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Group algebras and tensor operators

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Abstract. The conditions under which class sum operators for a finite group are hermitian are discussed. A class of linear mappings within the group algebra is treated, together with methods of obtaining elements which are symmetry adapted with respect to these mappings. Traditional tensor operators are treated as symmetry adapted elements of the group algebra, and the absence of certain types of tensor operator from the group algebra of direct product groups is discussed. The relevance of the work to operator equivalent theory is briefly indicated.

1. Introduction

The commuting operator approach to finite group theory (Killingbeck 1970a,b) treats group representation theory in the spirit of the Dirac approach to quantum mechanics. If we formally allow addition of group elements (ie use the group algebra) then the sum of the elements within one class of the group is called a class sum. The various class sums commute with one another and thus yield a set of commuting operators $\mathscr{C}_j$ if the group elements are represented by linear operators as is usual in quantum mechanics. Each irreducible representation of the group is then labelled by a set of eigenvalues of the commuting class sum operators $\mathscr{C}_j$, and within a two (or more) dimensional representation the different functions can be further labelled by eigenvalues of some single group operator (since each single group element also commutes with all the class sums). With this approach it is possible to simplify the theory of Kronecker products, projection operators and tensor operators. In an earlier paper (Killingbeck 1970a) the general theory was outlined, and the particular point group $\bar{6}m2$ which appears as the crystal field symmetry group for several rare earth salts, was used to illustrate the procedures of the theory. The present paper re-investigates the form of some of the particular results obtained for $\bar{6}m2$ and shows that it is common to a wide class of groups. This leads to some new topics within the general theory. Section 2 makes some comments concerning simply reducible groups and the hermiticity of the class sum operators. Section 3 describes several types of linear mapping within the group algebra and shows that one of them leads to the regular representation of the group while another is that needed in the traditional tensor operator definition of quantum mechanics. The adaptation of the usual projection operator and character analysis methods to the construction of tensor operator elements within the group algebra is described. Section 4 applies this to $\bar{6}m2$ pointing out that the nonappearance of certain types of tensor operator elements within the $\bar{6}m2$ group algebra is a special case of a general result concerning direct product groups. Section 5 concludes with some remarks on operator equivalent theory. At one or two points a distinction is drawn between abstract elements (of a group or algebra) and the operators which represent them. However, as noted previously (Killingbeck 1970b), questions involving hermiticity, unitarity, etc only arise for *groups of operators.*

2. Simple reducibility for point groups

Since each of the $n^{(\lambda)}$ functions belonging to the λth irreducible representation has an eigenvalue $\mu^{(\lambda)}(\mathscr{C}_j)$ for the jth class sum element, it follows that the characters $\chi_j^{(\lambda)}$ of the representations obey the relation

$$n^{(\lambda)}\mu^{(\lambda)}(\mathscr{C}_j) = \chi^{(\lambda)}(\mathscr{C}_j). \tag{1}$$

(This form of the relationship is independent of any numerical factors which may be included in the definition of the class sums.) Traditional character tables thus show, for example, that the eigenvalues of the class sum elements $\mathscr{C}_j$ for the group $\bar{6}m2$ are all real (Killingbeck 1970a). This feature can be maintained for any group within which the class sum operators are all hermitian, and it is in such cases that the analogy with Dirac theory will be strongest, since Dirac theory uses sets of commuting observables (ie hermitian operators). The individual group elements for the usual point groups are represented by unitary linear operators, and so for an abelian point group the class sum operators will be unitary. This will not be so for a nonabelian group, except for the special cases of the zero rotation and rotations through angle π, which are both unitary *and* hermitian when considered as operators. If, however, each unitary group operator R belongs to the same class as its inverse, $R^{-1} = R^{\dagger}$, it follows that each class sum operator is a sum of terms of form $R+R^{\dagger}$ and is accordingly hermitian. Wigner (1940) made a detailed study of *simply reducible groups*, which he defined to have the properties: (i) An element and its inverse always belong to the same class. (ii) The Kronecker product of two irreducible representations contains any given irreducible representation not more than once. The property (ii) means that various diagonal sum rule procedures work for simply reducible groups; Wigner's work was mainly directed to showing that much of the formalism concerning even and odd representations, $3j$ and $6j$ symbols etc, which applies for the rotation group R_3, can be naturally extended to apply to any simply reducible group. The definition of simple reducibility used by Wigner applies for both finite groups and continuous groups (such as R_3); Lomont (1959) gives an alternative definition for finite groups; a finite group is simply reducible if

