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The Splitting of a Degenerate Level Under the Action of a Symmetry-Breaking Hamiltonian

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The ***qualitative*** problem of the splitting of a degenerate level under the action of a symmetry-, breaking Hamiltonian was solved many years ago by Bethe, with a simple and now classic group-theoretical method. By contrast, the ***quantitative*** problem of actually computing the size of the splitting is far more elaborate and correspondingly inelegant. We present in this paper a new method to solve this second problem, which, we feel, shares much of the directness and economy of the Bethe solution to the first problem.

O problema ***qualitativo*** do desmembramento de um nível degenerado sob a ação de um hamiltoniano de quebra de simetria foi resolvido por Bethe, muitos anos atrás, por um método simples de teoria de grupos que **já** se tornou clássico. Por outro lado, o problema ***quantitativo*** de calcular efetivamente a magnitude do desmembramento é muito mais complicado e, consequentemente, deselegante. Apresentamos neste artigo um novo método para resolver o segundo problema que, em nossa opinião, tem muito da economia e concisão da solução de Bethe para o primeiro problema.

1. Motivating Physical Problem

Among the many applications of symmetry techniques to atomic spectroscopy, one may distinguish two types of problems, as exemplified below:

a) Qualitative problem. Given an atomic level of specified symmetry under the rotation group (say, a level $L = 3$), into *how* many terms does the level split when the rotational symmetry is replaced by a lower symmetry (say, a crystalline field of octohedral symmetry)?

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b) Quantitative problem. Under the same circumstances, determine how ***much*** the energy levels split under a field (operator) invariant under the lower symmetry (crystal symmetry), but having specified transformation properties under the rotation group (for example, it is a $L = 4$ tensor operator).

The fírst problem ("how many" levels) is elegantly solved by the use of character tables for the symmetry groups involved; this is well known from the classic work of Bethe[1].

In contrast to the case with which the first problem is solved, the second problem ("how much" splitting) is surprisingly messy, and involves relatively complicated techniques and methods[2]. This has been expressed very well by Judd[3]: "It is difficult to avoid the feeling that a more direct method exists, especially since many of the roots of what appear to be complex determinantal equations turn out to be very simple".

The purpose of the present paper is to present a method for solving problems of the second type (quantitative evaluation of level splitting) which has, we feel, much of the economy and directness with which the nonquantitative structural problem (problem a) is solved.

In order that the method be grasped most easily, Section 2 discusses a typical example – the splitting of rotational levels by an octohedral symmetry – in such a fashion as to induce the ideas and concepts of the new method. Section **3** abstracts and rephrases these concepts in the language of group theory and then presents a complete solution for speciíied groups. A concluding section discusses generalizations and open problems.

2. An Example

Let us consider the splitting of an atomic level (characterized by the angular momentum L under the rotation group R,) when placed in a crystalline field of octohedral symmetry.

A), To solve problem a) one needs the character table of the octohedral group (Table I), and the character table of the group R,, given by the formula

$$X_L(\beta) = \frac{\sin[(L + 1/2)\beta]}{\sin[(1/2)\beta]} \tag{1}$$

Then, by reducing (subducing) the representations of R, into the irreducible

N.° of group elements in each class	Representations → Classes ↓	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
1	$R_{0°}$	1	3	2	3	1
6	$R_{180°}$	1	1	0	−1	−1
8	$R_{120°}$	1	0	−1	0	1
6	$R_{90°}$	1	−1	0	1	−1
3	$R_{180°}$	1	−1	2	−1	1

Table I - Character table for the octohedral group $\mathcal{O}$ (isomorphic to the symmetric group S_4).

representations of $\mathcal{O}$ by the standard procedure, using the formula

$$X_L(\beta_i) = \sum_k a_k{}^L X_{\Gamma_k}(\beta_i), \tag{2}$$

one immediately gets the solution, as shown in Table II. For example, one immediately reads from the table that an L = 3 level splits into 3 levels, two triply degenerate (representations Γ_2 and Γ_4) and one non-degenerate (representation Γ_5).

	1	2	3	4	5
$L = 0$	1	0	0	0	0
$L = 1$	0	0	0	1	0
$L = 2$	0	1	1	0	0
$L = 3$	0	1	0	1	1
$L = 4$	1	1	1	1	0
—	—	—	—	—	—

Table II - Qualitative splitting of a level with angular momentum L in a field of octohedral symmetry.

