Space Group Subgroups generated by Sublattice Relations: Software for IBM-Compatible PCs

R. DIRL
Institut fur Theoretische Physik, T.U., Wien, Austria

B. L. DAVIES
School of Mathematics, U.C.N.W., Bangor, U.K.

Introduction

The role of symmetry considerations exploiting group-subgroup relations of space groups in structural phase transitions is widely accepted and presents an indispensible tool. Here we briefly discuss group-subgroup relations of space groups that are generated by sublattices. The present approach generalizes the task of identifying given sub-space groups [1] since the aim is to determine all compatible extensions [2].

Group-Subgroup Relations of Space Groups

To establish our conventions, we recall that every space group $\mathcal{G} = \mathcal{G}(\mathcal{T}, \mathcal{P}; \tau, \Phi)$ is fixed by its translation group $\mathcal{T}$, its point group $\mathcal{P}$, the mapping τ, and its extension Φ [3]. Every extension $\Phi \longleftrightarrow \{\mathbf{n}(\mathsf{R})\}$ which is uniquely assigned to a set of non-primitive lattice vectors (non-plv's) sensitively depends on the setting of the space group. The setting of space groups can be changed by shifts of the origin and/or re-orientation operations.

Two space groups, say $\mathcal{G}' = \mathcal{G}(\mathcal{T}', \mathcal{P}'; \tau', \Phi')$ and $\mathcal{G} = \mathcal{G}(\mathcal{T}, \mathcal{P}; \tau, \Phi)$, are group-subgroup related, i.e. $\mathcal{G}' \subset \mathcal{G}$, if in addition to $\mathcal{T}' \subset \mathcal{T}$ and/or $\mathcal{P}' \subset \mathcal{P}$ the mappings τ' and τ and the extensions Φ' and Φ are compatible [2]. We distinguish between

$$\begin{array}{lll} \{t\}\ \textbf{Sub-Space Group:} & \mathcal{T}' = \mathcal{T} & \mathcal{P}' \subset \mathcal{P} \\ \{k\}\ \textbf{Sub-Space Group:} & \mathcal{T}' \subset \mathcal{T} & \mathcal{P}' = \mathcal{P} \\ \{g\}\ \textbf{Sub-Space Group:} & \mathcal{T}' \subset \mathcal{T} & \mathcal{P}' \subset \mathcal{P} \end{array}$$

Every $\mathcal{G}'$ is called "maximal" subgroup of $\mathcal{G}$ if there does not exist an $\mathcal{M}$ such that the subgroup chain $\mathcal{G}' \subset \mathcal{M} \subset \mathcal{G}$ holds. Because of Hermann's Theorem [4] maximal subgroups of space groups $\mathcal{G}$ are either $\{t\}$ or $\{k\}$ subgroups. A non-trivial consequence of Hermann's theorem is that every sub-space group $\mathcal{G}'$ of a given space group $\mathcal{G}$ can be stepwise derived by linking appropriately maximal subgroups of type $\{t\}$ and $\{k\}$ respectively. However in practical applications it is tedious to sort out which chain of maximal subgroups leads to the desired $\{g\}$ subgroup relation.

Next we summarize the basic conditions for the validity of $\{t\}$, $\{k\}$, and $\{g\}$ subgroup relations where $\mathcal{G}_s$ and $\mathcal{G}_{ns}$ indicate symmorphic and non-symmorphic space groups.

Compatibility Relations for $\{t\}$ Space Groups		
$\mathcal{G}_s \supset \mathcal{G}'_s$	$\mathsf{n}(\mathsf{R}') = 0$	$\mathsf{t}(\mathsf{R}', \mathsf{S}') = 0$
$\mathcal{G}_{ns} \supset \mathcal{G}'_s$	$\mathsf{n}(\mathsf{R}') = 0$	$\mathsf{t}(\mathsf{R}', \mathsf{S}') = 0$
$\mathcal{G}_{ns} \supset \mathcal{G}'_{ns}$	$\mathsf{n}(\mathsf{R}') \neq 0$	$\mathsf{t}(\mathsf{R}', \mathsf{S}') \in \mathcal{T}$

