_i(w_j) \in V_i \cap W_j$ and $W_j = \bigoplus_{i=1}^{k} (V_i \cap W_j)$. This induces a further reduction of the complete typically orthogonal decomposition $V = \bigoplus_{j=1}^{m} W_j$, so we conclude at most one $V_i \cap W_j$ is non-zero, and $W_j \subseteq V_i$, some i. By a dimension argument, uniqueness (up to the order of the summands) follows.

This shows that there is a well-defined typically orthogonal decomposition type (abbreviated ODT) for $_H V$ and $_H QT$. This is clearly the same for all pairs (H, T) in the same geometric crystal class. Also, it is the same for all geometric classes in a family by the following.

<u>Proposition 3.13</u>. Let T be a minimal lattice in the arithmetic crystal class of (H, T). Then:

(i) $_H V = V_1 \oplus \dots \oplus V_k$ is a complete typically orthogonal decomposition if and only if $_{G(T)} V = V_1 \oplus \dots \oplus V_k$ is;

(ii) $_H QT = QT_1 \oplus \dots \oplus QT_k$ is a complete typically orthogonal decomposition if and only if $_{G(T)} QT = QT_1 \oplus \dots \oplus QT_k$ is.

<u>Proof</u>. By Lemma 2.9, C(H, Pos(V)) = C(G(T), Pos(V)). Using the polar decomposition and Proposition 2.4, we may

deduce that $\varphi H\varphi^{-1} \subseteq O(V)$ if and only if $\varphi G(T)\varphi^{-1} \subseteq O(V)$. The decompositions ${}_{G(T)}V = V_1 \oplus \dots \oplus V_k$ and ${}_{G(T)}QT = QT_1 \oplus \dots \oplus QT_k$ are both valid decompositions, by Proposition 3.4. The result now follows.

<u>Proposition 3.14</u>. (i) Suppose ${}_HV = V_1 \oplus \dots \oplus V_k$ is complete and for some $h \in H$, $h|_{V_i}$ has an eigenvalue $\lambda$ whereas $h|_{V_j}$ has no eigenvalue $\lambda$. Then for all $\varphi \in GL(V)$ such that $\varphi H\varphi^{-1} \subset O(V)$, $\varphi V_i$ is orthogonal to $\varphi V_j$.
(ii) Suppose ${}_HQT = QT_1 \oplus \dots \oplus QT_k$ is complete and for some $h \in H$, $h|_{RT_i}$ has an eigenvalue of order k whereas $h|_{RT_j}$ has no eigenvalue of order k. Then for all $\varphi \in GL(V)$ such that $\varphi H\varphi^{-1} \subset O(V)$, $\varphi(RT_i)$ is orthogonal to $\varphi(RT_j)$.
<u>Proof</u>. (i) Any vector v in $V_i$ in the eigenspace of $\lambda$ is orthogonal to $V_j$, by Lemma 3.6. Since $H \subset O(V)$ and ${}_HV_i$ is irreducible, it follows that $V_i$ is orthogonal to $V_j$. The same argument applies to $\varphi V_i$, $\varphi V_j$ and $\varphi H\varphi^{-1}$.
(ii) A similar argument applies, using Lemma 3.6 and Proposition 3.7.

<u>Theorem 3.15.</u> Any complete decomposition of ${}_HV$ or ${}_HQT$ is typically orthogonal if it has dimensions either

(i) $(n - 1, 1)$, $n \geq 3$;

or (ii) $(n - 2, 2)$, $n \geq 3$, $n \neq 4$.

<u>Proof</u>. <u>(i) for all n and (ii) for n odd</u>.

Use Proposition 3.14 and arguments similar to those in the proof of Theorem 3.8.

<u>(ii) for n even</u>. If we assume the decomposition is not typically orthogonal, then using Proposition 3.14 and similar arguments to those in Theorem 3.9, we establish

that ${}_HV$ (or ${}_HQT$) has DT = (2, 2,...,2). This is a contradiction unless n = 4.

We shall examine some crystallographic point groups for which the DT and ODT differ in Section 3.5, after looking at the relationship between decomposability and centralizers.

## 3.4. Decomposability and the Centralizer.

Theorem 3.16. Let H be a crystallographic point group and suppose ${}_HV$ is indecomposable. If $\varphi \in C(H, GL(V))$ and $\varphi$ has a real eigenvalue, then $\varphi = k\iota$, some $k \neq 0$. If $\varphi$ has a non-real eigenvalue $re^{i\eta}$, then $re^{-i\eta}$ is the only other eigenvalue and the eigenspace of $re^{i\eta}$ and $re^{-i\eta}$ spans V.

In particular, if n is odd, $C(H, GL(V)) = (R^*)\iota$.

For any n, $C(H, Pos(V)) = (R^+)\iota$.

Proof. Suppose $\varphi$ has a real eigenvalue k with $\varphi x = kx$, $x \neq 0$. Since ${}_HV$ is irreducible, the orbit Hx spans V. However, for all $h \in H$, $\varphi(hx) = h\varphi x = k(hx)$. It follows that $\varphi = k\iota$.

If $\varphi$ has a non-real eigenvalue $re^{i\eta}$ with $x + iy \in V + iV$ such that $\varphi^C(x+iy) = re^{i\eta}(x + iy)$, then $\varphi^C(x - iy) = re^{-i\eta}(x - iy)$. Also, $\varphi^C = r(e^{i\eta})\iota$ on $CH^C\{x + iy\}$ and $\varphi^C = r(e^{-i\eta})\iota$ on $CH^C\{x - iy\}$. Now $2x \in V$ and ${}_HV$ is irreducible, so $V + iV = CH^C\{2x\} = CH^C\{x + iy\} + CH^C\{x - iy\}$. The result follows.

If ${}_HV = V_1 \oplus \dots \oplus V_k$, then the external direct product $\prod_{i=1}^{k} GL(V_i)$ is easily identified with the subgroup of $GL(V)$ consisting of those transformations which leave each $V_i$ invariant. The isomorphism (which is also a homeomorphism) takes $(\varphi_1, \ldots, \varphi_k)$ to $\varphi$ where $\varphi(v_1 + \ldots + v_k) = \varphi_1 v_1 + \ldots + \varphi_k v_k$ and its inverse takes $\varphi$ to $(\varphi|_{V_1}, \ldots, \varphi|_{V_k})$.

Proposition 3.17. The product $\prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$ is a closed subgroup of $C(H, GL(V))$. The coset space

$$C(H, GL(V)) \Big/ \prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$$

is in one-to-one correspondence with the distinct decompositions ${}_HV = \varphi V_1 \oplus \ldots \oplus \varphi V_k$ produced from ${}_HV = V_1 \oplus \ldots \oplus V_k$ by elements $\varphi$ in $C(H, GL(V))$, where the order of the summands is considered.

Proof. The product $\prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$ is clearly a subgroup of $C(H, GL(V))$. Also,

$$\prod_{i=1}^{k} C(H|_{V_i}, GL(V_i)) = C(H, GL(V)) \cap \prod_{i=1}^{k} GL(V_i)$$

since each $h \in H$ is uniquely expressible in the form $(h_1, \ldots, h_k)$. Since $\prod_{i=1}^{k} GL(V_i)$ is closed in $GL(V)$, $\prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$ is closed in $C(H, GL(V))$.

If $\varphi, \psi \in C(H, GL(V))$, then $\varphi, \psi$ produce the same decomposition if and only if

$$\varphi V_i = \psi V_i, \ 1 \leq i \leq k$$

$$\Leftrightarrow \ \varphi^{-1}\psi V_i = V_i, \ 1 \leq i \leq k$$

$$\Leftrightarrow \ \varphi^{-1}\psi \in \prod_{i=1}^{k} GL(V_i)$$

$$\Leftrightarrow \ \varphi^{-1}\psi \in \prod_{i=1}^{k} C(H|_{V_i}, GL(V_i)) .$$

When the number of distinct decompositions produced by elements of $C(H, GL(V))$ is finite, $C(H, GL(V))$ is a finite union of open and closed cosets. We now give necessary and sufficient conditions for this.

Theorem 3.18. For a decomposition ${}_HV = V_1 \oplus \dots \oplus V_k$ the following are equivalent:

(1) ${}_HV = V_1 \oplus \dots \oplus V_k$ is typically orthogonal;

(2) $C(H, GL(V)) \Big/ \prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$ is finite;

(3) $C(H, GL(V)) \Big/ \prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$ has dimension 0;

(4) $C(H, Pos(V)) = \prod_{i=1}^{k} C(H|_{V_i}, Pos(V_i))$

(not a product of groups)

(5) $\dim C(H, Pos(V)) = \sum_{i=1}^{k} \dim C(H|_{V_i}, Pos(V_i))$.

Proof. (1) ⟹ (2). Reduce the decomposition in (1) to a complete typically orthogonal decomposition. By the uniqueness of this (up to the order of the summands), an element of $C(H, GL(V))$ can only permute the summands. Now use Proposition 3.17.

(2) ⟹ (3). Obvious.

(3) ⟹ (1). Suppose (1) is not true. Then if ${}_HV = V_1 \oplus \dots \oplus V_k$ is orthogonal, there exists $\varphi \in GL(V)$ such that $\varphi H \varphi^{-1} \subset O(V)$ and ${}_{\varphi H \varphi^{-1}}V = \varphi V_1 \oplus \dots \oplus \varphi V_k$ is not orthogonal. Taking p to be the positive definite symmetric part of $\varphi$, we deduce that $p \in C(H, Pos(V))$ and ${}_HV = pV_1 \oplus \dots \oplus pV_k$ is not orthogonal. If

${}_HV = V_1 \oplus \ldots \oplus V_k$ is not orthogonal we similarly can find $p \in C(H, Pos(V))$ such that ${}_HV = pV_1 \oplus \ldots \oplus pV_k$ is orthogonal by Proposition 3.11. In either case $p \notin \prod_{i=1}^{k} GL(V_i)$. Now the dimension of

$$C(H, GL(V)) \Big/ \prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$$

equals the dimension of the vector space

$$C(H, L(V)) \Big/ \bigoplus_{i=1}^{k} C(H|_{V_i}, L(V_i))$$

where $L(V)$ is the vector space of all linear transformations of $V$. However, there exists $p$ in $C(H, L(V))$ which is not in $\bigoplus_{i=1}^{k} L(V_i)$ . The result now follows.

<u>(1) $\Rightarrow$ (4)</u>. If (1) holds and $p \in C(H, Pos(V))$ then ${}_HV = pV_1 \oplus \ldots \oplus pV_k$ is orthogonal and $pV_i = V_i$, $1 \leq i \leq k$ (use the same argument as in the proof of Proposition 3.12). Therefore $p \in \prod_{i=1}^{k} GL(V_i)$ and so $p \in \prod_{i=1}^{k} C(H|_{V_i}, Pos(V_i))$.

The reverse inclusion is obvious.

<u>(4) $\Rightarrow$ (5)</u>. Obvious.

<u>(5) $\Rightarrow$ (1)</u>. Suppose (1) is not true. By the construction in Proposition 3.11 we obtain $\delta \in C(H, Pos(V))$ such that ${}_HV = \delta V_1 \oplus \ldots \oplus \delta V_k$ is orthogonal. Clearly $\dim C(H|_{V_i}, Pos(V_i)) = \dim C(H|_{\delta V_i}, Pos(\delta V_i))$, since conjugation by $\delta$ gives a homeomorphism. However, ${}_HV = \delta V_1 \oplus \ldots \oplus \delta V_k$ is not typically orthogonal, so there exists $p \in C(H, Pos(V))$ such that ${}_HV = p\delta V_1 + \ldots + p\delta V_k$ is not orthogonal, meaning $p \notin \prod_{i=1}^{k} GL(\delta V_i)$. We conclude that the vector space

$C(H, Sym(V)) \Big/ \bigoplus_{i=1}^{k} C(H|_{V_i}, Sym(V_i))$ is non-zero and hence

$$\dim C(H, Sym(V)) > \sum_{i=1}^{k} \dim C(H|_{\delta V_i}, Sym(V_i)).$$

As remarked in the proof of (1) $\Rightarrow$ (2), an element of C(H, GL(V)) may only permute the summands of a complete typically orthogonal decomposition. In practical cases, the possible permutations are limited by considering eigenvalues, since if $\varphi \in C(H, GL(V))$ and $\varphi V_i = V_j$, then for all $h \in H$, the eigenvalues of $h|_{V_i}$ must equal those of $h|_{V_j}$. A particularly good example of this, when the identity is the only possible permutation is:

<u>Proposition 3.19</u>. Suppose ${}_HV = V_1 \oplus \dots \oplus V_k$ is complete and $H = \prod_{i=1}^{k} H|_{V_i}$, where all the fixed points of H are contained in one $V_i$. Then $C(H, GL(V)) = \prod_{i=1}^{k} C(H|_{V_i}, GL(V_i))$.

<u>Proof</u>. Considering eigenvalues, we see that ${}_HV = V_1 \oplus \dots \oplus V_k$ is a complete typically orthogonal decomposition and elements of C(H, GL(V)) must leave invariant each $V_i$.

In 3 dimensions, the identity is also the only possible permutation that occurs and consequently the centralizers are all a product of lower dimensional ones, except, of course, when ODT = (3). In the following table, the ODT is obtained using Proposition 3.14 (i). The table is included to illustrate the results of this section and for later use. The information it contains does not appear elsewhere in the literature.

Table 3.1. Centralizers of the 3-Dimensional Point Groups.

| Geometric Crystal Class of H | DT of $_H V$ | ODT of $_H V$ | C(H, GL(V) | C(H, Pos(V)) |
|---|---|---|---|---|
| $1, \bar{1}$. | (1,1,1) | (3) | $GL_3$ | Pos(3) |
| $2, m, \frac{2}{m}$. | (1,1,1) | (2,1) | $GL_2 \times GL_1$ | Pos(2) x Pos(1) |
| 222, 2mm, mmm. | (1,1,1) | (1,1,1) | $GL_1 \times GL_1 \times GL_1$ | Pos(1) x Pos(1) x Pos(1) |
| $4, \bar{4}, \frac{4}{m}$. | (2,1) | (2,1) | $(R^*)SO_2 \times GL_1$ | $(R^+)\iota_2 \times Pos(1)$ |
| 422, 4mm, $\bar{4}2m$, $\frac{4}{m}mm$. | (2,1) | (2,1) | $(R^*)\iota_2 \times GL_1$ | $(R^+)\iota_2 \times Pos(1)$ |
| $3, \bar{3}, 6, \bar{6}, \frac{6}{m}$. | (2,1) | (2,1) | $(R^*)SO_2 \times GL_1$ | $(R^+)\iota_2 \times Pos(1)$ |
| 32, 622, 3m, $\bar{3}m$, 6mm, $\bar{6}m2$, $\frac{6}{m}mm$. | (2,1) | (2,1) | $(R^*)\iota_2 \times GL_1$ | $(R^+)\iota_2 \times Pos(1)$ |
| 23, 432, m3, $\bar{4}3m$, m3m. | (3) | (3) | $(R^*)\iota_3$ (Theorem 3.16) | $(R^+)\iota_3$. |

Remark about the Normalizer.