$$\sum_R [\mathscr{G}(R)]^3 = \sum_R [\mathscr{E}(R)]^2 \tag{2}$$

where the sums are over all group elements, $\mathscr{G}(R)$ is the number of square roots of R and $\mathscr{E}(R)$ is the number of elements which commute with R. Neither in Wigner's work nor in the rest of the literature does there seem to be any comment on the relationship between conditions (i) and (ii) mentioned above. However, a survey of the point groups known to solid state physicists actually provides sufficient examples to show that (i) and (ii) are logically independent (although they are both fulfilled by most crystal point groups used in practice). For example, the cyclic group 3 fulfills condition (ii) but not condition (i). The icosahedral group P (Judd 1957) fulfils condition (i) but not condition (ii). The group 23 of symmetry rotations of a regular tetrahedron fulfils neither (i) nor (ii): If $n^{(\lambda)}$ is the dimension of the λth irreducible representation of a group, and $n(\max)$ is the largest of the $n^{(\lambda)}$, it is clearly sufficient that the condition

$$[n(\max)]^2 > \sum_{\lambda} n^{(\lambda)} \tag{3}$$

should be obeyed in order to violate condition (ii). Both the icosahedral group P and the group 23 satisfy condition (3). 23 has $n^{(\lambda)}$ values $(1, 1, 1, 3)$ and also has rotations through angles $2\pi/3$ and $4\pi/3$ which belong to different classes. The interesting point about condition (i) as far as the present discussion is concerned is that any point group which satisfies it will give hermitian class sum operators $\mathscr{C}_j$; this makes the parallel between the class sum operator approach and the Dirac commuting observables approach as close as possible. As the discussion above shows, the group P satisfies (i), as do the simply reducible groups, whereas cyclic groups such as 3 and 6 do not. However, abelian groups such as 2 and 222 involving rotations through angle π have class sum operators which are simultaneously unitary and hermitian, and obey condition (i). Even non-hermitian class sum operators will have real eigenvalues for some of the irreducible representations (eg the identity representation), but the total array of eigenvalues must contain some complex elements. Criterion (i) as given above is also the sufficient condition to ensure that the coefficients c_{JKN} appearing in the class multiplication table are symmetric in any two subscripts (Killingbeck 1970a).

3. Linear mappings and tensor operators within the group algebra

The group algebra consists of all linear combinations of form $\Sigma\, z_k R_k$, the R_k being group elements (often represented by operators) and the z_k complex numbers. There are two types of linear mapping within this algebra which are immediately suggested by the usual procedures of quantum mechanics. The first one involves regarding the elements of the algebra as 'wavefunctions', with the individual group elements acting from the left as 'operators', according to the rule

$$R_m\left(\sum_k z_k R_k\right) = \sum_k z_k(R_m R_k) \tag{4}$$

with $R_m R_k$ being found from the group multiplication table. If we take the individual group elements as operands (ie we set all z_k equal to 0 or 1) then the result is that each group element (regarded as an operator) is represented by a $g \times g$ permutation matrix, g being the order of the group. This, of course, is the so-called regular representation of the group (Weyl 1931), and the mapping is traditionally called a left translation. By using the usual projection operator methods it is then possible to project out elements $F_j^{(\lambda)}$ within the group algebra which belong to the various irreducible representations of the group. A second kind of mapping which can be used in the group algebra is one which takes account of the fact that the group operators are often represented by quantum mechanical operators. The type of transformation appropriate to operators is of form

$$\sum_k z_k R_k \to \sum_k z_k(R_m R_k R_m^{-1}) \tag{5}$$

and we can apply this within the group algebra also. The definition of irreducible tensor operators for a finite group of operators (Wigner 1940) involves exactly this kind of mapping

$$RT_j^{(\lambda)}R^{-1} = \sum_k T_k^{(\lambda)}D_{kj}^{(\lambda)}(R). \tag{6}$$

Here R is any group operator and the $T_j^{(\lambda)}$ are the component operators belonging to the irreducible tensor family with representation matrices $D_{kj}^{(\lambda)}$. We can apply the same character analysis and projection techniques when dealing with transformation (5) as we use in connection with equation (4). Indeed, if we have *any* group of linear mappings $\mathscr{M}(R_k)$ which is in one-to-one correspondence with the group elements R_k and which operates within the group algebra, we can form the combination

$$\sum_{R_k} \chi^{(\lambda)*}(R_k)(\mathscr{M}(R_k)X) \tag{7}$$

for any X in the group algebra. The resulting element of the algebra then transforms according to the λth irreducible representation *under the mapping* $\mathscr{M}$. This last proviso is important, for the following reason. The regular representation of a group contains each irreducible representation at least once, so that we can apparently obtain elements of the group algebra belonging to *any* irreducible representation of the group. However, they only belong to their given symmetry types with respect to the mapping (4), and in general *do not* have such simple transformation properties under the mapping (5). For example, there are no elements in the $\bar{6}m2$ group algebra which belong to the B_1, B_2 or E_2 symmetry types of $\bar{6}m2$ for the mapping (6) (Killingbeck 1970a), although there are elements which belong to those symmetry types for the mapping (4). It is, of course, the mapping (5) which must be used if we wish to interpret the resulting symmetry adapted elements of the group algebra as tensor operators which act on quantum mechanical wavefunctions. As an example of a more general type of mapping which could be used in conjunction with (7), we may quote the group of mappings defined by

