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OPECHOWSKI'S THEOREM AND COMMUTATOR GROUPS

by

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ABSTRACT

This paper shows that the conditions of application of Opechowski's theorem for double groups of subgroups of **O**(3) are directly associated to the structure of their commutator groups. Some characteristics of the structure of classes are also discussed.

Key-words: Double groups.

I. INTRODUCTION

Forty-five years ago Opechowski (1940) defined the double groups and established his now famous theorem which describes their class structure. The theorem states that when a finite group **G**, subgroup of the three-dimensional rotation group **SO**(3) has among its elements two rotations by an angle π through mutually perpendicular axes, the number of classes of its double group **G*** is less than twice the number of classes of **G**.

In this paper we show that when the non trivial element z of $\mathbf{Z}_2$ (the group of the center of **SU**(2)) belongs to the commutator group **G***' of **G***, the theorem of Opechowski applies. In this case, the order of **G***' is always an even number and it is isomorphic to **G**'*, the double group of the commutator group. On the other hand, we also show that if $\mathbf{G}^{*\prime} \sim \mathbf{G}^{\prime *}$ holds, the group **G** contains at least two rotations in π around mutually perpendicular axes. Furthermore, if z does not belong to **G***', this group is of odd order and it is isomorphic to **G**' .

In section II we define a double group of a finite subgroup of **SO**(3) by means of its relation with central extensions.

In section III the commutator group and some of its properties are treated.

The main problem of this paper is discussed in section IV, where an extension to improper groups is also considered.

In section V, a simple treatment of the crystallographic point groups is presented using the results of the preceding sections.

II. THE DOUBLE GROUPS

The elements of the group **SO**(3) are specified completely by a rotation angle in the range $0 \leq \theta \leq \pi$ around a rotation axis $\hat{n}$. Rotations by angles $\theta > \pi$ can always be treated in the same interval using the well-known relation $R(2\pi-\theta,-\hat{n}) = R(\theta,\hat{n})$.

From the irreducible representations (irreps) $D^j(\theta,\hat{n})$, $0 \leq \theta \leq 2\pi$, of the group **SU**(2) it is possible to obtain a set of matrices which forms an irrep of **SO**(3). Taking into account that for $\theta > \pi$ we can write $D^j(\theta,\hat{n}) = (-1)^{2j} D^j(2\pi-\theta,-\hat{n})$, every set of parameters $(\theta,\hat{n})$ is associated to two matrices $D^j(\theta,\hat{n})$ and $(-1)^{2j} D^j(\theta,\hat{n})$. For j half-integer, these matrices form the so called double-valued representations of **SO**(3).

Let $R(\theta_{k\ell},\hat{n}_k)$ denote the elements of a finite group **G** < **SO**(3), where $\theta_{k\ell} = 2\pi\ell/r_k$, $\ell = 1,\ldots,r_k-1$, and $\hat{n}_k$ is the unitary vector in the direction of the r_k-fold rotation axis. Opechowski (1940) has defined the double group **G*** of a group **G** of order $|G|$ as the abstract group of $2|G|$ elements isomorphic to the matrix group of elements $\{\pm D^j(\theta_{k\ell},\hat{n}_k)\}$ for half-integral j .

An alternative definition is possible if we rewrite the set of matrices as $D^j(\theta,\hat{n})\mathbf{Z}_2$, $\mathbf{Z}_2$ being the group with elements $I = D^j(0,\hat{n})$, $-I = D^j(2\pi,\hat{n})$. It can be immediately shown that $D^j(\theta,\hat{n})Z_2$ is a matrix group isomorphic to **SO**(3). On the other hand, as the set of D^j matrices forms a faithful irrep of **SU**(2) for half-integer j, the elements $D^j(\theta,\hat{n})\mathbf{Z}_2$ form a group also isomorphic to the factor group $SU(2)/Z_2$ and then we have $SO(3) \sim \mathbf{SU}(2)/\mathbf{Z}_2$. Therefore, since **G*** must be a finite subgroup of **SU**(2) for **G** < **SO**(3), the isomorphism $G^*/Z_2 \sim \mathbf{G}$ must hold and **G*** is a solution of the central extension of $\mathbf{Z}_2$ by **G** .