We do not use the normalizer in this work, but it is worth noting how the ideas of this section apply to it. We know that N(H, Pos(V)) = C(H, Pos(V)) (Proposition 2.4) and N(H, GL(V)) is homeomorphic to N(H, O(V)) x C(H, Pos(V)), where the homeomorphism is given by the polar decomposition. It is not generally true that N(H, GL(V)) contains the product $\prod_{i=1}^{k} N(H|_{V_i}, GL(V_i))$ e.g. n = 3 and H is of class $\bar{4}2m$. When it is true we can establish that N(H, GL(V)) is a finite union of open and closed cosets when a decomposition is typically orthogonal. In the case $H = \prod_{i=1}^{k} H_{V_i}$, it is always true that $N(H, GL(V)) \supseteq \prod_{i=1}^{k} N(H|_{V_i}, GL(V_i))$. An example of this is when T is orthorhombic and H = G(T). Then ${}_HV$ has DT = (1,1,1) and ODT = (1,1,1). The normalizer N(H, GL(V)) is a union of six cosets of $GL_1 \times GL_1 \times GL_1$.

## 3.5. Inclined Crystallographic Point Groups.

<u>Definition</u>. A crystallographic point group H is <u>inclined</u> if for one and hence for all pairs (H,T), ${}_HQT$ is decomposable, but the ODT of ${}_HQT$ is (n).

We shall now describe all inclined crystallographic point groups for which the DT of ${}_HQT$ involves only the dimensions 1, 2 and 3. Using Proposition 3.14 and similar arguments to those in the proof of Theorem 3.15, we can deduce that for such groups the DT of ${}_HQT$ must, in fact, involve all 1's or all 2's or all 3's. Also, by Proposition 3.14 (ii), for each $h \in H$ and for each i,j, the orders of the eigenvalues of $h|_{RT_i}$ must be the same as those of $h|_{RT_j}$.

We now look at the possibilities for these groups and use Theorem 3.18 to check which have ODT = (n).

(1) The DT of ${}_{H}QT$ is (1,1,...,1). For each n, there are only two possibilities, $H = \{\iota\}$ and $H = \{\iota, -\iota\}$. Clearly, in each case C(H, Pos(V)) = Pos(V), and Theorem 3.18 ((1) $\Leftrightarrow$ (4)) implies that the ODT is (n), recalling that any complete decomposition can be built up to a complete typically orthogonal one. <u>For each n > 1, this gives two inclined geometric crystal classes for which ${}_{H}QT$ has DT = (1,1,...,1)</u>.

(2) The DT of ${}_{H}QT$ is (2,2,...,2), n is even. Let ${}_{H}QT = QT_1 \oplus \dots \oplus QT_k$ be complete. For any i, ${}_{H}QT_i$ is indecomposable and so $H|_{RT_i}$ is in one of the classes

<u>3</u>, <u>3m</u>, <u>4</u>, <u>4mm</u>, <u>6</u>, <u>6mm</u>. Looking at eigenvalue orders, we see that H is either cyclic of order 3, 4 or 6 or it is generated by an element of order 3, 4 or 6 <u>plus</u> an element whose restriction to each $RT_i$ is a reflection. This gives six possible geometric classes. If H is cyclic of order 3,4 or 6, it has a particularly simple matrix form, and it is not difficult to show that there is an orthonormal basis of V relative to which C(H, Pos(V)) is the set of matrices whose upper triangle has the form:

$$\begin{array}{ccccccc}
a_1 & 0 & b_{12} & c_{12} & \cdots & b_{1m} & c_{1m} \\
 & a_1 & \overline{c_{12}} & b_{12} & & \overline{c_{1m}} & b_{1m} \\
 & & a_2 & 0 & \cdots & b_{2m} & c_{2m} \\
 & & & a_2 & & \overline{c_{2m}} & b_{2m} \\
 & & & & \ddots & \vdots & \\
 & & & & & a_m & 0 \\
 & & & & & & a_m
\end{array}$$

where $m = \frac{n}{2}$ and $a_1, \ldots, a_m$, $b_{ij}$, $c_{ij}$ are arbitrary subject to positive definiteness. If H also contains the "reflection" element, this adds the restriction $c_{ij} = 0$. Using Theorem 3.18 ((1)$\Leftrightarrow$(4)) we conclude that in both cases the ODT of ${}_HQT$ is (n). <u>For n even, n > 2, this gives six inclined geometric crystal classes for which ${}_HQT$ has DT = (2,2,...,2)</u>. In the cyclic case,

$$\dim C(H, \mathrm{Pos}(V)) = \frac{n}{2} + \frac{n}{2}\left(\frac{n}{2} - 1\right) = \frac{n^2}{4}.$$ In the dihedral case, $$\dim C(H, \mathrm{Pos}(V)) = \frac{1}{2}\left(\frac{n}{2}\right)\left(\frac{n}{2} + 1\right) = \frac{n^2}{8} + \frac{n}{4}.$$

(3) The DT of ${}_HQT$ is (3,3,...,3), n a multiple of 3. Let ${}_HQT = QT_1 \oplus \ldots \oplus QT_k$ be complete. For each i, ${}_HQT_i$ is indecomposable and therefore $H|_{RT_i}$ must belong to one of the classes <u>23</u>, <u>m3</u>, <u>432</u>, <u>$\bar{4}$3m</u> or <u>m3m</u>. Looking at eigenvalue orders, it is easily deduced that each $H|_{RT_i}$ is in the same class.

When each $H|_{RT_i}$ is of class <u>23</u>, we can always choose an orthonormal basis of V relative to which H has generators;

$$\begin{pmatrix} \begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix} & & & 0 \\ & \begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix} & & \\ & & \ddots & \\ 0 & & & \begin{matrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{matrix} \end{pmatrix},$$

of order 3, and

$$\begin{pmatrix} 1 & & & & & & & & & \\ & \mathrm{T} & & & & & & & & \\ & & \mathrm{T} & & & & & & & \\ & & & 1 & & & & & & \\ & & & & \mathrm{T} & & & & & \\ & & & & & \mathrm{T} & & & & \\ & & & & & & \ddots & & & \\ & & & & & & & 1 & & \\ & & & & & & & & \mathrm{T} & \\ & & & & & & & & & \mathrm{T} \end{pmatrix}, \text{ of order 2.}$$

This follows from the properties of 23 and from Proposition 3.11. It is clear that all appropriate H are geometrically equivalent. A similar situation occurs when $H|_{RT_i}$ is of class m3. We can show in both cases C(H, Pos(V)) is the set of matrices whose upper triangle has form:

$$\begin{matrix}
a_1 & 0 & 0 & b_{12} & 0 & 0 & & b_{1m} & 0 & 0 \\
 & a_1 & 0 & 0 & b_{12} & 0 & & 0 & b_{1m} & 0 \\
 & & a_1 & 0 & 0 & b_{12} & & 0 & 0 & b_{1m} \\
 & & & a_2 & 0 & 0 & & b_{2m} & 0 & 0 \\
 & & & & a_2 & 0 & & 0 & b_{2m} & 0 \\
 & & & & & a_2 & & 0 & 0 & b_{2m} \\
 & & & & & & \ddots & & \vdots & \\
 & & & & & & & a_m & 0 & 0 \\
 & & & & & & & & a_m & 0 \\
 & & & & & & & & & a_m
\end{matrix}$$

where $m = \frac{n}{3}$ and $a_1,\dots,a_m$, $b_{ij}$ are arbitrary subject to positive definiteness.

When each $H|_{RT_i}$ is of class 432, the situation is more complicated. Consider the case n = 6. Again we can choose an orthonormal basis of V relative to which one generator of H, of order 3, has matrix:

$$\begin{pmatrix} 0 & 0 & 1 & & & \\ 1 & 0 & 0 & & 0 & \\ 0 & 1 & 0 & & & \\ & & & 0 & 0 & 1 \\ & 0 & & 1 & 0 & 0 \\ & & & 0 & 1 & 0 \end{pmatrix}.$$

However, the other generator (of order 4) can be either (a) $\begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & 0 & \bar{1} & & 0 & \\ 0 & 1 & 0 & & & \\ & & & 1 & 0 & 0 \\ & 0 & & 0 & 0 & \bar{1} \\ & & & 0 & 1 & 0 \end{pmatrix}$ or (b) $\begin{pmatrix} 1 & 0 & 0 & & & \\ 0 & 0 & \bar{1} & & 0 & \\ 0 & 1 & 0 & & & \\ & & & 1 & 0 & 0 \\ & 0 & & 0 & 0 & 1 \\ & & & 0 & \bar{1} & 0 \end{pmatrix}$.

The two possibilities for H are not geometrically equivalent. However, for (a), C(H, Pos(V)) has the same form as in the 23 case whereas for (b) $b_{12} = 0$. From Theorem 3.18 we conclude that for (a) the ODT is (6) whereas for (b) it is (3, 3). It is not difficult to see that in higher dimensions also the type (a) generator is the only one giving ODT = (n). The same type of situation occurs for the classes $\bar{4}3m$ and $m3m$. Therefore we get exactly one inclined class for each 3-dimensional indecomposable class. For $n > 3$, n a multiple of 3, there are five inclined geometric crystal classes for which ${}_HQT$ has DT = (3,3,...,3). For each, dim C(H, Pos(V)) $= \frac{1}{2}\left(\frac{n}{3}\right)\left(\frac{n}{3} + 1\right) =$

$$= \frac{n^2}{18} + \frac{n}{6} .$$

# CHAPTER FOUR. THE DECOMPOSITION OF FAMILIES.

Throughout this chapter, when we refer to the DT or ODT of a family we mean the DT or ODT of ${}_{H}QT$ for any pair (H,T) in that family, unless specifically stated otherwise. In fact, we concentrate on pairs of the form (G(T),T).

## 4.1. Distinguishing Between Decomposable Families.

Let ${}_{G(T)}QT = QT_1 \oplus \dots \oplus QT_k$, where $\dim QT_i = n_i$. Then $G(T)|_{RT_i}$ is a crystallographic point group in $RT_i$, determining an $n_i$-dimensional crystal family $F_i$. Associated with the decomposition we have a k-tuple of families $(F_1,\dots,F_k)$. If T is minimal in the arithmetic class of (H,T), then $H|_{RT_i}$ also determines the family $F_i$, since C(G(T), Pos(V)) = C(H, Pos(V)) by Lemma 2.9 and hence $C(G(T)|_{RT_i}, \mathrm{Pos}(RT_i)) = C(H|_{RT_i}, \mathrm{Pos}(RT_i))$.

Theorem 4.1. (i). If ${}_{G(T)}QT = QT_1 \oplus \dots \oplus QT_k$ and ${}_{G(T')}QT' = QT_1' \oplus \dots \oplus QT_k'$ are:(a) complete; or (b) complete typically orthogonal; where T and T' are lattices in the same family, then the associated k-tuples $(F_1,\dots,F_k)$ and $(F_1',\dots,F_k')$ are identical, up to possible variation in order.

(ii). If ${}_{G(T)}QT = QT_1 \oplus \dots \oplus QT_k$ and ${}_{G(T')}QT' = QT_1' \oplus \dots \oplus QT_k'$ are typically orthogonal and the k-tuples of families $(F_1,\dots,F_k)$ and $(F_1',\dots,F_k')$ are identical, up to possible variation in order, then T and T' are in the same family.

<u>Remark</u>. Part (i) is not true for arbitrary typically orthogonal decompositions. Part (ii) is not true for arbitrary complete decompositions. e.g. let n = 2, T be of class $\underline{P}$ and T' be of class $\underline{R}$.

<u>Proof</u>. (i) (a). Suppose that T is minimal in the arithmetic class of (H,T). Then ${}_HQT = QT_1 \oplus \dots \oplus QT_k$ is complete by Proposition 3.4. Moreover, $H|_{RT_i}$ determines the same family as $G(T)|_{RT_i}$. Now T and T' are related by a finite chain of equivalences and through these the decomposition ${}_{G(T)}QT = QT_1 \oplus \dots \oplus QT_k$ induces a complete decomposition of ${}_{G(T')}QT'$ with k-tuple $(F_1,\dots,F_k)$. By the Krull-Schmidt property, the result follows.

(b). The proof is similar, using Propositions 3.13 and 3.12 in that order.

(ii). Let $S_1$ be the lattice generated by $T_1,\dots,T_k$. Then ${}_{G(T)}S_1 = T_1 \oplus \dots \oplus T_k$. Let S be a minimal lattice in the arithmetic class of $(G(T),S_1)$. Then there exists $\varphi$ in GL(V) with $\varphi S_1 = S$, $\varphi G(T)\varphi^{-1} = H \subseteq G(S)$, $\varphi G(S_1)\varphi^{-1} \supseteq G(S)$. The decomposition ${}_HS = \varphi T_1 \oplus \dots \oplus \varphi T_k$ must be orthogonal. Moreover, since S is minimal in the arithmetic class of (H,S), ${}_{G(S)}S = \varphi T_1 \oplus \dots \oplus \varphi T_k$ by Proposition 3.4. We can now deduce that $G(S) = \prod_{i=1}^{k} G(\varphi T_i)$. Similarly, we may construct S' from T', where

$G(S')^{S'} = \varphi' T_1' \oplus \ldots \oplus \varphi' T_k'$ is orthogonal and $G(S') = \prod_{i=1}^{k} G(\varphi' T_i')$. Clearly S is in the same family as T and S' is in the same family as T'. We now show that S and S' are in the same family. We may assume without loss of generality that $R(\varphi T_i) = R(\varphi' T_i')$ and that $\varphi T_i$ and $\varphi' T_i'$ are in the same family - otherwise reorder the $T_i'$ and take $\theta S'$ for some $\theta \in O(V)$. Now $\varphi T_i$ and $\varphi' T_i'$ are related by a finite chain of equivalences. Consider the first link in such a chain, giving $\varphi T_i$ equivalent to, say, $U_i$, for $1 \leq i \leq k$. We have:

$\varphi T_i$ is minimal in the arithmetic class of $(H_i, \varphi T_i)$;

$U_i$ is minimal in the arithmetic class of $(L_i, U_i)$;

and $(H_i, \varphi T_i)$ is geometrically equivalent to $(L_i, U_i)$. Without loss of generality we may assume that $H_i$ and $L_i$ both contain $-\iota$.

Now S is minimal in the arithmetic class of $(\prod_{i=1}^{k} H_i, S)$, because $(\prod_{i=1}^{k} H_i)^S = \varphi T_1 \oplus \ldots \oplus \varphi T_k$ is typically orthogonal and $G(S) = \prod_{i=1}^{k} G(\varphi T_i)$. Putting $U = U_1 \oplus \ldots \oplus U_k$, we take U' to be minimal in the arithmetic class of $(\prod_{i=1}^{k} L_i, U)$, which is geometrically equivalent to $(\prod_{i=1}^{k} H_i, S)$. Therefore S and U' are in the same family. Treating the other links in the chain of equivalences in the same way, we conclude that S and S' are in the same family. This completes the proof.