Note that the $\{t\}$ subgroup conditions are always realizeable for any pair of $\{t\}$ space groups since the restriction $\{\mathsf{v}(\mathsf{R})\} \downarrow \mathcal{P}'$ by definition does not violate the compatibility of the corresponding extensions. The special plv's $\mathbf{t}(\mathsf{R},\mathsf{S}) = \mathbf{n}(\mathsf{R}) + \mathsf{R}\mathbf{n}(\mathsf{S}) - \mathbf{n}(\mathsf{RS}) \in \mathcal{T}$ define for $\mathsf{R},\mathsf{S} \in \mathcal{P}$ the extension Φ of $\mathcal{G}$ and for $\mathsf{R}',\mathsf{S}' \in \mathcal{P}'$ the extension Φ' of $\mathcal{G}'$ respectively. Group-subgroup relations of the type $\mathcal{G}_s \longmapsto \mathcal{G}'_{ns}$ are ruled out.

Compatibility Relations for $\{k\}$ Space Groups		
$\mathcal{G}_s \supset \mathcal{G}'_s$	$\mathbf{n}(\mathsf{R}) = \mathbf{0}, \mathbf{w}(\mathsf{R}) \in \mathcal{T}$	$\mathbf{w}(\mathsf{R},\mathsf{S}) = \mathbf{0}$
$\mathcal{G}_s \supset \mathcal{G}'_{ns}$	$\mathbf{n}(\mathsf{R}) = \mathbf{0}, \mathbf{w}(\mathsf{R}) \in \mathcal{T}$	$\mathbf{w}(\mathsf{R},\mathsf{S}) \in \mathcal{T}'$
$\mathcal{G}_{ns} \supset \mathcal{G}'_{ns}$	$\mathbf{n}(\mathsf{R}) \neq \mathbf{0}, \mathbf{w}(\mathsf{R}) \in \mathcal{T}$	$\mathbf{t}(\mathsf{R},\mathsf{S}) + \mathbf{w}(\mathsf{R},\mathsf{S}) \in \mathcal{T}'$

Note that the $\{k\}$ subgroup conditions are only realizeable for a given pair of $\{k\}$ space groups iff appropriate $\mathbf{w}(\mathsf{R}) \in \mathcal{T}$ exist such that for $\mathbf{n}'(\mathsf{R}) = \mathbf{n}(\mathsf{R}) + \mathbf{w}(\mathsf{R})$ the compatibility condition is satisfied, namely $\mathbf{t}'(\mathsf{R},\mathsf{S}) = \mathbf{t}(\mathsf{R},\mathsf{S}) + \mathbf{w}(\mathsf{R},\mathsf{S}) \in \mathcal{T}'$ where $\mathbf{w}(\mathsf{R},\mathsf{S}) = \mathbf{w}(\mathsf{R}) + \mathsf{R}\mathbf{w}(\mathsf{S}) - \mathbf{w}(\mathsf{RS})$. Here group-subgroup relations of the type $\mathcal{G}_{ns} \longmapsto \mathcal{G}'_s$ cannot be realized since one cannot find some $\mathbf{w}(\mathsf{R}) \in \mathcal{T}$ such that $\mathbf{t}(\mathsf{R},\mathsf{S}) + \mathbf{w}(\mathsf{R},\mathsf{S}) = \mathbf{0}$ is valid.