Before proceeding to the second problem b), let us remark, as a warming up exercise for our. method, that an equivalent solution to problem a) could be obtained with the following recursive procedure.

Recall the Clebsch-Gordan series for the representations D_L of R_3:

$$D_L \times D_{L'} = D_{L+L'} + D_{L+L'-1} + \ldots + D_{|L-L'|}, \tag{3}$$

and the corresponding results for the group O (Table III).

	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
Γ_1	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
Γ_2	Γ_2	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$	$\Gamma_2 + \Gamma_4$	$\Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5$	Γ_4
Γ_3	Γ_3	$\Gamma_2 + \Gamma_4$	$\Gamma_1 + \Gamma_3 + \Gamma_5$	$\Gamma_2 + \Gamma_4$	Γ_3
Γ_4	Γ_4	$\Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5$	Γ_4	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$	Γ_2
Γ_5	Γ_5	Γ_4	Γ_3	Γ_2	Γ_1

Table III - Multiplication table for the irreducible representations of the group $\mathcal{O}$

Assume known that the representations D_0, D, of R, reduce as follows under the group O:

$$D_0 = \Gamma_1 ; \quad D_1 = \Gamma_4 . \tag{4}$$

Then from

$$D_1 \times D_1 = D_0 + D_1 + D_2 \tag{5}$$

and

$$r, \times \Gamma_4 = r, + r, + r, + r,, \tag{6}$$

one immediately gets

$$D_2 = \Gamma_2 + \Gamma_3 . \tag{7}$$

From

$$D_2 \times D_1 = D_1 + D_2 + D_3 \tag{8}$$

and

$$(\Gamma_2 + \Gamma_3) \times \Gamma_4 = 2\Gamma_2 + \Gamma_3 + 2\Gamma_4 + \Gamma_5 , \tag{9}$$

one immediately gets

$$D_3 = \Gamma_2 + \Gamma_4 + \Gamma_5 \tag{10}$$

and so on.

B) Let us now go over to problem b) and consider the quantitative effects of a symmetry-breaking Hamiltonian, invariant under O, and transforming as a tensor V_k under R,. By working out explicitly the perturbation equations (see Ref. 2 for details), one can write the results as in Table **IV**. The

		Γ_1	Γ_2	Γ_3	Γ_4	Γ_5
$L = 0$	$V_0(0)$	1	0	0	0	0
$L = 1$	$V_0(1)$	0	0	0	1	0
$L = 2$	$V_0(2)$	0	1	1	0	0
	$V_4(2)$	0	−2	3	0	0
$L = 3$	$V_0(3)$	0	1	0	1	1
	$V_4(3)$	0	−1	0	3	−6
	$V_6(3)$	0	9	0	−5	−12
$L = 4$	$V_0(4)$	1	1	1	1	0
	$V_4(4)$	14	−13	2	7	0
	$V_6(4)$	−20	−5	16	1	0
	$V_8(4)$	−10	0	−7	8	0
	.....	..	..	..	..	..

Table IV - Quantitative splitting of a level with angular momentum L in a field of octohedral symmetry.

rows labelled $V_0(0)$, $V_0(1)$, $V_0(2)$, etc. are the same as in Table **II**, and give the "qualitative" splitting. The rows labelled $V_k(0)$, $V_k(1)$, $V_k(2)$, etc. (k $\neq$ O) give the "quantitative" splitting for the corresponding field. For example, from Table **IV** one can read off immediately that the energy of the three levels resulting from an L = **3** state are given by:

$$\begin{array}{ll} E, = a - b + 9c & \text{corresponding to } \Gamma_2, \\ E, = a + 3b - 5c & \text{corresponding to } \Gamma_4, \\ E, = a - 6b - 12c & \text{corresponding to } \Gamma_5, \end{array}$$

where a, b, c, are the strengths of the perturbing fields transforming as V_0, V_4, V_6, respectively.

It is the computation of this part of the table, that is, the rows $V_k(L)$ with $k \neq 0$ – which current methods can obtain only through a lengthy and indirect procedure – which is the purpose of the present paper to improve.

We begin by remarking that the rows $V_k(L)$ for k # 0 differ in two essential ways from the rows $V_0(L)$: the rows $V_0(L)$ have positive integral coefficients, and a significant normalization, both features being inherited from the fact that $V_0(L)$ denotes a (generally reducible) character of O. By contrast, the rows $V_k(L)$ involve negative coefficients and an arbitrary normalization (the strength of the perturbing field) – both aspects denying that a significant interpretation of $V_k(L)$ as a character exists.