Calling $R(2\pi\ell/r_k,\hat{n}_k)$ the elements of **G** < **SO**(3), the double-valued representation of **G** for j=1/2, is given by

$$\pm D^{1/2}(2\pi\ell/r_k,\hat{n}_k) = \pm\{\sigma_0\cos(\pi\ell/r_k) + i\,\vec{\sigma}\,.\hat{n}\,\sin(\pi\ell/r_k)\},$$

where σ_0 is the 2x2 unit matrix and $\vec{\sigma}$ are de Pauli matrices. Since in this equation r_k is the order of the element $g_k \in \mathbf{G}$, there is only one involution within the elements of **G***, i.e. the element $D^{1/2}(2\pi,\hat{n}) = z$, which corresponds to $r_k = 1$ in **G**. Caride and Zanette (1985) have shown that in order to **H** = **G*** it is necessary and sufficient that **H** should have only one involution and $\mathbf{H}/\mathbf{Z}_2 \sim \mathbf{G}$. From this , we can state the theorem of Opechowski in the following form. Let $(a,b) \in \mathbf{G} < \mathbf{SO}(3)$ be two rotations by π around perpendicular axes. Since z is the only element of order two in $\mathbf{G}^*$ and it is mapped onto the unit of $\mathbf{G}$, the orders of the pre-images α,β and $\alpha\beta$ of a, b and ab under the homomorphism $\mathbf{G}^*/\mathbf{Z}_2 \sim \mathbf{G}$ may be fixed by the relations $\alpha^2 = \beta^2 = (\alpha\beta)^2 = z$. Then, z may be written as $z = \alpha^{-1} \beta^{-1} \alpha\beta$ and one thus has that α and αz (and β and βz) belong to the same class in $\mathbf{G}^*$.

III. THE COMMUTATOR SUBGROUP

Let $\mathbf{G}'$ be the commutator subgroup of $\mathbf{G}$. Since $\mathbf{G}/\mathbf{G}'$ is abelian and the canonical mapping of $\mathbf{G}$ onto $\mathbf{G}/\mathbf{G}'$ is a homomorphism, the one-dimensional representations Γ_n of $\mathbf{G}$ are given by

$$\Gamma_n(g) = \gamma_n(g\mathbf{G}') ,$$

where γ_n is a representation of the factor group. The number of one-dimensional irreps is $|G/G'|$.

Since $\mathbf{G}'$ is self-conjugate, it consists of complete conjugacy classes C_i and the same is true for the set of generators of $\mathbf{G}'$ consisting of the commutators $(a^{-1}b^{-1}ab)$, $a,b \in \mathbf{G}$. For if an element $x = a^{-1} b^{-1} a b$ belongs to the set, its conjugate $g x g^{-1} = x^g = (a^g)^{-1} (b^g)^{-1} a^g b^g$ also belongs to it.

Let us now define the operator

$S = \sum_{a,b \in G} a^{-1}b^{-1}ab$ in the group algebra of **G**. It can be written as $S = \sum_i \nu(i) S_i$, where S_i is the class sum operator $S_i = \sum_{x \in C_i} x$ and $\nu(i)$ is the number of times the conjugacy class C_i is contained in the generator set of **G**'. In other words, $\nu(i)$ is the number of times that an element of C_i can be written as a commutator.

Using the orthogonality property of the irreps of **G**, Burnside (1955,p.319) obtained the following expression

$$\nu(i) = (1/|G|) \sum_{j,a,b} \chi^j(a^{-1}b^{-1}a\, b)\, \chi^j(C_i)$$

$$= |G| \sum_j \chi^j(C_i) \,/\, \chi^j(1) \;,$$

where $\chi^j(C)$ denotes the character of C in the representation j.