$$\mathscr{M}(R)X = RXU \qquad (U^2 = U) \tag{8}$$

for any idempotent element U of the group algebra. The choice $U = 1$ gives mapping (4).

Suppose that we use the character projection operator (7) and the mapping (5) to obtain an element of the algebra which belongs to the λth irreducible representation. We have, since all elements in the same class have the same character

$$\sum_{R_k} \chi^{(\lambda)*}(R_k)R_k = \sum_j \chi^{(\lambda)*}(j)\mathscr{C}_j \tag{9}$$

where j is a class label and $\mathscr{C}_j$ a class sum operator. Since every group element commutes with each $\mathscr{C}_j$, it follows that all the group algebra elements of type (9) are of A_1 (identity) type from the point of view of the mapping (5) and can be regarded as A_1 tensor operators. By acting on the identity element of the group with the operator (9) and varying the choice of λ we can obtain elements of the group algebra corresponding to each irreducible representation, but they will all be of A_1 type when regarded as tensor operators undergoing the mapping (5). The element displayed in equation (9) is, in fact, the *only* element of λ symmetry type (except for a trivial phase factor) if the λ representation is one dimensional. We have

$$\begin{aligned}\sum_{R_k} \chi^{(\lambda)*}(R_k)R_kX &= [\chi^{(\lambda)*}(X)]^{-1}\sum_{R_k} \chi^{(\lambda)*}(R_kX)R_kX \\ &= [\chi^{(\lambda)*}(X)]^{-1}\sum_{R_k} \chi^{(\lambda)*}(R_k)R_k \end{aligned} \tag{10}$$

by using the group multiplication property, and taking X to be *any* group element. This is in accord with the result that each one dimensional irreducible representation appears once in the regular representation. The character projection operator which yields a tensor operator of the λ symmetry type acts on a group element X as follows

$$P^{(\lambda)}X = \sum_{R_k} \chi^{(\lambda)*}(R_k)R_kXR_k^{-1} \tag{11}$$

and thus yields only linear combinations of elements from within the same class as X, whereas the operator (9) mixes elements from different classes. It is essentially this difference which leads to the fact that for some groups (eg $\bar{6}m2$) tensor operators of some symmetry types do not exist in the group algebra. The types of tensor operator which can be formed from the elements of a given class can be found by using character analysis in the standard way; for a mapping $\mathscr{M}(R_k)$ of the type discussed in connection with equation (8), the appropriate definition of character to be employed is as follows:

$$\begin{matrix}\text{character of set } j \\ \text{with respect to element } \mathscr{M}(R)\end{matrix} = \begin{matrix}\text{number of elements of } j \\ \text{mapped into themselves by } \mathscr{M}(R).\end{matrix} \tag{12}$$

This is adequate here, since both mappings (4) and (5) take one group element over into exactly one group element. It was in this way that the A_1, A_2 and E_1 tensor operators in the algebra of $\bar{6}m2$ were obtained, while B_1, B_2 and E_2 types were proved nonexistent within the algebra. The mechanism of the construction was not explained in the earlier paper (Killingbeck 1970a), which merely quoted the results; in the present paper the procedure has been described for more general types of mapping.

4. Tensor operators for direct product groups

The group algebra of the group $\bar{6}m2$ was previously found (Killingbeck 1970a) to contain only tensor operators of A_1, A_2 and E_1 types. We shall now show that this result can be explained by using the fact that $\bar{6}m2$ is a direct product group. The two groups involved in the product are the group 32 and the group $(1, \sigma)$ consisting of the identity element and the reflection operation in a mirror plane perpendicular to the three fold axis of 32.