Nonetheless, Table IV strongly suggests that one seek to interpret the rows as a generalized character. We accomplish this by considering the Γ_i as basis elements *for* an algebra and the $V_k(L)$ as the associated linear combinations over this basis. For example, the element $\hat{V}_4(3) = -\hat{\Gamma}_2 + 3\hat{\Gamma}_4 - 6\,f_6$, with $\hat{\Gamma}_i$ denoting basis elements (operators) in the algebra. For the algebra to be associated with the basis elements $\hat{\Gamma}_i$ there is a natural choice: the algebra of representations[4]. This is the algebra defined by the reduction of the Kronecker product of representations; that is,

$$\Gamma_i \times \Gamma_j = \sum_k \{ijk\}\, \Gamma_k \qquad \text{(the Clesbsch-Gordan series)}$$

with

$$\{ijk\} = [\sum_g X_i(g) X_j(g) X_k(g^{-1})]/(\text{group volume}).$$

There are two natural ways to realize this algebra in terms of matrices:

(1) Either associate the basis element $\hat{\Gamma}_j$ with a diagonal matrix whose diagonal elements are the entries in the character of the representation Γ_j, or,

(2) Take the matrix $\hat{\Gamma}_j$ to be the matrix: $(\hat{\Gamma}_j)_{ik} = \{ijk\}$. (These two realizations are equivalent and transform into each other using the character table itself as the transformation matrix[4].) The multiplication table for the algebra of representations of the octohedral group is the one already given in Table III.

It is an immediate consequence of this definition of $V_k(L)$ (as an element of the algebra of representations – which we denote henceforth by a circumflex) that there are several operations that are well defined. Let $\hat{V}_k(L) \overset{\text{def}}{\equiv} \sum_i a_i^{kL} \hat{\Gamma}_i$.

(a) Inner product:

$$\hat{V}_k(L) \cdot \hat{V}_{k'}(L) \overset{\text{def}}{\equiv} \sum_i a_i^{kL} a_i^{k'L} \hat{\Gamma}_i, \tag{12}$$

(b) Outer product:

$$\begin{aligned} \hat{V}_k(L) \times \hat{V}_{k'}(L') &\overset{\text{def}}{\equiv} (\sum_i a_i^{kL} \hat{\Gamma}_i) \times (\sum_j a_j^{k'L'} \hat{\Gamma}_j) \\ &= \sum_{i,j,t} a_i^{kL} a_j^{k'L'} \{ijt\} \hat{\Gamma}_t. \end{aligned} \tag{13}$$

There is one further operation to be defined, which is not quite so obvious. Let us define the trace of the element $\hat{V}_k(L)$ to be:

$$\operatorname{tr}(\hat{V}_k(L)) \overset{\text{def}}{\equiv} \sum_i a_i^{kL} (\dim \Gamma_i). \tag{14}$$

(This differs from what one might expect from the algebra of representations where one type of trace would already be defined over a matrix realization of the $\hat{\Gamma}_i$. This alternative trace would lead to unacceptable results.)

The thread of the reasoning has been interrupted by this listing of definitions. Let us return to the problem by posing the question: how do these concepts help us understand the structure of Table IV?

Recall first that all $\hat{V}_0(L)$ are readily calculated. Hence we look at the first row, $\hat{V}_4(2)$, having $k \neq 0$. There are two significant features of $\hat{V}_4(2)$: (a) $\operatorname{tr} \hat{V}_4(2) = 0$ and *(b)* $\operatorname{tr}(\hat{V}_0(2) \cdot \hat{V}_4(2)) = 0$. *Conversely, if* we assume these features, $\hat{V}_4(2)$ is *determined* (to within an overall constant).

Thus, we implement the rules for our algebra by assuming:

$$\text{(a)} \quad \operatorname{tr}(\hat{V}_k(L)) = (2L+1)\delta_k^0 \tag{15}$$

$$\text{(b)} \quad \operatorname{tr}(\hat{V}_k(L) \cdot \hat{V}_{k'}(L)) = 0, \quad k \neq k' \tag{16}$$

These two rules are insufficient to determine all the entries for L = 3. We can remedy this by using the outer product.