Applying the formula to $S^n = S \ldots S$ (n times) we find that the number of times an element of the class C_i can be written as the product of n commutators is

$$\nu_n(i) = |G|^{2n-1} \sum_j \chi^j(C_i)/[\chi^j(1)]^{2n-1} \;,$$

a formula due to Van Zanten and de Vries (1973).

As it will be seen in the next section, this expression is the key to obtain the structure of the group **G*** from the structure of **G***' or vice-versa .

IV. RESULTS AND CONCLUSIONS

Let us denote by Γ_j the irreps of the double group **G*** of **G** < **SO**(3). Since z belongs to the group of the center of **G*** and from Schur's lemma, $\Gamma_j(z) = \lambda_j I$, where I is the unit matrix. But $z^2 = 1$, therefore $\lambda_j = \pm 1$. When $\lambda_j = +1$ we have the so called integer irreps and when $\lambda_j = -1$ the half-integer irreps.

There is a very simple relation between the irreps of **G*** and those of **G**. Taking into account that

$$\chi^j(z) = \begin{cases} +\chi^j(1) & \text{for single-valued irreps} \\ -\chi^j(1) & \text{for double-valued irreps} \end{cases}$$

we can now rewrite $\nu_n(i)$ for $n = 1$ and $i = z$ as

$$\nu_1(z) = |G^*| \{2 \times \text{number of irreps of } \mathbf{G} - \text{number of irreps of } \mathbf{G}^*\}.$$

This equation shows that every time the number of irreps of G* is less than the number of irreps of **G**, it is possible to write z as a commutator. Consequently, $z = \alpha\beta\alpha^{-1}\beta^{-1}$ for at least one pair of elements $(\alpha,\beta) \in G^*$. Then, from the homomorphism $\mathbf{G}^*/Z_2 \sim \mathbf{G}$ which maps z onto the unit element of G we have that there are two elements, say $(a,b) \in \mathbf{G}$ such that ab = ba and hence, either a and b are two rotations around the same axis or they are two rotations by π around mutually perpendicular axes.

It will now be shown that if $\alpha\beta = \beta\alpha z$, the rotations a and b cannot be around the same axis. For if this were so, there would be an element d ϵ **G**, such that $a = d^{\kappa}$ and $b = d^{\ell}$, for some integers κ,ℓ .If δ and δz are the pre-images of the element d, the elements $\alpha = \delta^{\kappa}z_{\kappa}$ and $\beta = \delta^{\ell}z_{\ell}$ of **G***, with $(z_{\kappa},z_{\ell}) \epsilon \mathbf{Z}_2$, should be such that

$$\alpha\beta = \delta^{\kappa}z_{\kappa}\ \delta^{\ell}z_{\ell} = \delta^{\kappa+\ell}z_{\kappa}z_{\ell} = \delta^{\ell}z_{\ell}\delta^{\kappa}z_{\kappa} = \beta\alpha \ ,$$

which is contrary to the hypothesis. Thus, a and b are two rotations by π around mutually perpendicular axes.

Since z is the only involution of **G*** it is also the only one involution of **G***'. Then, if we arrange the elements of **G***' in pairs of the type ω,ω^{-1}, those two which are not among them are the unit element and z. Thus, when z ϵ **G***' we can also say that the order of **G***' is an even number.

Now let us suppose that $\nu_1(z) = 0$ and $\nu_n(z) \neq 0$ for $n > n_0 > 1$, i.e. z ϵ **G***' but **G** does not contain two rotations by π around mutually perpendicular axes. Then, the number of irreps of **G*** is twice the number of irreps of **G**. Moreover, since **G*** is a central extension of $\mathbf{Z}_2$ by **G** it will have two conjugacy classes $C(\alpha)$ and $C(\alpha z)$ with the same number of elements as $C(a)$ of **G**. Then, in order to satisfy the orthogonality relations,the character table of **G*** must have the structure of the table corresponding to the direct product **G** x Z_2. This fact would double the number $|G^*|/|G^{*\prime}|$ of one-dimensional irreps of $\mathbf{G}^*$ with respect to $\mathbf{G}$. Hence, the isomorphism $\mathbf{G}'^* \sim \mathbf{G}'$ must hold. But since $z \in \mathbf{G}^{*\prime}$, we have $\mathbf{G}^{*\prime}/\mathbf{Z}_2 \sim \mathbf{G}'$ and the isomorphism $\mathbf{G}^{*\prime} \sim \mathbf{G}'^*$ must hold. This contradiction clearly shows that if $z \in \mathbf{G}^{*\prime}$, $\nu_1(z) \neq 0$ always.

