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The New Double Space Groups

BY WALDEMAR GORZKOWSKI*

Universität Duisburg, Fachbereich 10, *Theoretische Physik, Duisburg, Federal Republic of Germany*

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Abstract

The definition of the double space groups is extended. All the new double space groups are classified.

The symmetry operations forming the space group G obey the following multiplication rule:

$$\{R_2|\mathbf{v}_2\}\{R_1|\mathbf{v}_1\} = \{R_2 R_1|\mathbf{v}_2 + R_2\,\mathbf{v}_1\}.$$

The space group G can be expressed as the sum of the left cosets of the translation group of one of the Bravais lattices T:

$$G = \{R_1|\mathbf{v}_1\}\,T + \{R_2|\mathbf{v}_2\}\,T + \cdots + \{R_h|\mathbf{v}_h\}\,T,$$

where the rotational parts $R_1, R_2, \ldots, R_h$ form one of the 32 crystallographic point groups.

In the case of double groups, for every element R_i of the single point group there are two corresponding elements: R_i and $\bar{R}_i$. We assume that both elements R_i and $\bar{R}_i$ have the same effect in acting on vectors $\mathbf{v}_j$:

$$\bar{R}_i\,\mathbf{v}_j = R_i\,\mathbf{v}_j.$$

The elements R_i and $\bar{R}_i$ obey the multiplication rule of the double point group.

The commonly used (*e.g.* Bradley & Cracknell, 1972) definition of the double space group G^+ corresponding to the single space group G is given by the formula:

$$G^+ = \{R_1|\mathbf{v}_1\}\,T + \{\bar{R}_1|\mathbf{v}_1\}\,T + \{R_2|\mathbf{v}_2\}\,T + \{\bar{R}_2|\mathbf{v}_2\}\,T + \cdots + \{R_h|\mathbf{v}_h\}\,T + \{\bar{R}_h|\mathbf{v}_h\}\,T,$$

where R_i and $\bar{R}_i$ are the elements of the double point group corresponding to the operation R_i in the single point group formed by $R_1, R_2, \ldots, R_h$. The multiplication rules for the members of the double space group G^+ have the form:

$$\{R_2|\mathbf{v}_2\}\{R_1|\mathbf{v}_1\} = \{R_2 R_1|\mathbf{v}_2 + R_2\,\mathbf{v}_1\}$$
$$\{\bar{R}_2|\mathbf{v}_2\}\{R_1|\mathbf{v}_1\} = \{\bar{R}_2 R_1|\mathbf{v}_2 + R_2\,\mathbf{v}_1\}$$
$$\{R_2|\mathbf{v}_2\}\{\bar{R}_1|\mathbf{v}_1\} = \{R_2 \bar{R}_1|\mathbf{v}_2 + R_2\,\mathbf{v}_1\}$$
$$\{\bar{R}_2|\mathbf{v}_2\}\{\bar{R}_1|\mathbf{v}_1\} = \{\bar{R}_2 \bar{R}_1|\mathbf{v}_2 + R_2\,\mathbf{v}_1\}.$$

According to the definition we have 230 double space groups (as in the case of the single space groups). Each of these groups contains the pairs of elements: $\{R_i|\mathbf{v}_i\}$ and $\{\bar{R}_i|\mathbf{v}_i\}$.

It seems that the above definition is not complete. For example, the subgroup G_1^+ of the group G^+ formed by the elements

$$\{E|0\}\,T,$$

where T is the translational group and E denotes the identity, is not the double space group in the sense of the definition given above. This is a rather trivial example. However, the following example is not so trivial.

It is easy to verify that the set G_2^+ given by the formula:

$$G_2^+ = \{E|0\}\,T + \{\overline{C_3^-}|0\}\,T + \{\overline{C_3^+}|0\}\,T,$$

* Permanent address: Instytut Fizyki PAN, al. Lotnikow 32/46, 02-668 Warszawa, Poland.

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where $\overline{C_3^+}$ is the rotation through the angle 240° (Bradley & Cracknell, 1972) and T is the translation group, is the group. It is an infinite group for which the hexagonal primitive translation subgroup T is the normal divisor. A similar remark applies to the subgroup T of the group G_1^+. This property is the characteristic feature of space groups and it would be rational to include the groups considered in the double space groups too.

It seems that the following definition of the double space group G^+ would be better.