## 4.2. The Descendants of One, Two and Three Dimensional Families.

Given a particular DT for ${}_{G(T)}QT$ in n dimensions, involving only the dimensions 1, 2 and 3, we wish to describe all the possible families corresponding to this. Suppose that the DT has $n_1$ 1's, $n_2$ 2's and $n_3$ 3's, meaning $n = n_1 + 2n_2 + 3n_3$. Then for any ${}_{G(T)}QT$ with the given DT, we can show, using Proposition 3.14, that there is a typically orthogonal decomposition ${}_{G(T)}QT = QT_1 \oplus QT_2 \oplus QT_3$, where the DT of ${}_{G(T)}QT_1$ is $(\underbrace{1,1,\ldots,1}_{n_1})$, the DT of ${}_{G(T)}QT_2$ is $(\underbrace{2,2,\ldots,2}_{n_2})$, and the DT of ${}_{G(T)}QT_3$ is $(\underbrace{3,3,\ldots,3}_{n_3})$. Some of the $QT_i$ may be zero. Corresponding to this decomposition there is a 3-tuple of families $(F_1,F_2,F_3)$. Using Theorem 4.1 (for complete typically orthogonal decompositions), it is easily shown that if T' has the same DT as T, but has corresponding 3-tuple $(F_1',F_2',F_3')$, then T and T' are in the same family if and only if $F_i$ and $F_i'$ are the same family for i = 1,2,3. Hence there is a distinct n-dimensional family for each distinct 3-tuple. If $\mathcal{F}^{(i)}(in_i)$ denotes the set of (i,i,...,i) families in dimension $(in_i)$ for i = 1,2,3, then the number of descendants in n dimensions of 1-, 2- and 3-dimensional families is:

$$|\mathcal{F}^{(1,2,3)}(n)| = \sum_{\substack{\text{all partitions}\\ \text{of n into parts}\\ \text{not greater}\\ \text{than 3}}} |\mathcal{F}^{(1)}(n_1)|\,|\mathcal{F}^{(2)}(2n_2)|\,|\mathcal{F}^{(3)}(3n_3)|;$$

where we assume $|\mathcal{F}^{(i)}(0)| = 1$, for the purposes of this formula.

If we can describe the $(i,i,\ldots,i)$ families for $i = 1,2,3$, then we can theoretically describe $\mathfrak{F}^{(1,2,3)}(n)$.

We now do describe all $(i,i,\ldots,i)$ families for $i = 1,2,3$.

## $(1,1,\ldots,1)$.

For any $m > 1$ there are only two inclined geometric crystal classes with DT = $(1,1,\ldots,1)$ in dimension $m$ (see Section 3.5), given by $H = \{\iota\}$ and $\{\iota, -\iota\}$. These clearly belong to the same family. Therefore by Theorem 4.1, there is just one family corresponding to each possible ODT in $n$ dimensions. (The existence of at least one is easily verified). We have:

Proposition 4.2. There are precisely $p(n)$ families in $n$ dimensions with DT = $(1,1,\ldots,1)$, where $p(n)$ is the number of unrestricted partitions of $n$ (i.e. partitions into positive parts, with order irrelevant ). The family corresponding to $n = m_1 + m_2 + \ldots + m_k$ has ODT = $(m_1, m_2, \ldots, m_k)$ and dimension $\left[\sum_{j=1}^{k} \frac{1}{2} m_j (m_j+1)\right] - 1$.

Proof. For the dimension part, use Theorem 3.18.

Remark. The function $p(n)$ is well known, but there is no known explicit expression for $p(n)$ in terms of $n$ ( see [8]). It is worth noting for studying growth in families that

$p(n) \to \frac{e^{K\sqrt{n}}}{4n\sqrt{3}}$ as $n \to \infty$, where $K = \pi(\frac{2}{3})^{\frac{1}{2}}$ (see [1; p.316]).

Hence $\frac{p(n+1)}{p(n)} \longrightarrow 1$ as $n \to \infty$.

If we can describe the $(i,i,\ldots,i)$ families for $i = 1,2,3$, then we can theoretically describe $\mathcal{F}^{(1,2,3)}(n)$.

We now do describe all $(i,i,\ldots,i)$ families for $i = 1,2,3$.

## (1,1,...,1).

For any $m > 1$ there are only two inclined geometric crystal classes with DT = $(1,1,\ldots,1)$ in dimension $m$ (see Section 3.5), given by $H = \{\iota\}$ and $\{\iota, -\iota\}$. These clearly belong to the same family. Therefore by Theorem 4.1, there is just one family corresponding to each possible ODT in $n$ dimensions. (The existence of at least one is easily verified). We have:

Proposition 4.2. There are precisely $p(n)$ families in $n$ dimensions with DT = $(1,1,\ldots,1)$, where $p(n)$ is the number of unrestricted partitions of $n$ (i.e. partitions into positive parts, with order irrelevant ). The family corresponding to $n = m_1 + m_2 + \ldots + m_k$ has ODT = $(m_1,m_2,\ldots,m_k)$ and dimension $\left[\sum_{j=1}^{k} \frac{1}{2}m_j(m_j+1)\right] - 1$.

Proof. For the dimension part, use Theorem 3.18.

Remark. The function $p(n)$ is well known, but there is no known explicit expression for $p(n)$ in terms of $n$ ( see [8]). It is worth noting for studying growth in families that

$p(n) \to \frac{e^{K\sqrt{n}}}{4n\sqrt{3}}$ as $n \to \infty$, where $K = \pi(\frac{2}{3})^{\frac{1}{2}}$ (see [1; p.316]).

Hence $\frac{p(n+1)}{p(n)} \to 1$ as $n \to \infty$.

Table 4.1. Families with DT = (1,1,....,1) up to n = 6.

| n | p(n)= Number of Families | Partition (ODT) | Usual Family Name | Dimension |
|---|---|---|---|---|
| 1 | 1 | 1=1 | Line | 0 |
| 2 | 2 | 2=2 | Parallelogram | 2 |
| | | 2=1+1 | Rectangle | 1 |
| 3 | 3 | 3=3 | Triclinic | 5 |
| | | 3=2+1 | Monoclinic | 3 |
| | | 3=1+1+1 | Orthorhombic | 2 |
| 4 | 5 | 4=4 | Hexaclinic | 9 |
| | | 4=3+1 | Triclinic | 6 |
| | | 4=2+2 | Diclinic | 5 |
| | | 4=2+1+1 | Monoclinic | 4 |
| | | 4=1+1+1+1 | Orthogonal | 3 |
| 5 | 7 | 5=5 | | 14 |
| | | 5=4+1 | | 10 |
| | | 5=3+2 | | 8 |
| | | 5=3+1+1 | | 7 |
| | | 5=2+2+1 | | 6 |
| | | 5=2+1+1+1 | | 5 |
| | | 5=1+1+1+1+1 | | 4 |
| 6 | 11 | 6=6 | | 20 |
| | | 6=5+1 | | 15 |
| | | 6=4+2 | | 12 |
| | | 6=3+3 | | 11 |
| | | 6=4+1+1 | | 11 |
| | | 6=3+2+1 | | 9 |
| | | 6=2+2+2 | | 8 |
| | | 6=3+1+1+1 | | 8 |
| | | 6=2+2+1+1 | | 7 |
| | | 6=2+1+1+1+1 | | 6 |
| | | 6=1+1+1+1+1+1 | | 5 |

Remarks. 1. Distinct ODT may result in the same dimension. The first examples are for $n = 6$.

2. Families with DT = $(1,1,\ldots,1)$ always have dimension larger than $n-1$, since $\left[\sum_{j=1}^{k} \frac{1}{2} m_j(m_j + 1)\right] - 1 = \left[\frac{1}{2}\sum_{j=1}^{k} m_j^2 + \frac{1}{2}\sum_{j=1}^{k} m_j\right] - 1 = \frac{1}{2}\left(\sum_{j=1}^{k} m_j^2\right) + \frac{1}{2}n - 1$, but $\sum_{j=1}^{k} m_j^2 \geq n$. This also shows that the lowest dimensional $(1,1,\ldots,1)$ family is the orthogonal one, with ODT = $(1,1,\ldots,1)$ and dimension $n-1$.

3. The highest dimensional family of all families is the $(1,1,\ldots,1)$ family with ODT = $(n)$. The next highest $(1,1,\ldots,1)$ family has ODT = $(n-1,1)$, since if $n = m_1 + \ldots + m_k$, then $(n-1)^2 + 1 \geq (n-m_1)^2 + m_1^2 \geq \sum_{j=1}^{k} m_j^2$.

## $\underline{(2,2,\ldots,2)}$

Lemma 4.3. For $m$ even, $m > 2$, there are 4 inclined families in $m$ dimensions with DT = $(2,2,\ldots,2)$.

Proof. Consider the six inclined geometric crystal classes with DT = $(2,2,\ldots,2)$ (see Section 3.5). Of the cyclic classes, those of order 3 and 6 are in the same family, since that of order 6 is generated by adding $-\iota$ to that of order 3. Similarly, the two dihedral classes obtained from these by adding the 'reflection' element are in the same family. By looking at dim C(H, Pos(V)), however, (see Section 3.5 again) we see that the cyclic and dihedral classes are in different families, since $\frac{m^2}{4} \neq \frac{m^2}{8} + \frac{m}{4}$ unless $m = 2$. The same applies to the cyclic and dihedral classes of $\underline{4}$ and $\underline{4mm}$. These determine different families from those of $\underline{6}$ and $\underline{6mm}$, by Theorem 4.1 (i). This gives 4 families in all.

Now consider a possible ODT corresponding to DT = (2,2,...,2). In contrast to the (1,1,...,1) case we now have many families associated with this ODT. Suppose the ODT has $q_1$ 2's, $q_2$ 4's and, in general, $q_i$ (2i)'s, for $i = 1,2,\ldots,\frac{n}{2}$, meaning $\sum_i q_i(2i) = n$. If $_{G(T)}QT$ has DT = (2,2,...,2) and the given ODT, then we have a typically orthogonal decomposition $_{G(T)}QT = QT_1 \oplus \cdots \oplus QT_{\frac{n}{2}}$, where $_{G(T)}QT_i$ has DT = (2,2,...,2) and ODT = (2i,2i,...,2i). Some $QT_i$ may be zero. Corresponding to this decomposition there is a $\frac{n}{2}$-tuple of families $(F_1,F_2,\ldots,F_{\frac{n}{2}})$, where some $F_i$ are missing for $n > 2$, namely those corresponding to zero $QT_i$. If $_{G(T')}QT'$ has the same DT and ODT as $_{G(T)}QT$, with $\frac{n}{2}$-tuple $(F_1',\ldots,F_{\frac{n}{2}}')$, then, using Theorem 4.1 for complete typically orthogonal decompositions, we can deduce that T and T' are in the same family if and only if $F_i$ and $F_i'$ are the same family for $i = 1,\ldots,\frac{n}{2}$. So the number of n-dimensional families corresponding to the given ODT is:

$$\prod_{i=1}^{\frac{n}{2}} M^i(q_i),$$

where $M^i(x)$ is the number of (2,2,...,2) families in dimension (2i)x with ODT = (2i,2i,...,2i). Again, existence is easily verified. We define $M^i(0) = 1$.

We introduce the symbol $\Delta^s_{(j_1,\ldots,j_l)}(x)$ to denote the number of partitions of x into s positive parts, $j_1$ of one kind, $j_2$ of another kind, $j_3$ of another kind etc. (order is irrelevant). Using Theorem 4.1 and the fact that there are two 2-dimensional indecomposable families, we deduce that, for $x \neq 0$, $M^1(x) = 2[\Delta^2_{(1,1)}(x) + \Delta^1_{(1)}(x)] + 1[\Delta^2_{(2)}(x)]$. If $i \neq 1$, then by Lemma 4.3 we get, for $x \neq 0$:

$$\begin{aligned}
M^i(x) = 24 &\left[\Delta^4_{(1,1,1,1)}(x) + \Delta^3_{(1,1,1)}(x)\right] \\
&+ 12\left[\Delta^4_{(2,1,1)}(x) + \Delta^3_{(2,1)}(x) + \Delta^2_{(1,1)}(x)\right] \\
&+ 6\left[\Delta^4_{(2,2)}(x) + \Delta^2_{(2)}(x)\right] \\
&+ 4\left[\Delta^4_{(3,1)}(x) + \Delta^3_{(3)}(x) + \Delta^1_{(1)}(x)\right] \\
&+ 1\left[\Delta^4_{(4)}(x)\right].
\end{aligned}$$

Note that this expression is independent of i.

We now have:

<u>Proposition 4.4</u>. In n dimensions (n even), there are

$$\sum_{\substack{\text{unrestricted} \\ \text{partitions} \\ \text{of } \frac{n}{2}}} \left(\prod_{i=1}^{\frac{n}{2}} M^i(q_i)\right)$$

families with DT = (2,2,...,2), where $q_i$ is the number of i's in a given partition and $M^i(q_i)$ is as described above.

<u>Remarks</u>. 1. We could give an explicit expression for the dimensions of the (2,2,...,2) families, but we do

not feel that this is sufficiently enlightening to merit inclusion.

2. Notice that many of the terms in the expression for $M^i(x)$ are zero in low dimensions. Also, $M^1(x)$ is always equal to $x + 1$. Some values of $M^i(x)$, $i \neq 1$, for small $x$ are: $M^i(1) = 4$, $M^i(2) = 10$, $M^i(3) = 20$, $M^i(4) = 35$, $M^i(5) = 56$.

In the following table, we do include the dimensions. The word in brackets after a particular dimension indicates the number of families in that row with that dimension, if there is more than one.

Table 4.2. Families with DT = (2,2,...,2) up to n = 8.

| n | Partition of $\frac{n}{2}$ | ODT | Number of Families Belonging to Partition | Usual Family Names | Dimension |
|---|---|---|---|---|---|
| 2 | 1=1 | (2) | $M^1(1)=2$ | Square | 0 |
| | | | TOTAL=2 | Hexagon | 0 |
| 4 | 2=2 | (4) | $M^2(1)=4$ | Ditetragonal diclinic | 3 |
| | | | | Dihexagonal diclinic | 3 |
| | | | | Ditetragonal monoclinic | 2 |
| | | | | Dihexagonal monoclinic | 2 |
| | 2=1+1 | (2,2) | $M^1(2)=3$ | Ditetragonal orthogonal | 1 |
| | | | | Dihexagonal orthogonal | 1 |
| | | | TOTAL=7 | Hexagonal tetragonal | 1 |

Continued

Table 4.2. Continued.

| n | Partition of $\frac{n}{2}$ | ODT | Number of Families Belonging to Partition | There are no usual family names for $n > 4$ | Dimensions |
|---|---|---|---|---|---|
| 6 | 3=3 | (6) | $M^3(1)=4$ | | 8(two),5(two) |
| | 3=2+1 | (4,2) | $M^1(1)M^2(1)=8$ | | 4(four),3(four) |
| | 3=1+1+1 | (2,2,2) | $M^1(3)=4$ | | 2(four) |
| | | | TOTAL=16 | | |
| 8 | 4=4 | (8) | $M^4(1)=4$ | | 15(two),9(two) |
| | 4=3+1 | (6,2) | $M^1(1)M^3(1)=8$ | | 9(four),6(four) |
| | 4=2+2 | (4,4) | $M^2(2)=10$ | | 7(three),6(four 5(three) |
| | 4=2+1+1 | (4,2,2) | $M^2(1)M^1(2)=12$ | | 4(six),3(six) |
| | 4=1+1+1+1 | (2,2,2,2) | $M^1(4)=5$ | | 3(five) |
| | | | TOTAL=39 | | |

## (3,3,...,3)

Proposition 4.5. For n a multiple of 3, there are precisely $p(\frac{n}{3})$ families with DT = (3,3,...,3) in n dimensions. The family corresponding to $\frac{n}{3} = m_1 + \dots + m_k$ has ODT = $(3m_1,\dots,3m_k)$ and dimension $\left[\sum_{j=1}^{k} \frac{1}{2} m_j(m_j+1)\right] - 1$.