Consider the outer product: $\hat{V}_0(1) \times \hat{V}_4(2)$. Using Table IV, we find that:

$$\hat{V}_0(1) \times \hat{V}_4(2) = \hat{\Gamma}_2 - 2\hat{\Gamma}_3 + \hat{\Gamma}_4 - 2\hat{\Gamma}_5. \tag{17}$$

To interpret this result we note that the right hand side is just the linear combination:

$$0 \cdot \hat{V}_4(1) - \frac{2}{3}\hat{V}_4(2) + \frac{1}{3}\hat{V}_4(3). \tag{18}$$

A rule that will accord with this is to assume that:

$$\hat{V}_0(L) \times \hat{V}_k(L') = \text{linear combination of } \hat{V}_k(L''),$$

where

$$L'' = |L - L'|, \quad |L - L'| + 1, \ldots, L + L'. \tag{19}$$

Assuming this heuristic rule one can now complete the table for L = 3, since $\hat{V}_6(3)$ is defined (to within normalization) by the two equations:

$$\operatorname{tr}(\hat{V}_6(3) \cdot \hat{V}_0(3)) = 0 \tag{20}$$

$$\operatorname{tr}(\hat{V}_6(3) \cdot \hat{V}_4(3)) = 0. \tag{21}$$

The procedure is now clear. Find $\hat{V}_6(4)$ from

$$\hat{V}_6(3) \times \hat{V}_0(1) = A\hat{V}_6(2) + B\hat{V}_6(3) + C\hat{V}_6(4). \tag{22}$$

Find $\hat{V}_4(4)$ from

$$\hat{V}_4(3) \times \hat{V}_0(1) = A\hat{V}_4(2) + B\hat{V}_4(3) + C\hat{V}_4(4). \tag{23}$$

In the last case, one needs an extra equation, which is found by orthogonalizing $\hat{V}_4(4)$ with (the already obtained) $\hat{V}_6(4)$. $\hat{V}_8(4)$ can now be obtained by orthogonalizing it with $\hat{V}_0(4)$ and $\hat{V}_6(4)$. In this way we have completed the table for L = 4.

The careful reader will have noticed that the heuristic rules given above do indeed suffice to determine Table IV completely (to within normalizations for $\hat{V}_k(L)$ for $k \neq 0$) but that the *labelling* itself, $\hat{V}_k(L)$, is not determined by this procedure. This gap can be remedied by another heuristic rule for inner multiplication:

$$\hat{V}_k(\mathrm{L}) \, . \, \hat{V}_{k'}(\mathrm{L}) = \text{linear combination of } \hat{V}_{k''}(\mathrm{L}),$$

where

$$k'' = |k - k'|, \quad k - k' + 1, \; . \qquad k + k'. \tag{24}$$

(Note that this rule has a nice analogy to the rule assumed for outer products.)

Let us now summarize. By a study of the solution of the quantitative splitting problem for R, restricted to $\mathcal{O}$, as given in the solution Table IV, we have been led to several heuristic rules *that give a meaning to an algebra which extends the concept of character.*

We will show in the following sections how this heuristic process can be given a precise meaning. Before leaving our motivating example, R, $\supset$ O, several remarks are in order. Firstly, the induction process really did occur this way and is not a contrived example; it is, in fact, a natural generalization of the recursive process used at the end of part A) of this section. The second remark is cautionary: if the table for R, $\supset$ O is extended beyond L = 4, multiple entries appear in the rows for $\hat{V}_0(L)$. As always, multiplicities present additional complications, which are in a sense extraneous to the method. (We discuss this further in the concluding section.)

One further remark. It should be clearly noted that the construction of Table I – using the heuristic rules given above – is very considerably easier than the complicated construction in the literature. And it is quite general. As an exercise, the reader is suggested to rederive the Gell-Mann--Okubo formula for the octet and the decuplet, reducing $SU(3)$ to $[U(1) \times SU(2)]/Z(3)$, with a symmetry breaking Hamiltonian transforming as an octet under $SU(3)$ (and, of course, invariant under $[U(1) \times SU(2)]/Z(3)$.)

3. Group Theoretic Re-Interpretation

Let us now re-phrase the problem considered in Section 2 in a more abstract, group theoretic, way. We are given a group, G, (in the example R,) and a subgroup, H, (in the example O), and we wish to consider a given irreducible representation (abbreviated irrep) of G. This irrep of G is to be split by a set of operators $\{\hat{V}\}$, classified as having irreducible transformation properties under G but transforming invariantly under H.