Compatibility Relations for $\{g\}$ Space Groups		
$\mathcal{G}_s \supset \mathcal{G}^{\#}_s \supset \mathcal{G}'_s$	$\mathbf{n}(\mathsf{R}') = \mathbf{0}$	$\mathbf{n}'(\mathsf{R}') = \mathbf{0}$
$\mathcal{G}_s \supset \mathcal{G}^{\#}_s \supset \mathcal{G}'_{ns}$	$\mathbf{n}(\mathsf{R}') = \mathbf{0}$	$\mathbf{n}'(\mathsf{R}') = \mathbf{w}(\mathsf{R}')$
$\mathcal{G}_{ns} \supset \mathcal{G}^{\#}_s \supset \mathcal{G}'_s$	$\mathbf{n}(\mathsf{R}') = \mathbf{0}$	$\mathbf{n}'(\mathsf{R}') = \mathbf{0}$
$\mathcal{G}_{ns} \supset \mathcal{G}^{\#}_s \supset \mathcal{G}'_{ns}$	$\mathbf{n}(\mathsf{R}') = \mathbf{0}$	$\mathbf{n}'(\mathsf{R}') = \mathbf{w}(\mathsf{R}')$
$\mathcal{G}_{ns} \supset \mathcal{G}^{\#}_{ns} \supset \mathcal{G}'_{ns}$	$\mathbf{n}(\mathsf{R}') \neq \mathbf{0}$	$\mathbf{n}'(\mathsf{R}') = \mathbf{n}(\mathsf{R}') + \mathbf{w}(\mathsf{R}')$

The space groups $\mathcal{G}^{\#} = \mathcal{G}(\mathcal{T},\mathcal{P}';\tau^{\#},\Phi^{\#})$ with $\mathcal{P}' \subset \mathcal{P}$ are $\{t\}$ sub-space groups of $\mathcal{G}$. Note that the $\{g\}$ subgroup conditions are only realizeable for a given pair of $\{g\}$ space groups iff appropriate $\mathbf{w}(\mathsf{R}') \in \mathcal{T}$ exist such that for $\mathbf{n}'(\mathsf{R}') = \mathbf{n}(\mathsf{R}') + \mathbf{w}(\mathsf{R}')$ the compatibility condition is satisfied for all $\mathsf{R}',\mathsf{S}' \in \mathcal{P}'$, namely $\mathbf{t}'(\mathsf{R}',\mathsf{S}') = \mathbf{t}(\mathsf{R}',\mathsf{S}') + \mathbf{w}(\mathsf{R}',\mathsf{S}') \in \mathcal{T}'$. Here the combinations $\mathcal{G}_s \longmapsto \mathcal{G}^{\#}_{ns} \longmapsto \mathcal{G}'_s$ and $\mathcal{G}_s \longmapsto \mathcal{G}^{\#}_{ns} \longmapsto \mathcal{G}'_{ns}$ and $\mathcal{G}_{ns} \longmapsto \mathcal{G}^{\#}_{ns} \longmapsto \mathcal{G}'_s$ cannot be realized since one cannot find appropriate $\mathbf{w}(\mathsf{R}') \in \mathcal{T}$ such that the corresponding $\{g\}$ subgroup criterion is valid.

Sub-Space Groups generated by Sub-Lattices

The present approach is the following step-by step procedure where for lack of space subtle details are ignored. One starts from a super-space group $\mathcal{G}(\mathbf{0})$ in standard setting, then one fixes a sub-lattice $\mathcal{T}(\mathsf{Z}_0)$ of $\mathcal{T}$ by some element $\mathcal{N}(\mathsf{Z}_0) \in \mathcal{L}^+(3,\mathbf{Z})$, this determines the maximal "surviving" point group $\mathcal{P}(\mathsf{Z}_0) \subseteq \mathcal{P}$ which leaves the sub-lattice $\mathcal{T}(\mathsf{Z}_0)$ invariant, then the crucial problem is to find all inequivalent extensions Φ'_j which are compatible with Φ, and finally admissible sub-space groups $\mathcal{G}'_j$ are identified in terms of their image-space groups $\mathcal{G}^\sigma_j$ in standard settings which requires the determination of some shifts $\mathbf{v}'_j \in \mathcal{T}(3,\mathbf{R})$ and/or some re-orientation operations $\mathsf{S}_0 \in \mathcal{SO}(3,\mathbf{R})$ respectively.

