Commun. math. Phys. 36, 157—170 (1974)


# Selection Rules for $G_2$ Vectors in the Atomic $f$ Shell*

B. R. Judd

The Johns Hopkins University, Baltimore, Maryland, USA

Received December 12, 1973

**Abstract.** In various tabulations of such spectroscopic coefficients as the matrix elements of tensor operators or fractional parentage coefficients, it is found that many entries are unexpectedly zero. A survey is made of all cases that occur in the atomic $f$ shell and that involve the 7-dimensional vector representation of the group $G_2$. Direct explanations are given in terms of the group structure of the electronic configurations that comprise the shell. The techniques used depend on a splitting of the state space into "spin-up" and "spin-down" parts, and, for other cases, the extensive use of the methods of second quantization. The $F$ terms of the atomic $f$ shell are found to split into three classes. The separation that this classification provides for the two $F$ terms belonging to the irreducible representation (31) of $G_2$ coincides with Racah's separation. An improved separation of the $H$ states of (31) is described.

## 1. Introduction

It is a curiosity of considerable interest that the theory of Racah [1] for the atomic $f$ shell works much better, and has a more elegant structure, than might reasonably have been anticipated. One of the manifestations of this is the frequent vanishing of matrix elements for no apparent reason. A general survey has recently been made [2] of the kind of methods that can be used to understand many of these results; but the unexpected simplifications are so numerous and diverse in character that it seems far too optimistic to hope that a single guiding principle, if it were found, could account for all of them. In the present article an attempt is made to fully explain a single class of these kinds of puzzles, namely, those that involve the seven-dimensional vector representation of the group $G_2$. Following the notation of Racah [1], this representation is denoted by (10). The importance to us of (10) lies in the fact that it describes the transformation properties of the annihilation and creation operators of a single $f$ particle (whether boson or fermion). It thus plays a fundamental role in shell theory. There is the added attraction that (10) is associated with a particularly large number of matrix elements that are unexpectedly zero.

* Supported in part by the U.S. National Science Foundation.

In the theory of Racah [1], operators and states are assigned the irreducible representations of groups as labels. It can thus be seen that the vanishing matrix elements must correspond to Clebsch-Gordan (CG) coefficients whose values, for one reason or another, happen to be zero. This connection does not usually get us very far, since the methods for calculating the CG coefficients for such groups as $G_2$ are rarely sufficiently transparent to allay the feeling that a more direct approach should exist. If, however, we take the view that the CG coefficients exist in their own right, independent, for example, of their role in atomic shell theory, then the analysis that follows can be regarded as showing that fermion or boson states provide a convenient basis for exposing an otherwise hidden structure in the CG coefficients.

## 2. Tensors

Consider, first of all, spinless $f$ bosons. The tensor $\boldsymbol{b}^\dagger$, whose seven components $b_m^\dagger\,(-3 \leqq m \leqq 3)$ create the seven possible angular-momentum states of a single boson, spans (10), as do the components $b_m$ of the annihilation tensor $\boldsymbol{b}$. Both $\boldsymbol{b}^\dagger$ and $\boldsymbol{b}$ are spherical tensors of rank 3 in $R_3$ (the group of rotations in ordinary three-dimensional space), since $b_m^\dagger$ and $b_m$ transform like the spherical harmonics $Y_{3m}$ and $Y_{3m}^*$ respectively. The decomposition law for $G_2 \to R_3$ is fixed by $(10) \to F$, where the traditional spectroscopic notation is used for the irreducible representation of $R_3$. (In general, we shall use the symbol $L$ for such representations.) The representation (10) also appears when pairs of creation or annihilation operators are coupled to a total rank of 3. That is, the three tensors

$$(\boldsymbol{b}^\dagger \boldsymbol{b}^\dagger)^{(3)}, \qquad (\boldsymbol{b}^\dagger \boldsymbol{b})^{(3)}, \qquad (\boldsymbol{b}\,\boldsymbol{b})^{(3)} \tag{1}$$

can all be assigned the representation (10) of $G_2$. The reason for this is that the Kronecker square of (10) decomposes as follows [3]:

$$(10) \times (10) = (00) + (10) + (11) + (20)\,,$$

and, of all the representations on the right-hand side of this equation, an $F$ state only occurs in (10). Racah [1] showed that $G_2$ can be embedded in $R_7$ according to the scheme $(100) \to (10)$, and it turns out that the coupled tensors (1) belong to (110) of $R_7$, while the single annihilation or creation operators belong to (100).