The problem is then: what is the precise nature (spectrum, eigenvectors, eigenvalues) of this splitting?

Consider now the special features of the group G taken in the example of Section 2, *($G = R,$)*. For an irrep {L) of $R,$ we know in complete generality *all* of the operators that take the space { L) into itself: these are the diagonal Wigner operators (unit tensor operators having A J = 0) denoted by $\mathbf{S}_k = \{S_k^M\}$, for which the matrix elements are the Wigner coefficients: $C^{L\ k\ L}_{M'MM''}$. Expressed differently, these canonical operators $\mathbf{S}_k$ are polynomials over the generators **J.**

The feature which underlies the simplicity of the calculations given in Section 2 is the fact that in the restriction $R, \to 0$, the irreps L = 1, 2, 3, 4 contained no irrep of $\mathcal{O}$ more than once. Expressed conventionally one says that the restriction $R, \to$ O is ***multiplicity-free*** for L < 5. The property of being multiplicity-free is a very basic one, and much of the success in applying group theory to physics hinges on the fact that in these applications the multiplicity-free property holds. (For example, the construction of tensor operators in $R,$ is relatively easy since $R,$ x $R,$ (with group elements $g_1 g_2$) restricted to the diagonal subgroup $R, \otimes R,$ (with group elements $g_1 = g_2$) is multiplicity-free.)

Hence, to simplify the analysis – and to understand the essentials of the problem – let us assume that restriction of irreps of G to the subgroup H will always be multiplicity-free. For $G = R,,$ there are two sub-groups H which satisfy. this requirement:

a. the Abelian group $R,,$
b. the non-Abelian dihedral group D_∞.

We will carry out the analysis in detail for both these cases. It is fortunate that one of these cases is non-Abelian, since case (a) by itself is a bit too simple.

(a) $R, \supset R,$:

The operators which carry the irrep space {L) of $R,$ into itself are, as mentioned, the tensor operators $\{V_K^M\}$ whose matrix elements are:

$$\langle LM_f | V_K{}^M | LM_i \rangle = (\text{constant})\ C^{L\ K\ L}_{M_i M M_f}. \tag{25}$$

The requirement that this set of operators transform invariantly under $R,$ [whose group elements are $g(\beta) = \exp(i\beta L_z)$] can easily be seen to be the condition that $M = 0$. Thus the set $\{V_K^M(L)\}$ is restricted to the sub-set $\{V_K{}^0(L)\}$.

The irreps of R, are all one-dimensional and have the character: $X_M(\beta) = \exp(iM\beta)$. The restriction of {L) to R, (as is very familiar) involves the quantities:

$$M = -L, \quad -L+1, \ldots, \quad L.$$

The algebra of representations of R, is equally elementary, since for Abelian groups this is just the dual group:

$$\hat{\Gamma}_M \times \hat{\Gamma}_{M'} = \hat{\Gamma}_{M+M'}. \tag{26}$$

We can now write out explicitly and precisely the algebraic generalization guessed at in Section 2. For the irrep (L) we have the algebraic elements:

$$\hat{V}_k(L) \overset{\text{def}}{\equiv} \sum_{M=-L}^{L} C_{M0M}^{LkL}\, \hat{\Gamma}_M. \tag{27}$$

It should be recognized that for the case R, $\supset R_2$, the fact that we know at once the matrix elements of $V_k^0(L)$ suffices to determine completely the analogue to Table IV. The point of the algebraic generalization given above is that we can now verify in detail the precise form of the algebraic rules assumed heuristically in Section 2.

Consider first the trace operation. Using $\mathrm{tr}(\hat{\Gamma}_M) = \dim \Gamma_M = 1$ we find[5]:

$$\mathrm{tr}(\hat{V}_k(L)) = \sum_{M=-L}^{L} C_{M0M}^{LkL} = (2L+1)\delta_k^0 \tag{28}$$

Next consider the inner product operation:

$$\hat{V}_k(L)\cdot \hat{V}_{k'}(L) = \sum_M C_{M0M}^{LkL} C_{M0M}^{Lk'L}\, \hat{\Gamma}_M,$$

$$\hat{V}_k(L)\cdot \hat{V}_{k'}(L) = \sum_{k''} \{[(2k''+1)(2L+1)]^{1/2}\cdot C_{000}^{kk'k''}\cdot W(LkLk';\, Lk'')\}\, \hat{V}_{k''}(L). \tag{29}$$

(The W(...) in eq. (29) denotes a Racah coefficient[5].)