When $z \notin \mathbf{G}^{*\prime}$ the theorem of Opechowski does not apply and the character table of $\mathbf{G}^*$ appears to be one corresponding to a group that can be written as a direct product. However, if the group $\mathbf{G}$, subgroup of $\mathbf{SO}(3)$, is of even order it has at least one element of order two. Hence, if α and αz are the pre-images in $\mathbf{G}^*$ of that element, they must be such that $\alpha^2 = (\alpha z)^2 = z$, and therefore it is not possible to write $\mathbf{G}^*$ as $\mathbf{G} \times \mathbf{Z}_2$. If $\mathbf{G}$ is of odd order, we can write

$$\mathbf{G} \sim \mathbf{C}_{2m+1} = \langle u \,||\, u^{2m+1} = 1 \rangle \quad ,$$

and therefore, only in this case we can write its double group

$$\mathbf{C}^*_{2m+1} = \langle\, u \,||\, u^{2m+1} = z,\ z^2 = 1 \,\rangle$$

as a direct product given by

$$\mathbf{C}^*_{2m+1} = \langle\, uz \,||\, (uz)^{2m+1} = 1 \,\rangle \times \mathbf{Z}_2 \ .$$

Let us now see how these results apply to improper subgroups of $\mathbf{O}(3)$.

When $\mathbf{G}$ is an improper group not isomorphic to a direct product of a group by the inversion, the preceding discussion is also valid since **G*** has only the element z as involution. Improper rotations belonging to these groups which do not contain the inversion explicitly, can be written in the form ig, where g is a proper rotation of even order. Thus, the order of the pre-images of ig in **G*** is always twice the order of ig .

When **G** is an improper group that can be written as $\mathbf{G} = \mathrm{H} \times \mathbf{C}_i$ where $\mathbf{H} < \mathbf{SO}(3)$, **G*** is isomorphic to $\mathbf{H}^* \times \mathbf{C}_i$ (Altmann, 1979). In this case, the results obtained can be directly applied to **H**. Furthermore, although in this case **G*** has three involutions, i, z and iz, the results are still valid because the inversion cannot be written as a commutator and therefore z is still the unique element of order two of **G*'**.

V. CRYSTALLOGRAPHIC POINT GROUPS

We now show that if **G'** is of even order, **G*'** is of even order and then $z \in \mathbf{G}^{*'}$. This was to be expected since if the order of **G'** is even there is at least one element of order two in **G'** and one of its pre-images, either α or αz must belong to **G*'**. But since $\alpha^2 = (\alpha z)^2 = z$, it follows that $z \in \mathbf{G}^{*'}$ and then $\mathbf{G}^{*'} \sim \mathbf{G}'^{*}$.

Point groups with commutator groups of even order for which the Opechowski theorem applies are $\mathbf{C}_{4n,v} \sim \mathbf{D}_{2n,d} \sim \mathbf{D}_{4n}$; $\mathbf{D}_{4n,h} \sim \mathbf{D}_{4n} \times \mathbf{C}_i$; $\mathbf{T}$; $\mathbf{T}_h = \mathbf{T} \times \mathbf{C}_i$; $\mathbf{O}_h = \mathbf{O} \times \mathbf{C}_i$; $\mathbf{T}_d \sim \mathbf{O}$; $\mathbf{Y}$ and $\mathbf{Y}_h = \mathbf{Y} \times \mathbf{C}_i$.

