LETTERS TO THE EDITOR

EXTENDED POINT GROUPS

The introduction of the anti-identity operation increases the number of the point groups from 32 to 122. These 122 groups are generally classified into three categories, namely: (*i*) the 32 crystallographic point groups, (*ii*) 32 grey groups containing the anti-identity operation explicitly and (*iii*) 58 double-coloured point groups consisting of one or more of the complementary symmetry operations introduced by Zheludev.[1] The classification of symmetry groups and the groups of various kinds of anti-symmetry has been defined more precisely by Zamorzaev[2] and Galyarskii and Zamorzaev.[3] The connection between coloured symmetry point groups and one-dimensional complex representations of the ordinary crystallographic point groups has been investigated, without the use of the representation theory, by Indenbom, Belov and Neronova.[4] Introducing a new definition of equivalence, which is a generalisation of the concept adopted earlier by Krishnamurty and Gopalakrishnamurty,[5] of two irreducible representations of the same dimension and nature of a crystallographic point group, it is shown, in this note, that the number of the point groups can be extended from 122 to 174.

Two alternating representations of a crystallographic point group G have been regarded[5] as magnetically equivalent, if the associated subgroups of index 2 of G are isomorphous. From the above concept, we observe that the magnetic equivalence of two alternating representations of a point group G arises only in the case of those point groups which have two conjugate classes of equal order consisting of isomorphous (or equivalent) elements.[6] Further we note that by interchanging two such conjugate classes, the characters of the elements of the conjugate classes are also interchanged. If, in the process of interchange of two such classes, an alternating representation A of G goes over into istelf, then A is an inequivalent representation. But if A goes over to B of G and B, in turn, goes over to A, then they are to be regarded as magnetically equivalent. For instance, the alternating representations A_2, B_1 and B_2 of the point group 222 are magnetically equivalent. Generalising these ideas, we are lead to the following definition: two irreducible representations of the same dimension and of the same nature (both real or complex) of a crystallographic point group G are regarded as physically (or magnetically) equivalent, if one goes over into the other by an interchange of two conjugate classes of G, which are of the same order and consist of isomorphous elements.

This definition has been applied to the various irreducible representations of the 32 crystallographic point groups. Consequently, 18 one-dimensional complex representations, 23 two-dimensional real representations and 11 three-dimensional real representations are found to be distinct, in addition to the known 58 alternating representations and the 32 identity representations. The distribution of the 18 distinct one-dimensional complex representations is indicated below against the corresponding point groups:

$$4\,(1);\quad \bar{4}\,(1);\quad \frac{4}{m}\,(2);\quad 3\,(1);\quad \bar{3}\,(2);\quad \frac{3}{m}\,(2);$$

$$6\,(2);\quad \frac{6}{m}\,(4);\quad 23\,(1) \text{ and } m\,3\,(2).$$

In the light of this definition, all the 23 real two-dimensional and 11 three-dimensional real representations present in the 32 point groups are found to be distinct. Assuming that each distinct representation induces a new group, as is true in the case of alternating representations, we conclude that 52 new groups can be induced by the 52 distinct representations enlisted above. These 52 groups together with the 122 groups described earlier constitute the 174 extended point groups. The validity of the definition introduced in this note can also be judged from the fact that it leads to known results in the case of one-dimensional complex,[4] alternating[5] and identity representations.

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