Proof. The five inclined geometric crystal classes with DT = (3,3,...,3) (see Section 3.5) all belong to one family, since each is contained in the class of m3m and C(H, Pos(V)) is the same (up to conjugacy) for each class. Therefore, by Theorem 4.1, there is precisely one family corresponding to each possible ODT. The dimension part follows from Section 3.5 and Theorem 3.18.

Table 4.3. Families with DT = (3,3,...,3) up to n = 9.

| n | $p(\frac{n}{3})$ = Number of Families | Partition of $\frac{n}{3}$ | ODT | Dimension |
|---|---|---|---|---|
| 3 | 1 (Cubic) | 1=1 | (3) | 0 |
| 6 | 2 | 2=2 | (6) | 2 |
| | | 2=1+1 | (3,3) | 1 |
| 9 | 3 | 3=3 | (9) | 5 |
| | | 3=2+1 | (6,3) | 3 |
| | | 3=1+1+1 | (3,3,3) | 2 |

Problem. For which k in general is it likely to be true that the number of (k,k,...,k) families in dimension n (where k divides n) is $p(\frac{n}{k})$ ? Clearly this depends on there being just one inclined (k,k,...,k) family.

The descendants of one, two and three dimensional families up to n = 6 are described in Table 4.4 in the next section. The actual values of $|\mathfrak{F}^{(1,2,3)}(n)|$ for the first eight dimensions are: 1, 4, 6, 17, 24, 58, 84, 178. Our description of $\mathfrak{F}^{(1,2,3)}(n)$ gives at least a lower bound for the total number of families in n dimensions.

We hope that our description can be used to discover the rate of growth of $\mathfrak{F}^{(1,2,3)}(n)$. We conjecture from looking at our results that $\frac{|\mathfrak{F}^{(1,2,3)}(n+1)|}{|\mathfrak{F}^{(1,2,3)}(n)|} \longrightarrow 1$ as $n \to \infty$, so heavily does $\mathfrak{F}^{(1,2,3)}(n)$ depend on partitions.

The main problem in confirming this conjecture (or otherwise) is to see if there exists a lower bound for the number of (2,2,...,2) families corresponding to a given ODT i.e. for $\Pi(M^1(q_1))$.

We wonder if the rate of growth of $\mathfrak{F}^{(1,2,3)}(n)$ matches the rate of growth of all families. A slow rate of growth such as that conjectured would be interesting because estimates for some other quantities in crystallography (see [13;p.31]) are of the form $2^{q(n)}$, where q(n) is a quadratic in n.

## 4.3. Using Decomposition Types to Describe Families in General.

The results of Chapter 3 and Section 4.1 actually allow us to do more than describe $\mathcal{F}^{(1,2,3)}(n)$. Although we do not have enough information to give a complete description of any other descendants, we can make some general observations. We can make deductions about typical orthogonality for some other decomposition types, by virtue of the fact that any indecomposable summand of ${}_{H}QT$ of dimension 1 (respectively 2) is always orthogonal to another summand of dimension other than 1 (respectively 2), using Proposition 3.14 and arguments like those in the proof of Theorem 3.15. In particular, by Theorem 4.1 we have:

Proposition 4.6. If the DT $(m_1,\ldots,m_k)$ has x corresponding n-dimensional families and no $m_i$ is 1, then the DT $(m_1,\ldots,m_k,1)$ has x corresponding (n+1)-dimensional families. If no $m_i$ is 2, then the DT $(m_1,\ldots,m_k,2)$ has 2x corresponding (n+2)-dimensional families.

A general statement about dimension using Proposition 3.11, Theorem 3.16 and Theorem 3.18 is:

<u>Proposition 4.7</u>. If the family F has m parts in its DT, then dim F $\geq$ m - 1.

Theorem 3.8 allows us to decide for some situations whether $_HV$ can be decomposable when $_HQT$ is not.

To illustrate these ideas we now enumerate as far as possible the families up to n = 6. In the following table we denote by $r_n$ the number of families in n dimensions for which $_HV$ is indecomposable i.e. which have dimension 0. We denote by $q_n$ the number of families in n dimensions for which $_HQT$ is indecomposable but $_HV$ is not - these all have dimension larger than 0. The dimensions of families are calculated using Theorem 3.18. Note that this also applies to cyclic and dihedral transitive classes, which always have dimension $\frac{n}{2} - 1$.

Some information in the table duplicates information in Tables 4.1 - 4.3, but this is necessary for completeness.

<u>Note</u>. We could substitute $r_4 = 3$ from the results of Bülow et al. in [3] and hence obtain a complete description of <u>all</u> decomposable families in 5 dimensions. We then can see that there are 30 of these. Since $q_5 = r_5$ (Proposition 3.10) the only other families have dimension 0.

As in Table 4.2 the word in brackets after a particular dimension indicates the number of families in that row with that dimension, if there is more than one.

Table 4.4. Description of Families up to n = 6.

| n | DT | Dimensions of a Typically Orthogonal Decomposition Suitable for all Families with DT | Names and Number of Families | | Dimensions |
|---|---|---|---|---|---|
| 1 | (1) | | See Table 4.1 | 1 | 0 |
| | | | | TOTAL=1 | |
| 2 | (1,1) | | See Table 4.1 | 2 | 2,1 |
| | (2) | | See Table 4.2 | 2 | 0(two) |
| | | | | TOTAL=4 | |
| 3 | (1,1,1) | | See Table 4.1 | 3 | 5,3,2 |
| | (2,1) | (2,1) | Tetragonal, Hexagonal | 2 | 1(two) |
| | (3) | | See Table 4.3 | 1 | 0 |
| | | | | TOTAL=6 | |
| 4 | (1,1,1,1) | | See Table 4.1 | 5 | 9,6,5,4,3 |
| | (2,1,1) | (2,2) | Tetragonal monoclinic, Hexagonal monoclinic, Tetragonal orthogonal, Hexagonal orthogonal | 4 | 3(two), 2(two) |
| | (2,2) | | See Table 4.2 | 7 | 3(two), 2(two), 1(three) |
| | (3,1) | (3,1) | Cubic orthogonal | 1 | 1 |
| | (4) | (4) | Octagonal, Decagonal, Dodecagonal | $q_4=3$ | 1(three) |
| | | | | $r_4$ | 0($r_4$ times) |
| | | | TOTAL=20+$r_4$ | | |

Continued

Table 4.4. Continued.

| n | DT | Dimensions of.. ..with DT | Number of Families | Dimensions |
|---|---|---|---|---|
| 5 | (1,1,1,1,1) | See Table 4.1 .. | 7 | 14,10,8,7,6,5,4 |
| | (2,1,1,1) | (2,3) | 6 | 6(two),4(two),3(two) |
| | (2,2,1) | (4,1) | 7 | 4(two),3(two),2(thre |
| | (3,1,1) | (3,2) | 2 | 3,2 |
| | (3,2) | (3,2) | 2 | 1(two) |
| | (4,1) | (4,1) | $r_4 + 3$ | 2(three),1($r_4$ times) |
| | (5) | (5) | $q_5 = r_5$ | 0($r_5$ times) |
| | | | TOTAL=$27+r_4+r_5$ | |
| 6 | (1,1,1,1,1,1) | See Table 4.1 | 11 | 20,15,12,11(two),9 8(two),7,6,5 |
| | (2,1,1,1,1) | (2,4) | 10 | 10(two),7(two),6(two) 5(two),4(two) |
| | (2,2,1,1) | (4,2) | 14 | 6(two).5(four), 4(five),3(three) |
| | (2,2,2) | See Table 4.2 | 16 | 8(two).5(two), 4(four),3(four), 2(four) |
| | (3,1,1,1) | (3,3) | 3 | 6,4,3 |
| | (3,2,1) | (3,2,1) | 2 | 2(two) |
| | (3,3) | SeeTable 4.3 | 2 | 2,1 |
| | (4,1,1) | (4,2) | $2r_4+6$ | 4(three),3(three+$r_4$), 2($r_4$ times) |
| | (4,2) | (4,2) | $2r_4+6$ | 2(six),0($r_4$ times) |
| | (5,1) | (5,1) | $r_5$ | 1($r_5$ times) |
| | (6) | (6) | $q_6(\geq 2)+r_6$ | 2(two),1($q_6$-2 times), 0($r_6$ times) |
| | | | TOTAL=$70+4r_4+r_5+r_6+q_6$ | |
| | | | where $q_6 \geq 2$ | |

<u>Remarks</u>. In dimension 7, there are 15 possible DT and new unknowns arise for (4,3) and (7) only. This is the first time we get unknowns not of the form $r_n$, $q_n$.

In dimension 8, there are 22 possible DT and new unknowns arise for (4,4), (5,3) and (8).

<u>Idea for Further Study</u>.

Families can be partially ordered according to dimension. However, we feel that this is only a guide to a much more useful ordering, that of 'special case'. e.g. in 3 dimensions, tetragonal is a special case of orthorhombic. This ordering seems likely to lead to useful statements about higher dimensional families.

Not only does dimension give a guide to this ordering, but also the DT and ODT do, and we feel that this is further justification for our emphasis on these.

We consider $F_1$ to be a special case of $F_2$ if every lattice in $F_1$ is a special case of a lattice in $F_2$, but not necessarily vice versa.

<u>Definition</u>. The family $F_1$ is a <u>special case</u> of the family $F_2$ if and only if $\mathcal{L}_n^{F_2}$ is dense in $\mathcal{L}_n^{F_1} \cup \mathcal{L}_n^{F_2}$.

<u>Proposition 4.8</u>. (i). If $F_1$ is a special case of $F_2$ then:

(a) $\dim F_1 < \dim F_2$;

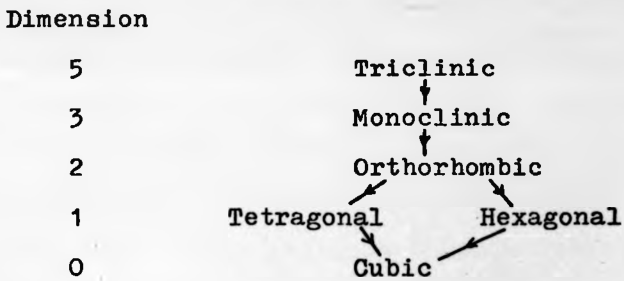
(b) the DT of $F_2$ can be 'built up' to that of $F_1$ by grouping parts.

(ii). If $F_1$ is a special case of $F_2$ and the DT of $F_1$ equals that of $F_2$, then the ODT of $F_1$ can be 'built up' to that of

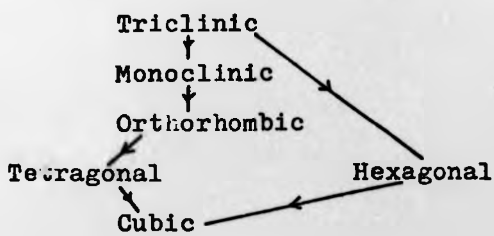
$F_2$ by grouping parts.

Proof. By Theorem 1.7, for any lattice $T_1$ in $F_1$ we may choose $T_2$ in $F_2$ with $G(T_2) \subsetneqq G(T_1)$. Part (i)(b) follows immediately. Part (i)(a) needs Lemma 2.9 also.
Part (ii) is true because a complete typically orthogonal decomposition can always be 'built up' from a complete decomposition.

In 3 dimensions, Proposition 4.8 (i)(b) and (ii) give the same amount of information about possible special cases as that given by (i)(a). The diagram of possible special case relationships which are allowed by Proposition 4.8 is:




The true diagram (see, for example, [12]) is:




In 4 dimensions, the decomposition type conditions actually contribute new information. The (1,1,1,1) family with ODT = (2,2) i.e. diclinic, has dimension 5 but cannot be a special case of the (1,1,1,1) family with ODT = (3,1) i.e. triclinic, of dimension 6, by (ii).

The two (2,1,1) families of dimension 2 cannot be special cases of the two (2,2) families of dimension 3, by (i)(b). The one (3,1) family of dimension 1 cannot be a special case of any of the four (2,2) families of dimension $> 1$, by (i)(b).

The decomposition type conditions are more significant in higher dimensions. This can be seen from looking at Table 4.4, in which it is noticeable that the overlap in dimensions between different decomposition types gets larger as n gets larger.

# CHAPTER FIVE. THE STABILITY OF SYMMETRY IN LATTICE HYPERPLANES.

## 5.1. Preliminaries Concerning Lattice Hyperplanes.

Let V be an n-dimensional real vector space with scalar product and let T be a lattice of rank n in V. We make the following standard definition.

Definition. W is a hyperplane in V if and only if it is of the form $f^{-1}(c)$, where $c \in R$ and f is a non-zero linear functional in V*.

Clearly, W is a hyperplane through 0 if and only if $c = 0$.

For $W = f^{-1}(c)$, we are interested in the set $T \cap W$. Either $T \cap W$ is empty or, for all $t \in T \cap W$, $T \cap W = t + (T \cap f^{-1}(0))$. Therefore we subsequently restrict attention to hyperplanes through 0 and by 'hyperplane' we mean 'hyperplane through 0.'

The following is a standard result, whose proof we omit.

Proposition 5.1 (a). Non-zero linear functionals $f, g \in V^*$ determine the same hyperplane if and only if $f = kg$, for some $k \neq 0$.

Let W be a hyperplane, $W = f^{-1}(0)$. Choose a basis $\{v_1, \ldots, v_n\}$ of V and write f as a matrix $(a_1 a_2 \ldots a_n)$ relative to this basis. We call $(a_1 a_2 \ldots a_n)$ a set of

<u>indices</u> of W relative to $\{v_1,\dots,v_n\}$. Following directly from Proposition 5.1 (a) we get:

<u>Proposition 5.1 (b)</u>. Two sets of indices $(a_1\dots a_n)$ and $(b_1\dots b_n)$ relative to $\{v_1,\dots,v_n\}$ represent the same hyperplane if and only if there exists $k \neq 0$ such that $a_i = kb_i$, for $1 \leq i \leq n$.

<u>Remarks</u>. 1. Under a change of basis represented by a matrix A in GL(n,R), the indices $(a_1\dots a_n)$ transform to the indices $(a_1\dots a_n)A$, relative to the new basis .
2. If W has indices $(a_1\dots a_n)$ relative to $\{v_1,\dots,v_n\}$ and $\varphi \in GL(V)$, then $\varphi W$ has indices $(a_1\dots a_n)$ relative to $\{\varphi v_1,\dots,\varphi v_n\}$.