When the commutator group is of odd order we have two alternatives: either $\mathbf{G}^{*\prime} \sim \mathbf{G}'$ or $\mathbf{G}^{*\prime} \sim \mathbf{G}'^{*}$. First case includes the cyclic groups $\mathbf{C}_n$, $\mathbf{C}_{n,h}$ and $\mathbf{S}_{2n}$, since the central extensions of $\mathbf{Z}_2$ by them are also cyclic and consequently, $\mathbf{G}^{*\prime} \sim \mathbf{G}' \sim \mathbf{C}_1$.

Let us now see the remaining crystallographic point groups which are isomorphic to $\mathbf{D}_n$ or to $\mathbf{D}_n \times \mathbf{C}_i$. The dihedral groups can be presented (Suzuki,1982) as

$$\mathbf{D}_n = < \rho,\varepsilon \; || \; \rho^n = \varepsilon^2 = (\rho\varepsilon)^2 = 1 >$$

and their double groups (Opechowski, 1940) as

$$\mathbf{D}_n^* = < u,v \; || \; u^n = v^2 = (uv)^2 = z, \; z^2 = 1 > ,$$

where $u = (\rho,1)$ and $v = (\varepsilon,1)$. Thus, the corresponding commutator groups are

$$\mathbf{D}_n' = < \rho^2 \; || \; \rho^n = 1 > \text{ and } \mathbf{D}_n^{*\prime} = < u^2 \; || \; u^n = z, \; z^2 = 1 > .$$

Therefore we see that if $n = 2m+1$,

$$\mathbf{D}'_{2m+1} = < \rho \; || \; (\rho)^{2m+1} = 1 > , \quad \mathbf{D}^{*\prime}_{2m+1} = < u^2 \; || \; (u^2)^{2m+1} = 1 >$$

and consequently, the commutator groups of the double groups of $\mathbf{C}_{2n+1,v} \sim \mathbf{D}_{2n+1}$ and $\mathbf{D}_{2n+1,d} \sim \mathbf{D}_{2n+1} \times \mathbf{C}_i$ are isomorphic to their commutator groups, i.e. for these groups $\mathbf{G}^{*\prime} \sim \mathbf{G}'$.

When $n = 4m+2$ we have

$$\mathbf{D}^{*\prime}_{4m+2} = < u^2 \; || \; (u^2)^{2m+1} = z, \; z^2 = 1 > .$$

Since $z \in D^{*'}_{4m+2}$ the double groups of the point groups $C_{4n+2,v} \sim D_{2n+1,h} \sim D_{4n+2}$ and $D_{4n+2,h} \sim D_{4n+2} \times C_i$ will have a number of classes which is less than twice the number of classes of its corresponding groups, and $G^{*'} \sim G^{'*}$.

Finally, we can say that in order to have a character table for G^* of the type corresponding to a direct product of G by Z_2 it is necessary and sufficient that $|G^*/G^{*'}| = 2\,|G/G'|$. This is so because $\nu_n(z)$ is by definition a positive function. Moreover, since the unit element can always be written as a commutator, ν_n is also a non decreasing function of n, i.e. $\nu_n(z) \leq \nu_{n+1}(z)$ and since $\lim_{n\to\infty} \nu_n(z) = |G^*|^{2n+1} \{2|G/G'| - |G^*/G^{*'}|\}$ we see that if $|G^*/G^{*'}| \neq 2|G/G'|$, $\nu_n(z) \neq 0$.

REFERENCES

Altmann, S.L. 1979 Mol.Phys. 38 2 .

Burnside, W. 1955 Theory of Groups of Finite Order (New York: Dover) (2nd ed.).

Caride, A.O. and Zanette, S.I. 1985 Mol.Phys. Vol.55

Opechowski, W. 1940 Physica VII nº 6 552.

Suzuki, M. 1982 Group Theory I (New York: Springer-Verlag).

Van Zanten, A.J. and de Vries, E. 1973 J.Math.Phys. 14 1423.