Similar statements can be made about the orbital transformation properties of the creation and annihilation operators $\boldsymbol{a}^\dagger$ and $\boldsymbol{a}$ for $f$ electrons. The presence of spin slightly complicates matters, however. Both $\boldsymbol{a}^\dagger$ and $\boldsymbol{a}$ are double tensors, possessing ranks 3 in the orbital space and $\frac{1}{2}$ in the spin space. Four kinds of non-vanishing coupled products are now possible, namely

$$(\boldsymbol{a}^\dagger \boldsymbol{a}^\dagger)^{(13)}, \quad (\boldsymbol{a}^\dagger \boldsymbol{a})^{(13)}, \quad (\boldsymbol{a}^\dagger \boldsymbol{a})^{(03)}, \quad (\boldsymbol{a}\,\boldsymbol{a})^{(13)}, \tag{2}$$

where the total spin rank is placed before the total orbital rank in the superscripts.

Matrix elements of the single annihilation and creation operators are proportional to coefficients of fractional parentage (cfp) [4]. They have been given by Nielson and Koster [5] for all states of the atomic $f$ shell. It is often useful to supplement these tables with those of Nutter and Nielson [6], where the factors making up the cfp are set out. The matrix elements of $(\boldsymbol{a}^\dagger \boldsymbol{a}^\dagger)^{(13)}$ and $(\boldsymbol{a}\,\boldsymbol{a})^{(13)}$ are directly related to certain two-particle cfp. A complete tabulation of the latter has been made by Donlan [7]. Nielson and Koster [5] have calculated all matrix elements of $\boldsymbol{U}^{(k)}$ for the atomic $f$ shell, where $\boldsymbol{U}^{(k)}$ is defined through the equations

$$\begin{aligned} \boldsymbol{U}^{(k)} &= (2k+1)^{-\frac{1}{2}} \boldsymbol{V}^{(k)}, \\ \boldsymbol{V}^{(k)} &= -2^{\frac{1}{2}} (\boldsymbol{a}^\dagger \boldsymbol{a})^{(0k)}. \end{aligned} \tag{3}$$

These various tables can be rapidly scanned to find vanishing matrix elements. Most of the zeros that appear can be given an immediate explanation. A typical matrix element

$$(UL|(10)F|U'L'),$$

where $U$ and $U'$ denote irreducible representations of $G_2$, automatically vanishes if $(10) \times U'$ does not contain $U$ in its reduction to irreducible components. Similarly, $F \times L'$ must contain $L$ for the matrix element to be non-zero. The tables of Wybourne [3] or of Nutter [8] enable $(10) \times U'$ to be quickly found. The condition on $L$ is simply that it must be possible to form a triangle (possibly collapsed to a straight line doubled back on itself) whose sides are of lengths $L$, 3, and $L'$.

We must also bear in mind that the representations $U$ of $G_2$ can be embedded in representations $W$ of $R_7$. The criteria that we applied to $U$ and $L$ can be readily extended to $W$. An additional selection rule appears for the operator $\boldsymbol{V}^{(3)}$. This tensor, which possesses the group labels $(110)\,(10)F$, forms, with $\boldsymbol{V}^{(1)}$ and $\boldsymbol{V}^{(5)}$, the generators of $R_7$ [1]. It follows that $\boldsymbol{V}^{(3)}$ is diagonal with respect to $W$. (For similar reasons, $\boldsymbol{V}^{(1)}$ and $\boldsymbol{V}^{(5)}$, the generators of $G_2$, are diagonal with respect to $U$.)

We could follow the thread connecting $R_3$, $G_2$, and $R_7$ even further; for $R_7$ can be embedded in the symplectic group $Sp_{14}$, and this, in turn, in $U_{14}$, and so on [9]. Zeros which depend exclusively on the properties of these higher groups are of no immediate interest to us. In any case, they are usually quite easy to interpret, since the relevant irreducible representations, although of a higher dimension, possess a simpler

Table 1. Branching rules for $G_2 \to R_3$

| $U$ | $L$ | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| (00) | $S$ | | | | | | | | | | |
| (10) | $F$ | | | | | | | | | | |
| (11) | $P$ | $H$ | | | | | | | | | |
| (20) | $D$ | $G$ | $I$ | | | | | | | | |
| (21) | $D$ | $F$ | $G$ | $H$ | $K$ | $L$ | | | | | |
| (22) | $S$ | $D$ | $G$ | $H$ | $I$ | $L$ | $N$ | | | | |
| (30) | $P$ | $F$ | $G$ | $H$ | $I$ | $K$ | $M$ | | | | |
| (31) | $P$ | $D$ | $F^2$ | $G$ | $H^2$ | $I^2$ | $K^2$ | $L$ | $M$ | $N$ | $O$ |
| (40) | $S$ | $D$ | $F$ | $G^2$ | $H$ | $I^2$ | $K$ | $L^2$ | $M$ | $N$ | $Q$ |

structure. For reference purposes, the $L$ structures of those irreducible representations $U$ that appear in the electronic $f$ shell are listed in Table 1.