We see at once from Eq. (29) that the inner product involves a linear combination over k'' whose values range from $|k-k'|$ to (k + k'). *This verifies the heuristic rule assumed in Section* 2, (cf. Eq. 24).

Note also that if we take the trace in Eq. (29) we obtain:

$$\mathrm{tr}(\hat{V}_k(L)\,.\,\hat{V}_{k'}(L)) = [(2L+1)/(2k+1)]\,\delta_k^{k'}. \tag{30}$$

This verifies the orthogonality rule of Section 2, Eq. (16).

The outer product can be treated equally easily (see Appendix). For this one finds the result:

$$\hat{V}_k(L) \times \hat{V}_{k'}(L') = \sum_{L''k''} \left[(2L+1)(2L'+1)(2L''+1)(2k''+1)^{1/2} \cdot C^{k\,k'\,k''}_{0\,0\,0} \cdot \begin{pmatrix} L & L & k \\ L' & L' & k' \\ L'' & L'' & k'' \end{pmatrix} \right] \hat{V}_{k''}(L''). \tag{31}$$

(The $\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$ symbol in Eq. (31) denotes a $9j$ ("Fano") coefficient.)

Once again we see that the conjectured rôle given in Section 2 is verified completely, that is, the outer product gives a linear combination limited by the angular momentum rules for k x k' and L x L'.

(b) $R_3 \supset D_\infty$:

In a sense, case (a) treated above, is too easy, in that the relevant operators have been tailored in advance to the subgroup R,. The D_∞ sub-group provides a bit more structure.

Let us recall some details on the group ***D*, .** There is a single infinitesimal generator, L,, and one finite generator, an involution (reflection) which may be taken to be $R = \exp(i\pi L_x)$. The defining group relations are:

$$R^2 = E, \quad R \cdot g(\psi) \cdot R = (g(\psi))^{-1}, \quad g(\psi) g(\psi') = g(\psi + \psi'), \tag{32}$$

where $g(\psi) = \exp(i\psi L_z)$, $(0 \leq \psi < 2\pi)$. The group elements are: $g(\psi)$, $R \cdot g(\psi)$. The group volume is 4π.

There are two one-dimensional irreps Γ_+ and Γ_-; the remaining irreps are two-dimensional: Γ_M, M = 1, 2, ... ∞. The character table is:

D_∞	Γ_+	Γ_-	Γ_M
$\{\psi\}$	1	1	$2\cos M\psi$
$\{R\psi\}$	1	-1	0

The algebra of representations of D, is given by the table:

	Γ_+	Γ_-	Γ_M
Γ_+	Γ_+	Γ_-	Γ_M
Γ_-	Γ_-	Γ_+	Γ_M
Γ_M	Γ_M	Γ_M	$\begin{cases}\Gamma_{M+M'} + \Gamma_{\lvert M-M'\rvert}, & M \neq M', \\ \Gamma_{M+M'} + \Gamma_+ + \Gamma_-, & M = M'.\end{cases}$

There are two details to be carried out before the operator algebra $\{\hat{V}\}$ can be set up. First, we must determine how the irreps {L} of $\boldsymbol{R}$, split under restrictions to D,. This is elegantly solved using the character tables and one finds:

$$(L) = \Gamma_{(-)^L} + \Gamma_1 + \Gamma_2 + \ldots + \Gamma_L. \tag{33}$$

The second necessary detail is to identify the D, invariant operators in the set $\{S_k^q(L)\}$. Invariance under L, forces the quantum number q to be ***zero.*** Invariance under $\boldsymbol{R}$ forces k to be ***even.*** Thus the set is: $\{S_{2k}^0(L)\}$. Hence for the operators in our algebra we have explicitly:

$$\hat{V}_{2k}(L) = \left(\sum_{M=1}^{L} C_{M0\,M}^{L\,2kL} \cdot \hat{\Gamma}_M\right) + C_{00\,0}^{L2kL} \cdot \hat{\Gamma}_{(-)^L}. \tag{34}$$

With the explicit definition given in **Eq. 34,** one may establish the following properties:

***Orthogonality Properties of the Trace*:**

(*a*) $\operatorname{tr}(\hat{V}_{2k}(L)) = (2L + 1)\delta_k{}^0,$ (35*a*)