<u>Theorem 5.2</u>. Let $\mathfrak{L}(T)$ be the collection of all sets of n independent vectors in T and let $\mathcal{J}(T)$ be the subcollection of all bases of T. For a hyperplane W, $T \cap W$ is a lattice of rank m-1, where m is the maximum number of integers in a set of indices of W, taken over all sets in $\mathfrak{L}(T)$. This maximum is equal to that taken over $\mathcal{J}(T)$.
<u>Proof</u>. The set $T \cap W$ is a lattice of rank $\leq n-1$, by Proposition 1.4. Let $\{v_1,\dots,v_n\}$ be a basis of V contained in T and $(a_1\dots a_n)$ a set of indices of W relative to $\{v_1,\dots,v_n\}$ , such that $a_1,\dots,a_m \in Z$, $a_{m+1},\dots,a_n \notin Z$. Not all of $a_1,\dots,a_m$ are zero, so assume without loss of generality that $a_m \neq 0$. For $j = 1,\dots,m-1$, define $w_j \in T \cap W$ by $w_j = (-a_m)v_j + a_jv_m$. The set $\{w_1,\dots,w_{m-1}\}$ is independent, since $\det(w_1,\dots,w_{m-1},v_m) = (-a_m)^{m-1} \neq 0$. Therefore, rank $T \cap W \geq m-1$.

Suppose rank $T \cap W = r$. Let $\{t_1, \ldots, t_r\}$ be a basis for $T \cap W$ and extend it to a basis $\{t_1, \ldots, t_n\}$ of T (see Proposition 1.5). Relative to this basis, W has indices of the form $(0 \ldots 0 b_{r+1} \ldots b_n)$. By taking a suitable multiple we obtain a set of indices, relative to a basis of T, with r+1 integers. The only possibility is that $r = m-1$.

Remark. The maximum number of integers in a set of indices of W, taken over one basis, may be different from that taken over another basis. For example, when $n = 3$, let W have indices $(\sqrt{2}11)$ relative to a lattice basis and change to the basis $\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.

Corollary. The lattice $T \cap W$ has rank n-1 if and only if W has a set of all integer indices relative to one (and hence all) of the sets in $\mathfrak{B}(T)$.

Proof. Note that a change from one set in $\mathfrak{B}(T)$ to another is given by $A \in GL(n, Q)$.

We shall concentrate subsequently on hyperplanes W for which rank $T \cap W = n-1$. We call these rational hyperplanes for T. The lattice $T \cap W$ is called a lattice hyperplane. These terms are consistent with the terms rational plane and lattice plane used by crystallographers in 3 dimensions. For any given set in $\mathfrak{B}(T)$, we always choose the unique integer indices for W for which $HCF(a_1, \ldots, a_n) = 1$ (unique, at least, up to sign).

## 5.2. Description of the Problem in n Dimensions.

In this section we formulate an approach to the problem of stability of symmetry in n dimensions and in Section 5.3 we present the corresponding solution in 3 dimensions.

Small symmetry preserving perturbations of a lattice T are represented by maps $\varphi$ close to $\iota$ in GL(V) for which $G(\varphi T) \geq \psi G(T)\psi^{-1}$, for some $\psi \in GL(V)$. If W is rational for T, then $\varphi W$ is rational for $\varphi T$ and $\varphi T \cap \varphi W = \varphi(T \cap W)$. Since orthogonal maps always preserve the symmetry of $T \cap W$, we restrict attention to $p \in Pos(V)$. In order to compare $G(T \cap W) \subseteq O(W)$ with $G(p(T \cap W)) \subseteq O(pW)$, we can choose any $\theta \in O(V)$ such that $\theta pW = W$ and compare $G(T \cap W)$ with $G(\theta p(T \cap W)) \subseteq O(W)$. In fact, if $\theta$, $\beta \in O(V)$ and $(\theta p)W = (\beta p)W = W$, then

$$\begin{aligned}(\beta p)|_W((\theta p)|_W)^{-1} &= (\beta p)|_W(p^{-1}\theta^{-1})|_W \\ &= (\beta\theta^{-1})|_W \in O(W).\end{aligned}$$

Therefore $(\beta p)|_W$ and $(\theta p)|_W$ have the same positive definite symmetric part, which is of the form $(\gamma p)|_W$ for some $\gamma \in O(V)$. We denote it by $\omega(p) \in Pos(V)$. It is convenient to use this for comparison - we now compare $G(T \cap W)$ with $G((\omega(p))(T \cap W))$. Note that $\omega$ is a continuous function from Pos(V) onto Pos(W) (see Proposition 2.3).

Subsequently we denote $\omega(p)$ by $p^{\omega}$.

<u>Definition</u>. The rational hyperplane W for T is <u>locally stable</u> if and only if there exists $\delta > 0$ such that:

$p \in Pos(V)$, $\| p - \iota \| < \delta$ and $G(pT) \supseteq \psi G(T)\psi^{-1}$, for some $\psi \in GL(V)$

$$\Longrightarrow \quad G(p^{\omega}(T \cap W)) \supseteq \gamma\, G(T \cap W)\gamma^{-1}, \text{ for some } \gamma \in GL(W).$$

By Theorem 1.7 and its Corollary, we obtain an equivalent definition by replacing $\psi$ by $p$, $\gamma$ by $p^{\omega}$ and $\supseteq$ by $=$ . In view of this and Proposition 2.4, the definition becomes:

<u>Definition</u>. The rational hyperplane W for T is <u>locally stable</u> if and only if there exists $\delta > 0$ such that:
$p \in C(G(T), Pos(V))$, $\| p - \iota \| < \delta$

$$\Longrightarrow \quad p^{\omega} \in C(G(T \cap W), Pos(W)).$$

Notice that we are now working in neighbourhoods of T in $\Lambda_n(G(T))$ and $T \cap W$ in $\Lambda_{n-1}(G(T \cap W)$.

We denote $C(G(T), Pos(V))$ by $C(T)$ and $C(G(T \cap W), Pos(W))$ by $C(T \cap W)$ in the sequel. The definition says that W is locally stable if and only if , locally at $\iota$, $\omega^{-1}(C(T \cap W)) \supseteq C(T)$.

<u>Proposition 5.3</u>. (i). If $G(T \cap W) = \{\iota_W, -\iota_W\}$, then W is locally stable.
(ii). If $G(T) = \{\iota, -\iota\}$, W is locally stable if and only if $G(T \cap W) = \{\iota_W, -\iota_W\}$.
(iii). If ${}_{G(T)}V$ is indecomposable, any rational plane W is locally stable.
<u>Proof</u>. (i). $C(T \cap W) = Pos(W)$, so $\omega^{-1}(C(T \cap W)) = Pos(V)$.

(ii). $C(T) = Pos(V)$. However, $\omega^{-1}(C(T\cap W)) = Pos(V)$ if and only if $C(T\cap W) = Pos(W)$, which in turn is true if and only if $G(T\cap W) = \{\iota_W, -\iota_W\}$.

(iii). Use Theorem 3.16 and note $\omega((R^+)\iota) = (R^+)\iota_W$.

We now show that $\omega^{-1}(C(T\cap W)) \supseteq C(T)$ is true globally if it is true locally, meaning that local stablility is equivalent to a type of global stability, in the entire Bravais class of T.

<u>Proposition 5.4</u>. The rational plane W is locally stable for T if and only if, for all $p \in Pos(V)$ with $G(pT) \supseteq pG(T)p^{-1}$, $G(p^{\omega}(T\cap W)) \supseteq G(T\cap W)$.

<u>Proof</u>. <u>If</u>. Obvious.

<u>Only if</u>. Take $p \in Pos(V)$ with $G(pT) \supseteq pG(T)p^{-1}$. Then $p \in C(T)$. Take a, b > 0 such that {eigenvalues of p} $\subset$ [a,b] and {eigenvalues of $p^{\omega}$} $\subset$ [a,b]. For any $\delta > 0$, define $f_\delta : [a,b] \to R^+$ by $f_\delta(s) = (1 + \delta s^2)^{\frac{1}{2}}$. Then $f_\delta$ is a one-to-one function. Let $\{y_1,\ldots,y_n\}$ be an orthonormal basis of V consisting of eigenvectors of p, with corresponding eigenvalues $\lambda_1,\ldots,\lambda_n$. Let $\{x_1,\ldots,x_{n-1}\}$ be an orthonormal basis of W, consisting of eigenvectors of $p^{\omega}$, with corresponding eigenvalues $\mu_1,\ldots,\mu_{n-1}$. Suppose $x_i = \sum_{j=1}^{n} x_{ij}y_j$, for $1 \le i \le n-1$. For $i \ne k$, $\langle px_i, px_k\rangle = 0$, giving $\sum_{j=1}^{n}\lambda_j^2 x_{ij}x_{kj} = 0$. Also, $\mu_i^2 = \langle px_i, px_i\rangle = \sum_{j=1}^{n}\lambda_j^2 x_{ij}^2$.

Now for any $\delta > 0$,

$$\begin{aligned}\langle f_\delta(p)x_i, f_\delta(p)x_k\rangle &= \sum_{j=1}^{n}(1+\delta\lambda_j^2)x_{ij}x_{kj}\\ &= \sum_{j=1}^{n}x_{ij}x_{kj} + \delta\sum_{j=1}^{n}\lambda_j^2 x_{ij}x_{kj}\\ &= \begin{cases}0 & \text{if } i \ne k\\ 1+\delta\mu_i^2 & \text{if } i = k.\end{cases}\end{aligned}$$

Therefore $(f_\delta(p))^\omega$ has eigenvectors $x_1,\ldots,x_{n-1}$ with eigenvalues $(1+\delta\mu_1{}^2)^{\frac{1}{2}},\ldots,(1+\delta\mu_{n-1}{}^2)^{\frac{1}{2}}$. Consequently, $(f_\delta(p))^\omega = f_\delta(p^\omega)$.

For small $\delta$, $f_\delta$ is close to 1 and $f_\delta(p)$ is close to $\iota$ by Proposition 2.1(i). Since $p \in C(T)$, so does $f_\delta(p)$ by Proposition 2.2. By local stability, $(f_\delta(p))^\omega \in C(T\cap W)$ and so $f_\delta(p^\omega) \in C(T\cap W)$. Since $f_\delta$ is invertible, $p^\omega \in C(T\cap W)$ and the result follows.

Using the bijection between unoriented hyperplanes through O in V and $P^{n-1}(R)$, let W correspond to $w \in P^{n-1}(R)$.

<u>Proposition 5.5</u>. Locally at $\iota$, there is a homeomorphism from Pos(V) to Pos(W) x $P^{n-1}(R)$ x $R^+$, carrying $\iota$ to $(\iota, w, 1)$. This restricts to a local homeomorphism from $\omega^{-1}(C(T\cap W))$ to $C(T\cap W)$ x $P^{n-1}(R)$ x $R^+$. In particular, $\omega^{-1}(C(T\cap W))$ is locally at $\iota$ a topological submanifold of Pos(V), of dimension $n + \dim C(T\cap W)$.

<u>Proof</u>. Let $e_n$ be a fixed unit normal to W. Suppose $p \in \text{Pos}(V)$, p is close to $\iota$, and $pW = X$ corresponding to $x \in P^{n-1}(R)$. Let $\{e_1,\ldots,e_{n-1}\}$ be an orthonormal basis of W such that $\{e_1,\ldots,e_{n-2}\} \subset X\cap W$. Let $e_{n+1}$ be the unique vector of unit length in X normal to $\{e_1,\ldots,e_{n-2}\}$ such that $\alpha = \langle e_{n+1}, e_{n-1}\rangle \geq 0$ (uniqueness follows because p is close to $\iota$). Let $\beta = \langle e_{n+1}, e_n\rangle$. Then there exists $\theta \in O(W)$ such that:

$$\theta p^\omega = \left( \left( \begin{array}{ccc|cc} & & & 0 & 0 \\ & I_{n-2} & & \vdots & \vdots \\ & & & 0 & 0 \\ \hline 0 & \cdots & 0 & \alpha & \beta \\ 0 & \cdots & 0 & \bar{\beta} & \alpha \end{array} \right) p \right) \Bigg|_W$$

where the matrix is relative to $\{e_1,\ldots,e_n\}$.

Therefore there exist $c_1, \dots, c_n \in R$ such that:

$$\left(\begin{array}{ccc|cc} & & & 0 & 0 \\ & I_{n-2} & & \vdots & \vdots \\ & & & 0 & 0 \\ \hline 0 & \cdots & 0 & \alpha & \beta \\ 0 & \cdots & 0 & \bar{\beta} & \alpha \end{array}\right) p = \left(\begin{array}{ccc|c} & & & c_1 \\ & \Theta p^{\omega} & & \vdots \\ & & & c_{n-1} \\ \hline 0 & \cdots & 0 & c_n \end{array}\right)$$

giving $p = \left(\begin{array}{ccc|cc} & & & 0 & 0 \\ & I_{n-2} & & \vdots & \vdots \\ & & & 0 & 0 \\ \hline 0 & \cdots & 0 & \alpha & \beta \\ 0 & \cdots & 0 & \beta & \alpha \end{array}\right) \left(\begin{array}{ccc|c} & & & c_1 \\ & \Theta p^{\omega} & & \vdots \\ & & & c_{n-1} \\ \hline 0 & \cdots & 0 & c_n \end{array}\right)$.

It is easily verified that any choice of $\{e_1, \dots, e_{n-1}\}$ produces the same $c_n$. Since $p \in \mathrm{Pos}(V)$, we have : $c_i = \beta\psi_{(n-1)i}$ for $1 \leq i \leq n-2$; $\alpha c_{n-1} = \beta(c_n + \psi_{(n-1)(n-1)})$ and $\Theta \in O(W) \cap A^{-1}(\mathrm{Sym}(W))(p^{\omega})^{-1}$, where $\psi = \Theta p^{\omega}$ and

$$A = \left(\begin{array}{ccc|c} & & & 0 \\ & I_{n-2} & & \vdots \\ & & & 0 \\ \hline 0 & \cdots & 0 & \alpha \end{array}\right).$$

Define $\xi(p)$ to be $(p^{\omega}, x, c_n) \in \mathrm{Pos}(W) \times P^{n-1}(R) \times R^{+}$. Clearly $p^{\omega}$ and $x$ depend continuously on $p$ and it is easily checked that $c_n$ also does. Therefore $\xi$ is continuous. Close to $\iota_W$, $O(W)$ and $\mathrm{Sym}(W)$ intersect only in $\iota_W$ and they intersect transversally. Hence there are open neighbourhoods $U_1$ and $U_2$ of $\iota_W$ in $GL(W)$ such that for $A$, $p^{\omega}$ in $U_1$, $O(W)$ and $A^{-1}(\mathrm{Sym}(W))(p^{\omega})^{-1}$ intersect in just one point in $U_2$. Consequently, $\xi$ is one-to-one on a neighbourhood of $\iota$ in $\mathrm{Pos}(V)$. Since the intersection also depends continuously on $A$ and $p^{\omega}$, $\xi$ must be open on a neighbourhood of $\iota$. The fact that $\xi$ restricts is clear.