STEP 1:	$\mathcal{G}(\mathbf{0}) = \mathcal{G}(\mathcal{T},\mathcal{P};\tau,\Phi)$
STEP 2:	$\mathcal{T}' \equiv \mathcal{T}(\mathsf{Z}_0) \subset \mathcal{T}$
STEP 3:	$\mathcal{P}' \equiv \mathcal{P}(\mathsf{Z}_0) \subseteq \mathcal{P}$
STEP 4:	$\Phi \downarrow (\mathcal{T}',\mathcal{P}') \sim \Phi'_j \iff \mathcal{G}'_j \equiv \mathcal{G}(\mathcal{T}',\mathcal{P}';\tau',\Phi'_j) \subset \mathcal{G}(\mathbf{0})$
STEP 5:	$\mathcal{G}'_j = (\mathsf{S}_0\vert\mathbf{v}'_j) * \mathcal{G}^\sigma_j * (\mathsf{S}_0\vert\mathbf{v}'_j)^{-1}$

Software for IBM-Compatible PCs

The steps 1-4 set out in section above are being implemented in a program SUBLÅT.C written in the "C" programming language while step 5 is accomplished by a Pascal program PCIR.PAS. The following example will serve as an illustration of the preceding theory and of the capability of the programs.

Let $\mathcal{G}$ = Ia3d (#230) in standard setting [5] (Step 1) and fix the sublattice $\mathcal{T}' = \mathcal{T}(\mathsf{Z}_0)$ of $\mathcal{T}$ by the integral matrix $\mathcal{N}^{prim}(\mathsf{Z}_0)$ (Step 2).

$$\mathcal{N}^{prim}(\mathsf{Z}_0) = \begin{pmatrix} 1 & 2 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \mathcal{N}^{conv}(\mathsf{Z}_0) = \begin{pmatrix} 1/2 & -3 & 0 \\ 1/2 & 2 & 1 \\ -1/2 & -2 & 1 \end{pmatrix}$$

Note that $det\,\mathcal{N}^{prim}(\mathsf{Z}_0) = 5$ which equals the index of $\mathcal{T}'$ in $\mathcal{T}$. The program SUBLAT.C determines the maximal "surviving" group $\mathcal{P}' = \{1, 18, 25, 42\} = \{\mathsf{E}, \mathsf{C}_{2d}, \mathsf{J}, \sigma_{dd}\} = 2/\mathrm{m}$ [5] and the Bravais lattice type of the sublattice $\mathcal{T}'$ is identified as Monoclinic A (Step 3). The program also identifies all possible orientations of the conventional unit cell of the sublattice [4]. This is done by computing, for each orientation, the (in general) rational matrix, the columns of which give the rational linear combinations of the conventional lattice vectors $\{\mathrm{a}, \mathrm{b}, \mathrm{c}\}$ of T which define the conventional lattice vectors $\{\mathrm{a}', \mathrm{b}', \mathrm{c}'\}$ of $\mathcal{T}'$. There are exactly two orientations in this example: the matrix for the first one is $\mathcal{N}^{conv}(\mathsf{Z}_0)$ and that for the second is obtained by multiplying columns 1 and 2 of $\mathcal{N}^{conv}(\mathsf{Z}_0)$ by -1. One inequivalent extension Φ' is found that is compatible with Φ (Step 4). Relative to the standard primitive lattice vectors $\{\mathrm{t}_1, \mathrm{t}_2, \mathrm{t}_3\}$ of the Monoclinic A lattice [5] this extension is defined by the non-primitive translation $\mathrm{w} = \frac{1}{2}[\mathrm{t}_1 + \mathrm{t}_2 + \mathrm{t}_3]$ which is assigned to C_{2d} and σ_{dd}, with $\mathbf{0}$ being assigned to E and J. Finally PCIR.PAS identifies the subspace group $\mathcal{G}'$ as A2/a (#15) (Step 5). A closer examination of this example reveals that there is a countable infinity of shifts of the standard origin [5] given by $\mathrm{t}_0 = \frac{1}{2}[-m\mathrm{t}_2 + (1-m)\mathrm{t}_3]$, m integral, which will yield extensions equal (modulo $\mathcal{T}'$) to Φ'.