(b) $\operatorname{tr}(\hat{V}_{2k}(L) \cdot \hat{V}_{2k'}(L)) = [(2L + 1)/(4k + 1)]\,\delta_k^{k'}.$ (35*b*)

Inner Product Rule

$$\hat{V}_{2k}(L) \cdot \hat{V}_{2k'}(L) = \sum_{2k''=2|k-k'|}^{2(k+k')} [(2L + 1)(4k'' + 1)]^{1/2} \cdot C_{0\,0\,0}^{2k2k'2k''} \cdot$$
$$\cdot\, W(L\,2k\,L\,2k';\; L\,2k'') \cdot \hat{V}_{2k''}(L). \tag{36}$$

It is clear that these results once again verify the conjectures of Section 2. More interesting is the outer product law which explicitly involves the non-Abelian nature of the D_∞ group. Despite the very great difference in detail (the reduction of $\hat{\Gamma}_M \times \hat{\Gamma}_{M'}$ using the D_∞ algebra of representations) the result for the outer product law involves precisely the same *formal* result as for the $R_3 \supset R_2$ case (with k restricted to be even however). One finds:

***Outer Product Rule*:**

$$\hat{V}_{2k}(L) \times \hat{V}_{2k'}(L') = \sum_{L'',2k''} [(2L+1)(2L'+1)(2L''+1)(4k''+1)]^{1/2} \cdot C^{2k\,2k'\,2k''}_{0\ \ 0\ \ 0} \begin{pmatrix} L & L & 2k \\ L' & L' & 2k' \\ L'' & L'' & 2k'' \end{pmatrix} \cdot \hat{V}_{2k''}(L''). \tag{37}$$

It is clear, once again, that the conjectures made in Section **2** are valid for the system $R_3 \supset D_\infty$.

4. Discussion

The essential content of the previous sections is to demonstrate, by explicit examples, that the quantitative problem of level splitting may, in favorable cases, have an equally elegant solution as the qualitative problem. The key element which assures this favorable situation is the assumption that the reduction $G \to H$ be multiplicity-free. Under this assumption, the restriction $G \to H$ will have an inner and an outer multiplication as conjectured in Section **2** and exemplified in Section **3.**

Viewed more generally, our constructions and examples suffice to show that there does indeed exist a well-defined generalization of the concept of a character, a generalization which leads to an algebra over the basis elements $\hat{\Gamma}$.

A more formal approach to this problem would recognize that our results are, in fact, simply a general form of a commutative normed ring[6] defined by the restriction $G \to H$.

It would be interesting to pursue this more formal, but more powerful, algebraic approach, but in the absence of any effective way to deal with multiplicity (which in practice nearly always occurs) it seems a bit premature to discuss such formalizations here.

Appendix

The derivation of the inner and outer products for the $R_3 \supset R_3$ and $R_3 \supset D_\infty$ cases involves manipulations familiar in the quantum theory of angular momentum[5]. Thus, for example, the derivation of the inner product involves the standard re-coupling of Wigner coefficients using the Racah functions. By contrast, the manipulations leading to the outer product rules is not so immediate, hence we will sketch the details here. The essential step is to replace the Wigner operator appearing in $\hat{V}_k(L)$ by the substitution:

$$C^{L\,k\,L}_{M\,0\,M} = \sum_{\lambda,k''} [(2L+1)(2\lambda+1)]^{1/2} (-)^{L-M} \cdot C^{k\,k'\,k''}_{0\,0\,0} \cdot W(LLk''k';\,k\lambda) \cdot C^{L\,\,k'\,\lambda}_{-M\,0\,-M}\, C^{L\,\,\lambda\,k''}_{M\,-M\,0}\,. \quad \text{(A-1)}$$

Once this step is made, the standard operations may be applied. That is, one next re-couples the $C^{L'\,k'\,L}_{M'\,0\,M'}$ (from $\hat{V}_{k'}(L')$) and the coefficient $C^{L\,\,k'\,\lambda}_{-M\,0\,-M}$ appearing in *Eq.* (A-1) above. After a further re-coupling, one finds the sum over λ leads to a 9j symbol. Carrying out the required operator product – using the algebra of representations (for $R_3 \supset R_3$ or $R_3 \supset D_\infty$) – one finally obtains the explicit formulas given in the text (Eqs. 31 and 37, respectively).

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