On Space Groups with Q-Reducible Point Groups

V. Kopsky* and D. B. Litvin

Department of Physics
The Pennsylvania State University
The Berks Campus P.O. Box 2150
Reading, PA 19608 U.S.A.

ABSTRACT

If a point group G of a space group $\mathcal{G}$ is Q-reducible, then the group $\mathcal{G}$ has the following properties: (1) The point group G is a direct or subdirect product of point groups H_1 and H_2 which act on G-invariant subspaces V_1 and V_2. (2) The translation subgroup T_G splits into a direct or subdirect product of its projections T_1 and T_2 onto V_1 and V_2. (3) The subgroups $T_1^o = T_G \cap V_1$ and $T_2^o = T_G \cap V_2$ are normal in $\mathcal{G}$ and the corresponding factor groups $\mathcal{G}/T_1^o$ and $\mathcal{G}/T_2^o$ have the structure of subperiodic groups. (4) The group $\mathcal{G}$ itself is a direct or subdirect product of space groups of lower dimensions. These properties can be used either for the analysis of space groups with Q-reducible point groups or for the construction of space groups on the basis of the knowledge of lower dimensional ones. These points are illustrated by an example of groups of Laue class D_4.

The concept of reducibility plays a central role in the theory of linear operator groups. We will show here how an analogous concept, Q-reducibility[1], works in the theory of space groups and subperiodic groups, i.e. of groups with a discrete translational subgroup.

Any such group $\mathcal{G} = (G;T_G;o;u_G)$ is uniquely defined by its point group G, translational subgroup T_G, and a system of non-primitive translations u_G: $G \longrightarrow V(n)$. The point group G is a group of linear operators on V(n), the vector space associated with the Euclidean space. Let us assume that the point group G is Q-reducible. That is, that the action of G on V(n) is reducible such that $V(n)=V_1(n_1) \oplus V_2(n_2)$ is a splitting of V(n) into G invariant subspaces. In this case, every element $(g\, t+u_G)$ of $\mathcal{G}$ can be written as

$$(g|t+u_G) = \{(g_1,g_2)|t_1+t_2+u_{G1}+u_{G2}\}$$
$$= \{(g_1,e_2)|t_1+u_{G1}\}\,\{(e_1,g_2)|t_2+u_{G2}\}$$

where, for i=1,2, $g_i \in O(n_i)$, $t_i, u_{Gi} \in V_i(n_i)$ and $O(n_i)$. Since the elements $\{(g_1,e_2)|t_1+u_{G1}\}$ and $\{(e_1,g_2)|t_2+u_{G2}\}$ commute, the group $\mathcal{G}$ is a subgroup of $\mathcal{E}(n_1) \oplus \mathcal{E}(n_2)$.

It follows that $\mathcal{G}$ is a subdirect products of subgroups $\mathcal{H}_1 \subset \mathcal{E}(n_1)$ and $\mathcal{H}_2 \subset \mathcal{E}(n_2)$ of two lower-dimensional Euclidean groups. $\mathcal{G}$ can then be expressed as

$$\mathcal{G} = \mathcal{H}_1^o \oplus \mathcal{H}_2^o\,[(e_1,e_2)+(\hat{\gamma}_1^{(2)},\hat{\gamma}_2^{(2)})+\ldots+(\hat{\gamma}_1^{(s)},\hat{\gamma}_2^{(s)})] \quad (1)$$

where

$$\mathcal{H}_1 = \mathcal{H}_1^o[e_1+\hat{\gamma}_1^{(2)}+\ldots+\hat{\gamma}_1^{(s)}]$$
$$\mathcal{H}_2 = \mathcal{H}_2^o[e_2+\hat{\gamma}_2^{(2)}+\ldots+\hat{\gamma}_2^{(s)}] \quad (2)$$
$$\mathcal{H}_1/\mathcal{H}_1^o \simeq \mathcal{H}_2/\mathcal{H}_2^o \simeq \mathcal{G}/[\mathcal{H}_1^o \oplus \mathcal{H}_2^o]$$