Example: Subgroup Relations of Cubic Space Groups

To gain some insight into the complexity of the problem of defining subgroup relations of space groups we briefly summarize the results for the full cubic space groups [6]. Here the first column of the first Table gives the superlattices, the first row the possible sublattices, and at the intersection points admissible $\mathcal{N}(\mathsf{Z}_0)$-matrices that define the corresponding sublattice $\mathcal{T}(\mathsf{Z}_0)$ where $u \in \mathbf{Z}^+$ respectively.

Compatible Cubic Lattices: $\mathcal{N}(\mathsf{Z}_0)$-Matrices

	PC	FCC	BCC
PC	$\begin{pmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{pmatrix}$	$\begin{pmatrix} 0 & u & u \\ u & 0 & u \\ u & u & 0 \end{pmatrix}$	$\begin{pmatrix} -u & u & u \\ u & -u & u \\ u & u & -u \end{pmatrix}$
FCC	$\begin{pmatrix} -u & u & u \\ u & -u & u \\ u & u & -u \end{pmatrix}$	$\begin{pmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{pmatrix}$	$\begin{pmatrix} 3u & -u & -u \\ -u & 3u & -u \\ -u & -u & 3u \end{pmatrix}$
BCC	$\begin{pmatrix} 0 & u & u \\ u & 0 & u \\ u & u & 0 \end{pmatrix}$	$\begin{pmatrix} 2u & u & u \\ u & 2u & u \\ u & u & 2u \end{pmatrix}$	$\begin{pmatrix} u & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u \end{pmatrix}$

The second Table fixes in the first column the super-space groups $\mathcal{G}$, the first row contains all possible sub-space groups $\mathcal{G}'_j$. We indicate at the intersection points whether $u \in \mathbf{Z}^+$ can be arbitrary, has to be even $u = 2k$ or has to be odd $u = 2k+1$ respectively. We also indicate whether the sub-space groups $\mathcal{G}'_j = \mathcal{G}'_j(\mathbf{0})$ are in standard settings, or have to be reset by some appropriate shift of the origin. If for some reasons some subgroups cannot exist the corresponding intersection fields are empty.

Compatible Cubic Space Groups: $\mathcal{P} = \mathcal{O}_h$

	221	222	223	224	225	226	227	228	229	230
221	u 0	$2k$ 0	$2k$ 0	$2k$ 0	u 0	$2k$ 0	$2k$ 0	$2k$ 0	u 0	$2k$ 0
222		$2k+1$ 0								
223			$2k+1$ 0							$2k+1$ 0
224				$2k+1$ 0			$2k+1$ $\mathbf{v}_0$	$2k+1$ $\mathbf{v}_0$		
225	u 0	$2k$ 0	$2k$ 0	$2k$ 0	u 0	$2k$ 0	$2k$ 0	$2k$ 0	u 0	$2k$ 0
226		$2k+1$ $\mathbf{v}_0$	$2k+1$ 0			$2k+1$ 0				$2k+1$ 0
227							$2k+1$ 0			
228								$2k+1$ 0		
229	u 0	u 0	u 0	u 0	u 0	u 0	$2k$ 0	$2k$ 0	u 0	$2k$ 0
230										$2k+1$ 0

References

[1] D.M. Hatch, H.T. Stokes: Phys.Rev. **31**, 2908 (1985)

[2] M. Senechal: Acta Cryst. **A 36**, 845 (1980)

[3] E. Ascher, A. Janner: Helv.Acta **38**, 551 (1965)
E. Ascher, A. Janner: Comm.Math.Phys. **11**, 138 (1968/69)
J. Mozrzymas: Preprint ITP-SB-75-56 (1975)

[4] T. Hahn
International Tables for Crystallography
(Reidel, Dordrecht, Holland, 1983)

[5] A.P. Cracknell, B.L. Davies, S.C. Miller, W.F. Love
Kronecker Product Tables, Volume 1
(Plenum, New York, 1979)

[6] R. Dirl, B.L. Davies
Space Group Subgroups generated by Sublattice Relations: Practical Algorithm for identifying admissible Sub-Space Groups
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