<u>Corollary</u>. A necessary condition for $W$ to be stable is $\dim C(T \cap W) \geq \dim C(T) - n$.

This condition is rather weak in 3 dimensions, but is somewhat stronger in higher dimensions (cf. Section 4.3). It is the best general dimensional condition that we can expect, as if $\dim C(T \cap W) = \frac{1}{2}n(n-1)$ and $\dim C(T) = \frac{1}{2}n(n+1)$, then $W$ must be stable by Proposition 5.3 (i).

Even if $W$ is not stable for $T$, we are interested in the set $C(T) \cap \omega^{-1}(C(T \cap W))$. Globally, this is <u>a</u> subset of $C(T)$ on which the symmetry of $T \cap W$ is preserved. Locally at $\iota$, it is <u>the</u> subset of $C(T)$ on which the symmetry of $T \cap W$ is preserved. It always contains $(R^+)\iota$.

<u>We shall show in Section 5.3 that when n = 3 the situation is as follows.</u>

The set $\omega^{-1}(C(T \cap W))$ is locally at $\iota$ a differentiable submanifold of some submanifold $S(T,W)$ of $Pos(V)$ which also contains $C(T)$ ($S(T,W)$ may equal $Pos(V)$). The manifolds $C(T)$ and $\omega^{-1}(C(T \cap W))$ intersect transversally within $S(T,W)$ near $\iota$, meaning that $C(T) \cap \omega^{-1}(C(T \cap W))$ is locally a submanifold of $Pos(V)$ with dimension $d = \dim C(T) + \dim C(T \cap W) + 3 - \dim S(T,W)$, where $\dim S(T,W) \leq m = \text{minimum}\{\frac{1}{2}(3)(3+1), \dim C(T) + \dim C(T \cap W) + 3-1\}$. For a 3-dimensional Bravais class $B_3$ and a 2-dimensional Bravais class $B_2$, if $T \in B_3$ and $T \cap W \in B_2$, the dimension of $S(T,W)$ depends in general not only on $B_3$ and $B_2$, but on the particular position of $W$ in $T$ also. However, except for certain special planes which we shall fully describe in Section 5.3, dim $S(T,W) = m$ and consequently, except for the special planes,

$$d = (\dim \Lambda_n^{B}1) + (\dim \Lambda_n^{B}2) - \tfrac{1}{2}(3)(3-1) \text{ if } m = \tfrac{1}{2}(3)(3+1)$$
$$= 1 \text{ if } m = (\dim \Lambda_n^{B}1) + (\dim \Lambda_n^{B}2) + 3-1.$$

It is reasonable to conjecture that a similar pattern of dimensional relationships occurs in higher dimensions.

## 5.3. The Solution in 3 Dimensions.

In this section we need the following lemma.

Lemma 5.6. Let $T$ be a lattice of rank $n$ in $V$ with basis $\{s_1,\dots,s_n\}$. Let $\{f_1,\dots,f_{n-1}\}$ be a set of lattice vectors, where $f_i = \sum_{j=1}^{n} q_{ij}s_j$ $(q_{ij} \in Z)$. Then $\{f_1,\dots,f_{n-1}\}$ is a primitive set in $T$ if and only if the $n$ determinants

$$\begin{vmatrix} q_{11} & q_{12} & \cdots & \hat{q}_{1j} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & \hat{q}_{2j} & \cdots & q_{2n} \\ \vdots & \vdots & & \vdots & & \vdots \\ q_{(n-1)1} & q_{(n-1)2} & \cdots & \hat{q}_{(n-1)j} & \cdots & q_{(n-1)n} \end{vmatrix} \qquad j = 1,\dots,n$$

have highest common factor 1, where ^ denotes omission.

Proof. The set $\{f_1,\dots,f_{n-1}\}$ is primitive if and only if there exists $f_n \in T$ such that $\{f_1,\dots,f_{n-1},f_n\}$ is a basis of $T$ (Proposition 1.5). However, $\{f_1,\dots,f_n\}$ is a basis if and only if the matrix$(q_{ij})(i,j = 1,\dots,n)$, representing $\{f_1,\dots,f_n\}$ relative to $\{s_1,\dots,s_n\}$, is in $GL(n,Z)$. The result now follows easily from the fact that $\det(q_{ij}) = \pm 1$.

In 3 dimensions, we write indices relative to a set $\{\tau_1, \tau_2, \tau_3\}$ in $\mathcal{B}(T)$, where $\tau_1$, $\tau_2$, $\tau_3$ are shortest lattice vectors in the conventional axes (as described, for example, in [2; p.100 et seq.]). We take $\tau_3$ to be in an axis of highest order and, in the rhombohedral case, further restrict $\tau_1$ and $\tau_2$ by insisting that $\frac{2}{3}\tau_1 + \frac{1}{3}\tau_2 + \frac{1}{3}\tau_3 \in T$. We do not, incidentally, require right-handedness or an ordering on $\tau_1$ and $\tau_2$ determined by their relative lengths. The set $\{\tau_1, \tau_2, \tau_3\}$ need not be a basis of T, nor is it uniquely determined by the above. This non-uniqueness does not affect our results, since any result we give involving explicit plane indices is valid relative to any conventional set. Notice that if T and T' are in the same Bravais class and $\{\tau_1, \tau_2, \tau_3\}$ is a conventional set for T, then $\{\tau_1', \tau_2', \tau_3'\}$ is a conventional set for T' if and only if there exists $\varphi$ in GL(V) such that $\varphi T = T'$, $\varphi G(T)\varphi^{-1} = G(T')$ and $\varphi\tau_i = \tau_i'$ for $1 \leq i \leq 3$. If W has indices $(a_1a_2a_3)$ relative to $\{\tau_1, \tau_2, \tau_3\}$, then $\varphi W$ has indices $(a_1a_2a_3)$ relative to $\{\tau_1', \tau_2', \tau_3'\}$.

Recall that we always take the unique integer indices $(a_1a_2a_3)$ such that $HCF(a_1, a_2, a_3) = 1$.

When V has dimension 3, Pos(V) has dimension 6 and, having chosen an orthonormal basis for V, (we do not use conventional sets at this stage) we may write elements of Pos(V) as matrices $\begin{pmatrix} p_1 & p_4 & p_5 \\ p_4 & p_2 & p_6 \\ p_5 & p_6 & p_3 \end{pmatrix}$ relative to this.

First we look at $\omega^{-1}(C(T \cap W))$ for the five Bravais classes to which the 2-dimensional lattice $T \cap W$ may belong. If $T \cap W$ is of class $\underline{P}$ we know that $\omega^{-1}(C(T \cap W)) = Pos(V)$, since $\omega$

is onto. The remaining classes fall naturally into two groups: (i) $T \cap W$ is of class $\underline{R}$ or $\underline{D}$ and hence $C(T \cap W) = (R^+)\iota_{V_1} \times (R^+)\iota_{V_2}$, where $V_1$ and $V_2$ are orthogonal subspaces containing the mirror lines; (ii) $T \cap W$ is of class $\underline{S}$ or $\underline{H}$, and hence $C(T \cap W) = (R^+)\iota$.

(i). Suppose that $T \cap W$ is of class $\underline{R}$ or $\underline{D}$. Let $v_1 \in V_1$ and $v_2 \in V_2$, $v_1, v_2 \neq 0$. If $\{e_1, e_2, e_3\}$ is our chosen orthonormal basis, let $v_1 = x_1e_1 + y_1e_2 + z_1e_3$, $v_2 = x_2e_1 + y_2e_2 + z_2e_3$. Then a necessary and sufficient condition for $P = \begin{pmatrix} p_1 & p_4 & p_5 \\ p_4 & p_2 & p_6 \\ p_5 & p_6 & p_3 \end{pmatrix}$ to lie in $\omega^{-1}(C(T \cap W))$ is:

$(Pv_1)'(Pv_2) = 0$. This gives the following equation:

$$p_1{}^2(x_1x_2) + p_2{}^2(y_1y_2) + p_3{}^2(z_1z_2) + p_4{}^2(x_1x_2 + y_1y_2) + p_5{}^2(x_1x_2 + z_1z_2) + p_6{}^2(y_1y_2 + z_1z_2) + p_1p_4(x_1y_2 + x_2y_1) + p_1p_5(x_1z_2 + x_2z_1) + p_2p_4(x_1y_2 + x_2y_1) + p_2p_6(y_1z_2 + y_2z_1) + p_3p_5(x_1z_2 + x_2z_1) + p_3p_6(y_1z_2 + y_2z_1) + p_4p_5(y_1z_2 + y_2z_1) + p_4p_6(x_1z_2 + x_2z_1) + p_5p_6(x_1y_2 + x_2y_1) = 0 \tag{1}$$

Regarding this equation as $\alpha(p_1, p_2, p_3, p_4, p_5, p_6) = 0$ ($\alpha : R^6 \rightarrow R$), it is easily verified that:

$$D\alpha_{(1,1,1,0,0,0)} = (2x_1x_2,\ 2y_1y_2,\ 2z_1z_2,\ 2(x_1y_2 + x_2y_1),\ 2(x_1z_2 + x_2z_1),\ 2(y_1z_2 + y_2z_1)),$$

which is non-zero for non-zero $v_1$, $v_2$. Since $D\alpha$ is continuous, locally at $\iota$, $\omega^{-1}(C(T \cap W))$ is a smooth submanifold of Pos(V) of dimension 5.

(ii). Suppose $T \cap W$ is of class $\underline{S}$ or $\underline{H}$. Let W have indices $(c_1 c_2 c_3)$ relative to $\{e_1, e_2, e_3\}$ and suppose that $c_1 \neq 0$. Then $-c_2 e_1 + c_1 e_2$ and $-c_3 e_1 + c_1 e_3$ are independent vectors in W. Normalise these to get $v_1 = x_1 e_1 + y_1 e_2$, $v_2 = x_2 e_1 + z_2 e_3$, where $y_1 \neq 0$ and $z_2 \neq 0$. Now P lies in $\omega^{-1}(C(T \cap W))$ if and only if there exists $\Theta \in O(V)$ and $b \in R^+$ such that $(\Theta P)v_1 = bv_1$, $(\Theta P)v_2 = bv_2$. So necessary and sufficient conditions are:

$$(Pv_1)'(Pv_1) = (Pv_2)'(Pv_2) \qquad (2)$$

$$(Pv_1)'(Pv_2) = (Pv_1)'(Pv_1)v_1'v_2 \qquad (3)$$

Equation (2) gives:

$$p_1^2(x_1^2 - x_2^2) + p_2^2(y_1^2) - p_3^2(z_2^2) + p_4^2(1 - x_2^2) + p_5^2(x_1^2 - 1) + p_6^2(y_1^2 - z_2^2) + p_1p_4(2x_1y_1) - p_1p_5(2x_2z_2) + p_2p_4(2x_1y_1) - p_3p_5(2x_2z_2) - p_4p_6(2x_2z_2) + p_5p_6(2x_1y_1) = 0$$

Regard this as $\beta(p_1, \dots, p_6) = 0$.

Equation (3) gives:

$$p_1^2(x_1y_1^2x_2) - p_2^2(x_1y_1^2x_2) + p_5^2(x_1y_1^2x_2) - p_6^2(x_1y_1^2x_2) + p_1p_4(y_1x_2 - 2x_1^2y_1x_2) + p_1p_5(x_1z_2) + p_2p_4(y_1x_2 - 2x_1^2y_1x_2) + p_2p_6(y_1z_2) + p_3p_5(x_1z_2) + p_3p_6(y_1z_2) + p_4p_5(y_1z_2) + p_4p_6(x_1z_2) + p_5p_6(y_1x_2 - 2x_1^2y_1x_2) = 0$$

Regard this as $\gamma(p_1, \dots, p_6) = 0$.

We have:

$$D\beta_{(1,1,1,0,0,0)} = (2(x_1^2 - x_2^2),\ 2y_1^2,\ -2z_2^2,\ 4x_1y_1,\ -4x_2z_2,\ 0)$$

and

$$D\gamma_{(1,1,1,0,0,0)} = (2x_1y_1^2x_2,\ -2x_1y_1^2x_2,\ 0,\ 2(y_1x_2 - 2x_1^2y_1x_2),\ 2x_2z_2,\ 2y_1z_2).$$

Since $y_1, z_2 \neq 0$, these are non-zero and locally at $\iota$, $\beta^{-1}(0)$ and $\gamma^{-1}(0)$ intersect transversally. Therefore $\omega^{-1}(C(T \cap W))$ is locally at $\iota$ a smooth submanifold of Pos(V) of dimension 4. Assuming $c_2 \neq 0$ or $c_3 \neq 0$ gives the same result in this situation. In other situations later, we may have to consider the possibilities $c_1 = 0$, $c_2 \neq 0$; $c_1 = c_2 = 0$ but $c_3 \neq 0$.

Notice that the results in (i) and (ii) are in agreement with Proposition 5.5.

We now look at the centralizer C(T) and its intersection with $\omega^{-1}(C(T \cap W))$. If T is triclinic, C(T) = Pos(V) and $\omega^{-1}(C(T \cap W)) \cap C(T) = \omega^{-1}(C(T \cap W))$. If T is cubic, $C(T) = (R^+)\iota$ and $\omega^{-1}(C(T \cap W)) \cap C(T) = C(T)$. If $T \cap W$ is of class P, then $\omega^{-1}(C(T \cap W)) \cap C(T) = C(T)$. These three cases are easily seen to conform to the description in Section 5.2, and there are no special planes for them. They are summarised in Table 5.1.

For the remaining cases, we choose $\{e_1, e_2, e_3\}$ such that $e_2 = \frac{\tau_2}{\|\tau_2\|}$ and $e_3 = \frac{\tau_3}{\|\tau_3\|}$ forma conventional set in $\mathcal{B}(T)$. Therefore C(T) is determined as follows, no matter what the conventional set:

T monoclinic: $p_5 = p_6 = 0$;

T orthorhombic: $p_4 = p_5 = p_6 = 0$;

T tetragonal, hexagonal or rhombohedral:

$$p_1 = p_2,\ p_4 = p_5 = p_6 = 0.$$

For verification of this, refer to Table 3.1.

We now look at $\omega^{-1}(C(T\cap W)) \cap C(T)$ for these remaining cases.

(A). T Monoclinic.