The double space group G^+ is the group of the form

$$G^+ = \{P_1|\mathbf{t}_1\}\,T + \{P_2|\mathbf{t}_2\}\,T + \cdots + \{P_q|\mathbf{t}_q\}\,T,$$

where T is the translation group of one of the Bravais lattices, P_1, P_2, ..., P_q forming the evident or non-evident double point group, and $\mathbf{t}_1, \mathbf{t}_2, \ldots, \mathbf{t}_q$ are the fractional translations: the translation $\mathbf{t}_l$ associated with the translation P_l should be equal to the translation $\mathbf{v}_j$ associated with the single operation R_j corresponding to the double operation P_l.

Similar to the case of the double point groups (Gorzkowski & Suffczynski, 1978; Gorzkowski, 1982) the double space groups containing both operations $\{E|0\}$ and $\{\bar{E}|0\}$ will be called evident double space groups. It is clear that the first definition refers to the evident double space groups only.

The problem is to find all the non-evident double space groups, *i.e.* the double space groups which do not contain the operation $\{\bar{E}|0\}$.

At first, it should be remarked that in the non-evident double space groups the rotational parts must form the crystallographic non-evident double point groups. There are six such point groups:

$$\bar{C}_{\frac{1}{2}},\ \bar{C}_{\frac{1}{2}i},\ \bar{C}_{\frac{1}{2}\bar{i}},\ \bar{C}_{\frac{3}{2}},\ \bar{C}_{\frac{3}{2}i},\ \bar{C}_{\frac{3}{2}\bar{i}}.$$

The notation according to Gorzkowski (1982) has been used here. The corresponding single point groups are C_1, C_i, C_i, C_3, C_{3i}, C_{3i} respectively. Therefore, the non-evident double space groups should be subgroups of the double space groups corresponding to the single space groups belonging to the classes C_1, C_i, C_3 and C_{3i}. A very simple analysis shows that there are 11 non-evident double space groups listed in Table 1.

Table 1. *The non-evident double space groups*

E: the identity; I: the inversion; $\bar{I} = I\bar{E}$; $C_{\frac{3}{2}}$: rotation through 240° around the z axis.

Number	Suggested symbol	Translation subgroup	Generators	Corresponding single space group
1	$\bar{C}^1_{\frac{1}{2}}$	Arbitrary (P, Γ_t)	$\{E\|000\}$	$C_1^1\,(P1)$
2	$\bar{C}^1_{\frac{1}{2}i}$	Arbitrary (P, Γ_t)	$\{I\|000\}$	$C_i^1\,(P\bar{1})$
3	$\bar{C}^1_{\frac{1}{2}\bar{i}}$	Arbitrary (P, Γ_t)	$\{\bar{I}\|000\}$	$C_i^1\,(P\bar{1})$
4	$\bar{C}^1_{\frac{3}{2}}$	Hexagonal primitive (P, Γ_h)	$\{C_{\frac{3}{2}}\|000\}$	$C_3^1\,(P3)$
5	$\bar{C}^2_{\frac{3}{2}}$	Hexagonal primitive (P, Γ_h)	$\{C_{\frac{3}{2}}\|00\frac{1}{3}\}$	$C_3^2\,(P3_1)$
6	$\bar{C}^3_{\frac{3}{2}}$	Hexagonal primitive (P, Γ_h)	$\{C_{\frac{3}{2}}\|00\frac{2}{3}\}$	$C_3^3\,(P3_2)$
7	$\bar{C}^4_{\frac{3}{2}}$	Trigonal primitive (R, Γ_{rh})	$\{C_{\frac{3}{2}}\|000\}$	$C_3^4\,(R3)$
8	$\bar{C}^1_{\frac{3}{2}i}$	Hexagonal primitive (P, Γ_h)	$\{IC_{\frac{3}{2}}\|000\}$	$C_{3i}^1\,(P\bar{3})$
9	$\bar{C}^1_{\frac{3}{2}\bar{i}}$	Hexagonal primitive (P, Γ_h)	$\{\bar{I}C_{\frac{3}{2}}\|000\}$	$C_{3i}^1\,(P\bar{3})$
10	$\bar{C}^2_{\frac{3}{2}i}$	Trigonal primitive (R, Γ_{rh})	$\{IC_{\frac{3}{2}}\|000\}$	$C_{3i}^2\,(R\bar{3})$
11	$\bar{C}^2_{\frac{3}{2}\bar{i}}$	Trigonal primitive (R, Γ_{rh})	$\{\bar{I}C_{\frac{3}{2}}\|000\}$	$C_{3i}^2\,(R\bar{3})$

Between the elements of the evident double space groups and the elements of the single space groups there is a two-to-one correspondence. In the case of the non-evident double groups this correspondence is one-to-one, but the term 'double' is conserved because these groups refer to the double space in which $E \neq \bar{E}$.

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