and

$$e_i,\ \hat{\gamma}_i^{(j)} \in \mathcal{E}(n_i).$$

The point group G is a subgroup of $O(n_1) \oplus O(n_2)$ and hence is of the form of a subdirect product of subgroups $H_i \subset O(n_i)$, i=1,2:

$$G = H_1^o \oplus H_2^o \,[(e_1,e_2) + (g_1^{(2)},g_2^{(2)}) + \ldots + (g_1^{(p)},g_2^{(p)})] \quad (3)$$

where

$$H_1 = H_1^o \,[e_1 + g_1^{(2)} + \ldots + g_1^{(p)}]$$
$$H_2 = H_2^o \,[e_2 + g_2^{(2)} + \ldots + g_2^{(p)}] \quad (4)$$
$$H_1/H_1^o \simeq H_2/H_2^o \simeq G/[H_1^o \oplus H_2^o]$$

Finally, the translation group T_G is a subdirect sum of its projections T_1 and T_2 onto $V(n_1)$ and $V(n_2)$, respectively:

$$T_G = T_1^o \oplus T_2^o \,\{0 \dotplus d_2 \dotplus \ldots \dotplus d_q\} \quad (5)$$

where

$$T_1 = T_1^o[o \dotplus d_{21} \dotplus \ldots \dotplus d_{q1}]$$
$$T_2 = T_2^o[o \dotplus d_{22} \dotplus \ldots \dotplus d_{q2}] \quad (6)$$
$$T_1/T_1^o \simeq T_2/T_2^o \simeq T_G/[T_1^o \oplus T_2^o]$$

and $T_i^o = T_G \cap V(n_i)$, $i=1,2$. The groups T_1^o and T_2^o are normal subgroups of the space group $\mathcal{G}$ and the corresponding factor groups $\mathcal{G}/T_1^o$ and $\mathcal{G}/T_2^o$ have the structure of subperiodic groups.

We have applied the above concepts of Q-reducibility to two-dimensional space groups and the subperiodic layer groups with Q-reducible point groups.[2] We shall illustrate these points here with the following tables for space groups of the Laue class D_4. For lack of space we

give only cases with primitive Bravais lattices, where the subdirect sum, Equation 5, becomes a direct sum.

In Table 1 we give the point groups H_1, H_2, H_1^o and H_2^o in the decompositions equations (3) and (4), for all point groups G of the Laue class D_4. The factor groups $\mathcal{G}/T_1^o$ and $\mathcal{G}/T_2^o$ have the structure of a rod group[3] and a layer group[4]. In Table 2 we list rod groups and the corresponding space groups $\mathcal{G}$ where the factor group $\mathcal{G}/T_1^o$ is isomorphic to the rod group. Lastly, in Table 3, we list layer groups and the corresponding space groups $\mathcal{G}$ where the factor group $\mathcal{G}/T_2^o$ is isomorphic to the layer group.

ACKNOWLEDGEMENTS

This work was supported in part by National Science Foundation Grant DMR-8406196. We also greatfully acknowledge the financial support given by the Berks Campus Faculty Development Fund and the Penn State Faculty Scholarship Support Fund.

*Permanent address: Institute of Physics
Czechoslovak Academy of Sciences,
NA Slovance 2, POB 24, 18040 Prague 8,
Czechoslovakia

REFERENCES

1) V. Kopsky, J. Phys A19 L181 (1986).
2) D. B. Litvin and V. Kopsky, J. Phys A in press.
3) J. Bohm and K. Dornberger-Schiff, Acta Cryst. 23 913 (1967).
4) E. A. Wood, Bell Telephone Tech. J. 43 541 (1964).