(i). The lattice $L^{T\cap W}$ is of class R or D. From equation (1), it follows that $C(T)$ and $\omega^{-1}(C(T\cap W))$ intersect transversally in Pos(V) near $\iota$ unless $x_1x_2 = y_1y_2 = z_1z_2 = x_1y_2 + x_2y_1 = 0$, in which case $\omega^{-1}(C(T\cap W)) \subseteq C(T)$ and $S(T,W) = C(T)$. Therefore the dimension d of the 'local stability manifold' is 3 unless $x_1 = y_1 = z_2 = 0$ or $x_2 = y_2 = z_1 = 0$, when $d = 4$. If W has indices $(a_1a_2a_3)$ relative to $\{\tau_1, \tau_2, \tau_3\}$, $d = 4$ occurs when $T\cap W$ is of class R if and only if $a_3 = 0$; $a_2\tau_1 - a_1\tau_2$ and $\tau_3$ are primitive in $T\cap W$; $\| a_2\tau_1 - a_1\tau_2\| \neq \|\tau_3\|$. The vectors $a_2\tau_1 - a_1\tau_2$ and $\tau_3$ are shortest non-zero lattice vectors in the proposed mirror lines, and the last restriction is to prevent $T\cap W$ being of class S. If T is primitive monoclinic, $a_2\tau_1 - a_1\tau_2$ and $\tau_3$ are automatically primitive if $a_3 = 0$, by Lemma 5.6, since $HCF(a_1,a_2) = 1$. If T is body-centred, $\{\tau_1,\tau_2,\tau_3\}$ is no longer a basis of T and the primitivity condition becomes: $HCF(a_1-a_2, 2a_1, 2a_2) = 1$. This holds if and only if $a_1 + a_2$ is odd.

The lattice $T\cap W$ is of class D with appropriate restrictions if and only if $a_3 = 0$; $\frac{1}{2}a_2\tau_1 - \frac{1}{2}a_1\tau_2 + \frac{1}{2}\tau_3$ and $\tau_3$ are primitive in $T\cap W$; $\dfrac{\|a_2\tau_1 - a_1\tau_2\|}{\|\tau_3\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$.

If T is primitive monoclinic, this is impossible. If T is body-centred, we need $a_1$ and $a_2$ to both be odd i.e. $a_1 + a_2$ to be even.

(ii). The lattice $T \cap W$ is of class $\underline{S}$ or $\underline{H}$. From equations (2) and (3), $C(T)$ and $\omega^{-1}(C(T \cap W))$ intersect transversally near $\iota$ in Pos(V) unless $x_2 = 0$, in which case $C(T) \subseteq \gamma^{-1}(0) = S(T,W)$, and $C(T)$ and $\omega^{-1}(C(T \cap W))$ intersect transversally in $S(T,W)$. Therefore $d = 2$ unless $x_2 = 0$, when $d = 3$. However, $x_2 = 0$ requires $a_3 = 0$ and we have already calculated when $\underline{S}$ or $\underline{H}$ occurs under this restriction in (i). Deriving the analogue of equations (2) and (3) under the assumption $c_1 = 0$, $c_2 \neq 0$ gives the same result. The case $c_1 = c_2 = 0$ is impossible, since for this $T \cap W$ is always of class $\underline{P}$.

<u>Notice that we have not only identified the planes for which d has a special value if a particular 2-dimensional Bravais class appears. We have determined exactly when this class appears with a special value for d.</u> We shall do this in all later results as well.

<u>(B). T Orthorhombic</u>.

(i). The lattice $T \cap W$ is of class $\underline{R}$ or $\underline{D}$. From equation (1) we see that $C(T)$ and $\omega^{-1}(C(T \cap W))$ intersect transversally near $\iota$ in Pos(V) unless $x_1x_2 = y_1y_2 = z_1z_2 = 0$, when $C(T) \subseteq \omega^{-1}(C(T \cap W)) = S(T,W)$. Therefore $d = 2$ unless $x_1x_2 = y_1y_2 = z_1z_2 = 0$, when $d = 3$. Now $d = 3$ requires one of the following: $x_1 = y_1 = z_2 = 0$; $x_1 = y_2 = z_1 = 0$; $x_1 = y_2 = z_2 = 0$; $x_2 = y_1 = z_1 = 0$; $x_2 = y_1 = z_2 = 0$; $x_2 = y_2 = z_1 = 0$. Take the case $x_1 = y_1 = z_2 = 0$. If T is <u>primitive orthorhombic</u>, $T \cap W$ is of class $\underline{R}$ with these restrictions if and only if $a_3 = 0$; $a_2\tau_1 - a_1\tau_2$ and $\tau_3$ are primitive in $T \cap W$; $\|a_2\tau_1 - a_1\tau_2\| \neq \|\tau_3\|$. Since if

$a_3 = 0$, $HCF(a_1,a_2) = 1$, the primitivity condition is always satisfied. <u>If T is body-centred</u>, we require: $a_3 = 0$; $HCF(a_1-a_2, 2a_1, 2a_2) = 1$ i.e. $a_1 + a_2$ to be odd; $\| a_2\tau_1 - a_1\tau_2 \| \neq \|\tau_3\|$. <u>If T is face-centred</u>, we require: $a_3 = 0$; $HCF(\frac{2a_1}{m_1}, \frac{2(a_1+a_2)}{m_1}, \frac{4a_1}{m_1}) = 1$ $(m_1 = HCF(a_1+a_2, 2a_1))$ i.e. $a_1 + a_2$ to be even; $\| \frac{1}{2}a_2\tau_1 - \frac{1}{2}a_1\tau_2 \| \neq \|\tau_3\|$. <u>If T is C-centred</u> (meaning $\frac{1}{2}\tau_1 + \frac{1}{2}\tau_2 \in T$) we require: $a_3 = 0$; $HCF(\frac{a_1+a_2}{m_1}, \frac{2a_1}{m_1}) = 1$ $(m_1 = HCF(a_1+a_2, 2a_1))$; $\| \frac{a_2}{m_1}\tau_1 - \frac{a_1}{m_1}\tau_2 \| \neq \|\tau_3\|$. If $a_1 + a_2$ is even, $m_1 = 2$ and $HCF(\frac{a_1+a_2}{2}, a_1) = 1$; if $a_1 + a_2$ is odd, $m_1 = 1$ and $HCF(a_1+a_2, 2a_1) = 1$.

For $T \cap W$ of class <u>D</u> we get no possibilities for T <u>primitive</u> or <u>C-centred</u>. For T <u>body-centred</u>, we get $a_3 = 0$; $a_1 + a_2$ even; $\frac{\|a_2\tau_1 - a_1\tau_2\|}{\|\tau_3\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$. For T <u>face-centred</u>, we get $a_3 = 0$, $a_1 + a_2$ odd; $\frac{\|a_2\tau_1 - a_1\tau_2\|}{\|\tau_3\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$.

Considering the other possibilities for $x_1$, $y_1$, $z_1$, $x_2$, $y_2$, $z_2$ gives similar results with $a_1 = 0$ or $a_2 = 0$, except that <u>D</u> may occur in the C-centred case if $a_1$ or $a_2$ is zero. The results are summarized in the tables at the end of this section.

(ii). The lattice $T \cap W$ is of class <u>S</u> or <u>H</u>. The manifolds $C(T)$ and $\omega^{-1}(C(T\cap W))$ intersect transversally near $\iota$ in $Pos(V)$ unless $x_1 = 0$ or $x_2 = 0$, when $C(T) \subseteq \gamma^{-1}(0) = S(T,W)$, and $C(T)$ and $\omega^{-1}(C(T\cap W))$ intersect transversally in $S(T,W)$. Therefore $d = 1$ unless $x_1$ or $x_2 = 0$, when $d = 2$. The calculations in (i) reveal all cases when $x_1$ or $x_2 = 0$ and $T \cap W$ is of class $\underline{S}$ or $\underline{H}$, since this corresponds to one index of the plane being 0. Again the results are summarized in the tables.

In deriving equations (2) and (3), assuming $c_2 \neq 0$ or $c_1 = c_2 = 0$, $c_3 \neq 0$ gives the same results.

(C). T Tetragonal.

(i). The lattice $T \cap W$ is of class $\underline{R}$ or $\underline{D}$. Equation (1) implies that $C(T)$ and $\omega^{-1}(C(T \cap W))$ intersect transversally near $\iota$ in $\mathrm{Pos}(V)$ unless $z_1 z_2 = 0$, when $S(T,W) = \omega^{-1}(C(T \cap W))$, which is bigger than $C(T)$. Therefore $d = 1$ unless $z_1 z_2 = 0$, when $d = 2$. For $d = 2$ and $T \cap W$ of class $\underline{R}$ one mirror line must lie in the plane (001). A shortest non-zero lattice vector in this is $t_1 = \frac{a_2}{m_1}\tau_1 - \frac{a_1}{m_1}\tau_2$, where $m_1 = \mathrm{HCF}(a_1, a_2)$. We are assuming that $a_1$ and $a_2$ are not both 0, since if this is the case $T \cap W$ is always of class $\underline{S}$. If T is primitive tetragonal, a shortest non-zero lattice vector in W normal to $t_1$ is $t_2 = \frac{a_1 a_3}{m_2}\tau_1 + \frac{a_2 a_3}{m_2}\tau_2 - \frac{a_1^2 + a_2^2}{m_2}\tau_3$, where $m_2 = \mathrm{HCF}(a_1 a_3,\ a_2 a_3,\ a_1^2 + a_2^2)$.

For $T \cap W$ of class $\underline{R}$, we require $\mathrm{HCF}\left(\frac{a_1(a_1^2+a_2^2)}{m_1 m_2}, \frac{a_2(a_1^2+a_2^2)}{m_1 m_2}, \frac{a_3(a_1^2+a_2^2)}{m_1 m_2}\right)$ to be 1 and $\|t_1\| \neq \|t_2\|$. This is true if and only if $a_1^2 + a_2^2 = m_1 m_2$ and $\|t_1\| \neq \|t_2\|$. For $T \cap W$ to be of class $\underline{D}$, we require $\frac{1}{2}\left(\frac{a_2}{m_1} + \frac{a_1 a_3}{m_2}\right)$ and $\frac{1}{2}\left(-\frac{a_1}{m_1} + \frac{a_2 a_3}{m_2}\right)$ to be integral;

$HCF(\frac{a_1(a_1^2+a_2^2)}{2m_1m_2}, \frac{a_2(a_1^2+a_2^2)}{2m_1m_2}, \frac{a_3(a_1^2+a_2^2)}{2m_1m_2})$ to be 1;

$\frac{\|t_1\|}{\|t_2\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$. The second condition is satisfied if and only if $a_1^2 + a_2^2 = 2m_1m_2$. However, if this holds, it is immediate that $\frac{a_1^2}{m_1}$ and $\frac{a_2^2}{m_1}$ are odd. Since $\frac{a_1^2 + a_2^2}{m_2}$ is even, $\frac{a_1a_3}{m_2}$ and $\frac{a_2a_3}{m_2}$ must be odd, meaning the first condition is satisfied. Therefore $T\cap W$ is of class D with d=2 if and only if $a_1^2 + a_2^2 = 2m_1m_2$, $\frac{\|t_1\|}{\|t_2\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$.

If T is body-centred tetragonal, we test for R and D with $z_1z_2 = 0$ in a similar way. Since $\{\tau_1, \tau_2, \tau_3\}$ is no longer a basis of T, we now have $m_2 = HCF(a_1a_3+a_1^2+a_2^2, a_2a_3+a_1^2+a_2^2, 2(a_1^2+a_2^2))$ and for $T\cap W$ of class R we require $HCF(\frac{2a_1(a_1^2+a_2^2)}{m_1m_2}, \frac{2a_2(a_1^2+a_2^2)}{m_1m_2}, \frac{(a_1+a_2+a_3)(a_1^2+a_2^2)}{m_1m_2})$ to be 1 and $\|t_1\| \neq \|t_2\|$. This holds for $a_1+a_2+a_3$ odd if and only if $a_1^2+a_2^2 = m_1m_2$, and $\|t_1\| \neq \|t_2\|$; for $a_1 + a_2 + a_3$ even if and only if $2(a_1^2+a_2^2) = m_1m_2$, and $\|t_1\| \neq \|t_2\|$.

For $T\cap W$ of class D we require $\frac{1}{2}(\frac{a_2}{m_1} + \frac{a_1a_3+a_1^2+a_2^2}{m_2})$ and $\frac{1}{2}(-\frac{a_1}{m_1} + \frac{a_2a_3+a_1^2+a_2^2}{m_2})$ to be integral;
$HCF(\frac{a_1(a_1^2+a_2^2)}{m_1m_2}, \frac{a_2(a_1^2+a_2^2)}{m_1m_2}, \frac{(a_1+a_2+a_3)(a_1^2+a_2^2)}{2m_1m_2})$ to be 1;

$\frac{\|t_1\|}{\|t_2\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$. This holds for $a_1 + a_2 + a_3$ odd if and only if $a_1^2 + a_2^2 = 2m_1m_2$; $\frac{\|t_1\|}{\|t_2\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$; for $a_1 + a_2 + a_3$ even if and only if $a_1^2 + a_2^2 = m_1m_2$; $\frac{\|t_1\|}{\|t_2\|} \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$.

(ii). The lattice $T \cap W$ is of class $\underline{S}$ or $\underline{H}$. Equations (2) and (3) show that $C(T)$ and $\omega^{-1}(C(T \cap W))$ always intersect transversally in $\gamma^{-1}(0) = S(T,W)$, meaning $d = 1$. Assuming $c_2 \neq 0$ in deriving equations (2) and (3) gives the same result. Assuming $c_1 = c_2 = 0$, $c_3 \neq 0$ means we are considering the plane (001). Clearly $\underline{S}$ always occurs here with $d = 2$, but $\underline{H}$ never occurs.

(D). T Hexagonal/Rhombohedral.

The results follow the same pattern as in the tetragonal case, but we spare the reader the details of the calculations. The results are summarized in the tables.

Table 5.1. Usual Dimension d of the Local Stability Manifold.

The numbers in brackets in the first row are the dimensions of $\Lambda_3(G)$ for each system.

| T→ / T∩W↓ | Triclinic (6) | Monoclinic (4) | Ortho-rhombic (3) | Tetr-agonal (2) | Hex-agonal (2) | Rhombo-hedral (2) | Cubic (1) |
|---|---|---|---|---|---|---|---|
| $\underline{P}$ | 6 | 4 | 3 | 2 | 2 | 2 | 1 |
| $\underline{R}$ | 5 | 3 | 2 | 1 | 1 | 1 | 1 |
| $\underline{D}$ | 5 | 3 | 2 | 1 | 1 | 1 | 1 |
| $\underline{S}$ | 4 | 2 | 1 | 1 | 1 | 1 | 1 |
| $\underline{H}$ | 4 | 2 | 1 | 1 | 1 | 1 | 1 |

Table 5.2. Description of When the Local Stability Manifold has Special Dimension.

(A). T Monoclinic.

Notation: $\eta = \eta(a_1,a_2) = \dfrac{\|a_2\tau_1 - a_1\tau_2\|}{\|\tau_3\|}$.

| $T \cap W$ | Special Dimension | T Primitive | T Body-centred |
|---|---|---|---|
| R | d=4 (STABLE) | $a_3=0,\ \eta\neq 1$ | $a_3=0$, $a_1+a_2$ odd, $\eta\neq 1$ |
| D | d=4 (STABLE) | Never | $a_3=0$, $a_1+a_2$ even, $\eta\neq 1, \sqrt{3}, \frac{1}{\sqrt{3}}$ |
| S | d=3 | $a_3=0, \eta=1$ | $a_3=0, \eta=1$ |
| H | d=3 | Never | $a_3=0$, $a_1+a_2$ even, $\eta=\sqrt{3}, \frac{1}{\sqrt{3}}$ |

(B). T Orthorhombic.