The classes of 32 may be set out as follows: (1); $(3, 3^2)$; $(2, 2', 2'')$. We start by giving some examples which illustrate the general theory of § 3. Suppose we wish for an element of symmetry type A_2 in the 32 group algebra. The three classes have characters $1, 1, -1$, respectively, for A_2 and we find the elements

$$1+3+3^2-2-2'-2'' \tag{13}$$

$$3-3^2 \tag{14}$$

where (13) refers to mapping (4) and (14) to mapping (5). A more complicated problem is the finding of two elements (tensor operators) of E symmetry type for the mapping (5). The traditional approach would involve using projection operators incorporating the detailed representation matrix elements. We can proceed in another way as follows. The group operator 3 has the eigenvalues 1 for those functions belonging to A_1 or A_2, and has the character -1 for the E family. It follows that the eigenvalues of 3 within the E family must be ω and ω^2, where $\omega = \exp(i2\pi/3)$. If we use this classification of the two members of the E family, we can project out the (E, ω) member by 'knocking out' that part of an operand which has eigenvalues 1 or ω^2 for the operator 3. We can apply this approach for either of the mappings (4), (5), but consider only (5) here. We find for the effect of the projection on element 2

$$323^2-2 = 2'-2 \tag{15a}$$

$$\begin{aligned}3(2'-2)3^2-\omega^2(2'-2) &= 2''-2'-\omega^2(2'-2)\\ &= 2''+\omega 2'+\omega^2 2.\end{aligned} \tag{15b}$$

In (15*a*) eigenvalue 1 is removed, in (15*b*) eigenvalue ω^2 is removed. The resulting element of the group algebra is a tensor operator of (E, ω) type. The (E, ω^2) element can be obtained by interchanging ω and ω^2 in (15*b*).

By using the methods of § 3, as exemplified in the last paragraph above, we can obtain the tensor operators in the 32 group algebra. On adjoining the reflection element σ to 32 in order to form $\bar{6}32$, the effect on the mappings (4) and (5) is *different*. For example, if T_j is a symmetry adapted element of the 32 algebra with respect to mapping (4) and X is any element of 32, we have

$$X(T_j \pm \sigma T_j) = \sum_k D_{kj}^{(\lambda)}(X)(T_k \pm \sigma T_k) \tag{16a}$$

$$\sigma X(T_j \pm \sigma T_j) = \pm \sum_k D_{kj}^{(\lambda)}(X)(T_k \pm \sigma T_k). \tag{16b}$$

This shows that $\bar{6}32$ symmetry adapted elements can be formed by taking the obvious linear combinations of the elements T_j and σT_j, and this can be done for every 32 irreducible representation. If we attempt to do the same for the mapping (5) we find

$$X(T_j \pm \sigma T_j)X^{-1} = \sum_k D_{kj}^{(\lambda)}(X)(T_k \pm \sigma T_k) \tag{17a}$$

$$\sigma X(T_j \pm \sigma T_j)(\sigma X)^{-1} = \sum_k D_{kj}^{(\lambda)}(X)(T_k \pm \sigma T_k). \tag{17b}$$

(We note that the T_j in equations (16) and (17) are *not* the same!) The result (17*b*) arises because σ commutes with every X in 32, and it shows that the only $\bar{6}32$ tensor operators obtainable within the $\bar{6}32$ group algebra are those which are invariant under the σ mapping. This is why no B_1, B_2 or E_2 tensor operators were found in the earlier paper. The group $(1, \sigma)$ has only A_1 (identity) type tensor operators, namely the class sums 1 and σ (or any linear combination of them), and this is also the case for any abelian group. The results obtained here for $\bar{6}32$ may at once be generalized as follows; if the group $G = A \times B$ is a direct product group, then tensor operators of the Kronecker product symmetry type $\Gamma(A) \times \Gamma'(B)$ cannot be found in the G group algebra if $\Gamma(A)$ tensor operators do not exist in the A algebra or $\Gamma'(B)$ tensor operators do not exist in the B algebra. The proof depends on the fact that every transformation of type (5) for G factors into separate A and B parts. It may be seen intuitively as follows; if we regard the A elements as 'coefficients' in a generalized B group algebra, we require a Γ' type element in this algebra. If we cannot find such an element using complex coefficients then we cannot find it by using A group elements as coefficients either. It follows that in this case there can be no G algebra element of $\Gamma(A) \times \Gamma'(B)$ type.

5. Conclusion

It should be stressed that this paper deals with the construction of tensor operators *within the group algebra.* If such operators can be found, then they could act as operator equivalents for quantum mechanical operators of the same symmetry type, as explained by Killingbeck (1970a). That they *cannot* be found, places no restriction on the allowed types of physical operator. For example, the operator z belongs to the B_2 symmetry type for $\bar{6}m2$, and to the A_2 symmetry type for $(1, \sigma)$, but has no operator equivalent within the $\bar{6}m2$ group algebra. Both the original operators and their operator equivalents must have the same transformation properties, of course. The 32 operators (E, ω), (E, ω^2) correspond to complex coordinate operators such as $x \pm iy$. To obtain an E pair equivalent to (x, y) we could use the eigenvalue (± 1) of operator 2 to label the two members of the E family, with the x axis taken as the rotation axis.

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