G	H_1	H_2	H_1^o	H_2^o
$D_{4h}(4_z/m_z m_x m_{xy})$	C_{4v}	C_{sz}	C_{4v}	C_{sz}
$D_4(4_z 2_x 2_{xy})$	C_{4v}	C_{sz}	C_4	C_1
$C_{4v}(4_z m_x m_{xy})$	C_{4v}	C_1	C_{4v}	C_1
$D_{2d}(\bar{4}_z 2_x m_{xy})$	C_{4v}	C_{sz}	$\hat{C}_{2v}$	C_1
$\hat{D}_{2d}(\bar{4}_z m_x 2_{xy})$	C_{4v}	C_{sz}	C_{2v}	C_1

Table 1: Q-reducible point groups of the Laue class D_4. $C_{2v}=2_z m_x m_y$ and $\hat{C}_{2v}=2_z m_{xy} m_{x\bar{y}}$. The groups H_1, H_2, H_1^o, and H_2^o are defined in equations (3) and (4).

Point Group	Rod Group	Space Group
D_4	p422	D_4^1, D_4^2
	$p4_122$	D_4^3, D_4^4
	$p4_222$	D_4^5, D_4^6
	$p4_322$	D_4^7, D_4^8
C_{4v}	p4mm	C_{4v}^1, C_{4v}^2
	p4cc	C_{4v}^5, C_{4v}^6
	$\langle$ $p4_2cm$	C_{4v}^3, C_{4v}^4
	$\langle$ $p4_2mc$	C_{4v}^7, C_{4v}^8
D_{2d}	$\langle$ $p\bar{4}2m$	D_{2d}^1, D_{2d}^3
	$\langle$ $p\bar{4}m2$	D_{2d}^5, D_{2d}^7
	$\langle$ $p\bar{4}2c$	D_{2d}^2, D_{2d}^4
	$\langle$ $p\bar{4}c2$	D_{2d}^6, D_{2d}^8
D_{4h}	p4/mmm	$D_{4h}^1, D_{4h}^3, D_{4h}^5, D_{4h}^7$
	p4/mcc	$D_{4h}^2, D_{4h}^4, D_{4h}^6, D_{4h}^8$
	$\langle$ p4/mmc	$D_{4h}^9, D_{4h}^{11}, D_{4h}^{13}, D_{4h}^{15}$
	$\langle$ p4/mcm	$D_{4h}^{10}, D_{4h}^{12}, D_{4h}^{14}, D_{4h}^{16}$

Table 2: Rod groups and corresponding space-groups $\mathcal{G}$ such that the factor group $\mathcal{G}/T_1^o$ is isomorphic to the rod group. A symbol $\langle$ denotes two rod groups of the same class.

Point Group	Layer Group	Space Group
D_4	p422	$D_4^1, D_4^3, D_4^5, D_4^7$
	$p42_12$	$D_4^2, D_4^4, D_4^6, D_4^8$
C_{4v}	p4mm	$C_{4v}^1, C_{4v}^3, C_{4v}^5, C_{4v}^7$
	p4bm	$C_{4v}^2, C_{4v}^4, C_{4v}^6, C_{4v}^8$
D_{2d}	$p\bar{4}2m$	D_{2d}^1, D_{2d}^2
	$p\bar{4}2_1m$	D_{2d}^3, D_{2d}^4
	$p\bar{4}m2$	D_{2d}^5, D_{2d}^6
	$p\bar{4}b2$	D_{2d}^7, D_{2d}^8
D_{4h}	p4/mmm	$D_{4h}^1, D_{4h}^2, D_{4h}^9, D_{4h}^{10}$
	p4/nbm	$D_{4h}^3, D_{4h}^4, D_{4h}^{11}, D_{4h}^{12}$
	p4/mbm	$D_{4h}^5, D_{4h}^6, D_{4h}^{13}, D_{4h}^{14}$
	p4/nmm	$D_{4h}^7, D_{4h}^8, D_{4h}^{15}, D_{4h}^{16}$

Table 3: Layer groups and corresponding space groups $\mathcal{G}$ such that the factor group $\mathcal{G}/T_2^o$ is isomorphic to the layer group.

XV International Colloquium on

GROUP THEORETICAL METHODS IN PHYSICS

October 20-24, 1986
Drexel University, Philadelphia, PA

Editor
R. Gilmore

World Scientific
Singapore • New Jersey • Hong Kong