Notation: $\eta(a_i,a_j) = \dfrac{\|a_j\tau_i - a_i\tau_j\|}{\|\tau_k\|}$, $k\neq i,j$.

| $T \cap W$ | Special Dimension | Primitive | Body-centred | Face-centred | C-centred |
|---|---|---|---|---|---|
| R | d=3 (STABLE) | $a_1=0$<br>$\eta(a_2,a_3)\neq 1$<br>or<br>$a_2=0$<br>$\eta(a_1,a_3)\neq 1$<br>or<br>$a_3=0$<br>$\eta(a_1,a_2)\neq 1$ | $a_1=0$,<br>$a_2+a_3$ odd,<br>$\eta(a_2,a_3)\neq 1$<br>or<br>$a_2=0$,<br>$a_1+a_3$ odd,<br>$\eta(a_1,a_3)\neq 1$<br>or<br>$a_3=0$,<br>$a_1+a_2$ odd,<br>$\eta(a_1,a_2)\neq 1$ | Same as body-centred for R but with $a_i+a_j$ even | $a_1=0, a_2$ odd,<br>$\eta(a_2,a_3)\neq 1$<br>or<br>$a_2=0, a_1$ odd,<br>$\eta(a_1,a_3)\neq 1$<br>or<br>$a_3=0, a_1+a_2$ odd,<br>$\eta(a_1,a_2)\neq 1$<br>or<br>$a_3=0, a_1+a_2$ even,<br>$\eta(a_1,a_2)\neq 2$ |
| D | d=3 (STABLE) | Never | Same as in R but with $a_i+a_j$ even and $\eta(a_i,a_j)\neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ | Same as body-centred for D but with $a_i+a_j$ odd | $a_1=0, a_2$ even,<br>$\eta(a_2,a_3)\neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$<br>or<br>$a_2=0, a_1$ even,<br>$\eta(a_1,a_3)\neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ |

Continued.

Table 5.2(B). Continued.

| $T \cap W$ | Special Dimension | Primitive | Body-centred | Face-centred | C-centred |
|---|---|---|---|---|---|
| $\underline{S}$ | d=2 | <br>or<br>or | $a_1=0, \eta(a_2,a_3)=1$<br>$a_2=0, \eta(a_1,a_3)=1$<br>$a_3=0, \eta(a_1,a_2)=1$ | | $a_1=0, \eta(a_2,a_3)=$<br>or<br>$a_2=0, \eta(a_1,a_3)=$<br>or<br>$a_3=0, a_1+a_2$ odd,<br>$\eta(a_1,a_2)=1$<br>or<br>$a_3=0, a_1+a_2$ even<br>$\eta(a_1,a_2)=2$ |
| $\underline{H}$ | d=2 | Never | Same conditions on $a_1, a_2, a_3$ as in the corresponding column for $\underline{D}$ above, but with the restriction that $\eta = \sqrt{3}$ or $\frac{1}{\sqrt{3}}$. | | |

(C). T Tetragonal.

Notation: ($a_1, a_2$ not both zero) $m_1 = HCF(a_1, a_2)$;

$$t_1 = \frac{a_2}{m_1}\tau_1 - \frac{a_1}{m_1}\tau_2; \quad t_2 = \frac{a_1a_3}{m_2}\tau_1 + \frac{a_2a_3}{m_2}\tau_2 - \frac{a_1^2+a_2^2}{m_2}\tau_3;$$

$$\eta = \eta(a_1, a_2, a_3) = \frac{\|t_1\|}{\|t_2\|}$$

For T primitive, $m_2 = HCF(a_1a_3,\ a_2a_3,\ a_1^2+a_2^2)$.

For T body-centred, $m_2 = HCF(a_1a_3+a_1^2+a_2^2, a_2a_3+a_1^2+a_2^2, 2(a_1^2+a_2^2)$

In the following table (overleaf), we assume $a_1$ and $a_2$ are not both zero in rows $\underline{R}$ and $\underline{D}$.

| $T \cap W$ | Special Dimension | Primitive | Body-centred |
|---|---|---|---|
| R | d=2 (STABLE) | $a_1^2+a_2^2=m_1m_2$, $\eta \neq 1$ | $a_1+a_2+a_3$ odd, $a_1^2+a_2^2=m_1m_2$, $\eta \neq 1$ or $a_1+a_2+a_3$ even, $2(a_1^2+a_2^2)=m_1m_2$, $\eta \neq 1$ |
| D | d=2 (STABLE) | $a_1^2+a_2^2=2m_1m_2$ $\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ | $a_1+a_2+a_3$ odd, $a_1^2+a_2^2=2m_1m_2$, $\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ or $a_1+a_2+a_3$ even, $a_1^2+a_2^2=m_1m_2$, $\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ |
| S | d=2 (STABLE) | $a_1=a_2=0$ | $a_1=a_2=0$ |

(D). T Hexagonal/Rhombohedral.

Notation: ($a_1, a_2$ not both zero) $m_1 = \mathrm{HCF}(a_1, a_2)$;

$$t_1 = \frac{a_2}{m_1}\tau_1 - \frac{a_1}{m_1}\tau_2; \quad t_2 = \left(\frac{(2a_1+a_2)a_3}{m_2}\right)\tau_1 + \left(\frac{(2a_2+a_1)a_3}{m_2}\right)\tau_2 - \left(\frac{2(a_1^2+a_2^2+a_1a_2)}{m_2}\right)\tau_3;$$

$$\eta = \eta(a_1, a_2, a_3) = \frac{\|t_1\|}{\|t_2\|}.$$

For T hexagonal, $m_2 = \mathrm{HCF}((2a_1+a_2)a_3, (2a_2+a_1)a_3, 2(a_1^2+a_2^2+a_1a_2))$.

For T rhombohedral,

$$m_2 = \mathrm{HCF}\left[(2a_1+a_2)a_3+4(a_1^2+a_2^2+a_1a_2), (2a_2+a_1)a_3+2(a_1^2+a_2^2+a_1a_2), 6(a_1^2+a_2^2+a_1a_2)\right].$$

Again in the table overleaf we assume $a_1$ and $a_2$ are not both zero in rows R and D.

| $T \cap W$ | Special Dimension | Hexagonal | Rhombohedral |
|---|---|---|---|
| $\underline{R}$ | d=2 (<u>STABLE</u>) | $2(a_1^2+a_2^2+a_1a_2)=m_1m_2$,<br>$\eta \neq 1$ | $2(a_1^2+a_2^2+a_1a_2)=m_1m_2$,<br>3 does not divide $2a_1+a_2+a_3$,<br>$\eta \neq 1$<br><u>or</u><br>$6(a_1^2+a_2^2+a_1a_2)=m_1m_2$,<br>3 divides $2a_1+a_2+a_3$<br>$\eta \neq 1$ |
| $\underline{D}$ | d=2 (<u>STABLE</u>) | $a_1^2+a_2^2+a_1a_2=m_1m_2$,<br>$\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ | $a_1^2+a_2^2+a_1a_2=m_1m_2$,<br>3 does not divide $2a_1+a_2+a_3$,<br>$\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$<br><u>or</u><br>$3(a_1^2+a_2^2+a_1a_2)=m_1m_2$,<br>3 divides $2a_1+a_2+a_3, \eta \neq 1, \sqrt{3}, \frac{1}{\sqrt{3}}$ or |
| $\underline{H}$ | d=2 (<u>STABLE</u>) | $a_1=a_2=0$ | $a_1=a_2=0$ |

<u>Some Examples of Interesting Special Planes</u>.

We give some examples of planes satisfying the special conditions in Table 5.2 (C) and (D) when $T \cap W$ is of class $\underline{R}$ or $\underline{D}$. This is by no means a complete list of such planes. We exclude the restrictions on $\eta$ in these examples. Except for these restrictions, the examples may be regarded as always being of class $\underline{R}$ or $\underline{D}$.

<u>T Primitive Tetragonal</u>.

$\underline{R}$. $a_3 = a_1^2 + a_2^2$ and HCF$(a_1,a_2) = 1$ e.g. (125);
$a_1 = a_2$ and $a_3$ even e.g. (112);
(245);
$(3\bar{6}5)$ i.e. the plane with equation $3x - 6y + 5z = 0$;
(46(13)) i.e. " " " " $4x + 6y + 13z = 0$.

| $T \cap W$ | Special Dimension | Hexagonal | Rhombohedral |
|---|---|---|---|
| $\underline{R}$ | d=2 (<u>STABLE</u>) | $2(a_1^2+a_2^2+a_1a_2)=m_1m_2$, $\eta \neq 1$ | $2(a_1^2+a_2^2+a_1a_2)=m_1m_2$, 3 does not divide $2a_1+a_2+a_3$, $\eta \neq 1$ <u>or</u> $6(a_1^2+a_2^2+a_1a_2)=m_1m_2$, 3 divides $2a_1+a_2+a_3$ $\eta \neq 1$ |
| $\underline{D}$ | d=2 (<u>STABLE</u>) | $a_1^2+a_2^2+a_1a_2=m_1m_2$, $\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ | $a_1^2+a_2^2+a_1a_2=m_1m_2$, 3 does not divide $2a_1+a_2+a_3$, $\eta \neq 1, \sqrt{3}$ or $\frac{1}{\sqrt{3}}$ <u>or</u> $3(a_1^2+a_2^2+a_1a_2)=m_1m_2$, 3 divides $2a_1+a_2+a_3, \eta \neq 1, \sqrt{3}, \frac{1}{\sqrt{3}}$ or $\frac{1}{\sqrt{3}}$ |
| $\underline{H}$ | d=2 (<u>STABLE</u>) | $a_1=a_2=0$ | $a_1=a_2=0$ |

<u>Some Examples of Interesting Special Planes</u>.

We give some examples of planes satisfying the special conditions in Table 5.2 (C) and (D) when $T \cap W$ is of class $\underline{R}$ or $\underline{D}$. This is by no means a complete list of such planes. We exclude the restrictions on $\eta$ in these examples. Except for these restrictions, the examples may be regarded as always being of class $\underline{R}$ or $\underline{D}$.

<u>T Primitive Tetragonal</u>.

$\underline{R}$. $a_3 = a_1^2 + a_2^2$ and $HCF(a_1,a_2) = 1$ e.g. (125);

$a_1 = a_2$ and $a_3$ even e.g. (112);

(245);

$(3\bar{6}5)$ i.e. the plane with equation $3x - 6y + 5z = 0$;

(46(13)) i.e. " " " " $4x + 6y + 13z = 0$.

**D.** $a_1 = a_2$ and $a_3$ odd e.g. (113);
(265);
$(1\bar{3}(15))$.

<u>T Body-centred Tetragonal</u>.

**R.** $a_1 = a_2$, $a_3$ even, $\frac{a_3}{2} + a_1$ even;
$a_3 = a_1^2 + a_2^2$, HCF$(a_1,a_2) = 1$, $a_1 + a_2$ even;
(46(13));
(245).

**D.** $a_3 = a_1^2 + a_2^2$, HCF $(a_1,a_2) = 1$, $a_1 + a_2$ odd;
$a_1 = a_2$, $a_3$ odd;
$a_1 = a_2$, $a_3$ even, $\frac{a_3}{2} + a_1$ odd;
$(3\bar{6}5)$;
(265);
$(1\bar{3}(15))$.

<u>T Hexagonal</u>.

**R.** $a_1 = a_2$, $a_3$ even;
( 127 ).

**D.** $a_1 = a_2$, $a_3$ odd;
$a_3 = a_1^2 + a_2^2 + a_1a_2$, HCF$(a_1,a_2) = 1$;
(247).

<u>T Rhombohedral</u>.

**R.** $a_1 = a_2$, $a_3$ even and not divisible by 3.

**D.** $a_1 = a_2$, $a_3$ odd and not divisible by 3;
(247);
(127).

<u>Final Remark</u>.

In [6], there are four specific examples given illustrating the use of the algorithm in that paper. Each involves taking a plane of fixed indices throughout a Bravais class. In each case the plane is a non-special one by our classification and the answers obtained for these examples all conform to the pattern predicted in Table 5.1. To see this it is necessary to notice that the space of free parameters over a particular Bravais class, used by crystallographers, corresponds to our space C(G(T), Pos(V)) (cf. Proposition 2.12). Also, in view of the remarks at the beginning of this section about conventional sets, fixing plane indices and varying parameters in the Bravais class corresponds to taking pW for p in C(G(T), Pos(V)).

By way of illustration, consider the case of a (123) plane in a primitive orthorhombic lattice. Gruber states (p. 623) that <u>R</u> occurs if and only if the parameters a,b,c, satisfy $6a^2 = 3b^2 \neq 2c^2$ or $a^2 - 2b^2 - c^2 = 0$. It is clear that this indicates a local stability manifold of dimension 2, as Table 5.1 predicts. The other parametric equations in Gruber's examples may be interpreted in the same way. We emphasize that the parameters a, b, c are <u>not</u> plane indices but <u>lattice</u> parameters. The plane indices in Gruber's examples are fixed.

REFERENCES.

1. Apostol, T.M. Introduction to Analytic Number Theory. Springer Verlag, 1976.

2. Buerger, M.J. Elementary Crystallography. Wiley, New York, 1956.

3. Bülow, R., Neubüser, J. and Wondratschek, H. On Crystallography in Higher Dimensions I, II, III. Acta Cryst. 27A (1971), 517-535.

4. Burckhardt, J.J. Die Bewegungsgruppen der Kristallographie. Birkhäuser Verlag, Basel, 1966.

5. Curtis, C.W. and Reiner, I. Representation Theory of Finite Groups and Associative Algebras. Wiley, New York, 1962.

6. Gruber, B. Algorithm for Determining the Symmetry and Stacking Properties of the Planes (hkl) in a Bravais Lattice. Acta Cryst. 26A (1970), 622-627.

7. Halmos, P.R. Finite Dimensional Vector Spaces. Van Nostrand, 1958.

8. Hardy, G.H. and Wright, E.M. An Introduction to the Theory of Numbers. Oxford University Press, 1938.

9. Hermann, C. Kristallographie in Räumen Beliebiger Dimensionszahl I. Acta Cryst. 2 (1949), 139-145.

10. International Tables for X-ray Crystallography. Volume I. Edited by Henry, N.F.M. and Lonsdale, K. The Kynoch Press, 1965.

Continued.

REFERENCES (Continued).


11. Jaswon, M.A. and Dove, D.B. The Geometry of Lattice Planes. Acta Cryst. 8 (1955), 88-91.

12. Schwarzenberger, R.L.E. Classification of Crystal Lattices. Proc. Camb. Phil. Soc. 72 (1972), 325-349.

13. Schwarzenberger, R.L.E. Crystallography in Spaces of Arbitrary Dimension. Proc. Camb. Phil. Soc. 76 (1974), 23-32.

14. Van der Waerden, B.L. Die Reduktionstheorie der Positiven Quadratischen Formen. Acta Math. 96 (1956), 265-293.

15. Wolf, J.A. Spaces of Constant Curvature. Publish or Perish, 1974.