## 3. Simple Configurations

An obvious place to begin our analysis is the fermion or boson configurations $f^N$ for small $N$. No matrix elements of any of the tensors (1) and (2), taken between the states of $f$ or $f^2$, vanish unexpectedly. It is, however, worth noting that the $H$ states of $f^2$ belong to (11) of $G_2$, and that (11) does not occur in the reduction of $(10)\times(11)$. Thus

$$(f^2 H|V^{(3)}|f^2 H)=0\,. \tag{4}$$

If standard angular-momentum techniques are used to evaluate the matrix element – such as applying Eq. (7.1.8) of Edmonds [10] – we at once obtain

$$\begin{Bmatrix} 3 & 5 & 3 \\ 5 & 3 & 3 \end{Bmatrix}=0\,. \tag{5}$$

The vanishing of this 6-$j$ symbol is well known. It corresponds to the fact that the commutators $[V^{(5)}, V^{(5)}]$ do not contain $V^{(3)}$ in their development, and this is directly related to the very existence of $G_2$ as a subgroup of $R_7$ (see Racah [11]).

The first null matrix element of the kind we are searching for occurs in $f^3$. It runs

$$(f^3(21)F|V^{(3)}|f^3(21)H)=0\,. \tag{6}$$

Other states of (21) have non-vanishing matrix elements of $V^{(3)}$, and so Eq. (6) implies the vanishing of a CG coefficient for $G_2$. After factoring out the $R_3$ part, we are left with an isoscalar factor for which, in Racah's notation,

$$((21)F|(21)H+(10)F)=0\,. \tag{7}$$

This is a stronger statement than (6), since neither $N$ nor $V^{(3)}$ appears. We can deduce, for example, that no $(21)H$ states of $f^N$ possess any $(21)F$ states of $f^{N-1}$ as parents.

To understand results of this kind, we refer back to Eq. (6). Taking the $f$ particles to be electrons, we can factor the state space into a "spin-up" space (space $A$) and a "spin-down" space (space $B$). If we pick a total spin projection quantum number $M_S$ of $\frac{1}{2}$, there must be two electrons in space $A$ and one in space $B$. The representation (21) can only be formed from the product $(11)_A \times (10)_B$, where the optional subscripts assign the representations to the appropriate spaces. (The representation $(20)_A$ would violate the Pauli Exclusion Principle and can be disregarded.) Since $(11) \to P + H$ under the reduction $G_2 \to R_3$ [3], we are greatly limited in our choice of angular-momentum states for the $A$ and $B$ spaces. In fact, for bra, operator, and ket, only one option is open. Denoting the parts to be coupled in curly brackets, the structure of the matrix element of Eq. (6) is

$$(\{(11)H \times (10)F\}\,F\,|\{(00)S \times (10)F\}\,F\,|\{(11)H \times (10)F\}\,H)\,. \tag{8}$$

It is essential to write $S \times F$ for the operator rather than $F \times S$, for the latter would immediately give a null result in virtue of Eq. (4), when applied to space $A$. However, even in the form of (8), the matrix element is seen to be zero. We have only to use Eq. (7.1.8) of Edmonds [10] again, and a 6-$j$ symbol appears that is directly related, by a mere permutation of its arguments, to the one given in Eq. (5).

Whether the reader finds the above explanation satisfying or not is, of course, a subjective matter. But at least it is very much shorter than actually calculating the matrix element by the standard fractional-parentage techniques. Moreover, the device works well in other instances. In $f^4$, for example, we find, for no obvious reason, that

$$(f^4(30)L\,|V^{(3)}|\,f^4(30)L') = 0$$

for all $L$ and $L'$. However, if we pick $M_S = 0$, we find that we can form the representation (30) only from $(11)_A \times (11)_B$. Whether the operator is written in the form $(10)_A \times (00)_B$ or $(00)_A \times (10)_B$, we cannot escape the fact that (11) does not occur in the reduction of $(10) \times (11)$; and hence the matrix element vanishes. For $f^4$, the representation (30) belongs to (211) of $R_7$, for which some matrix elements of $V^{(3)}$ are non-zero. We can thus deduce that

$$((211)\,(30)\,|(211)\,(30) + (110)\,(10)) = 0\,, \tag{9}$$

where the isoscalar factor is labelled by representations of $R_7$ and $G_2$. This relation is useful in accounting for many zeros in the tables of matrix elements for more complex configurations of $f$ electrons.

## 4. Separation of the *F* States

In the electronic configuration $f^4$, the first signs become apparent of a remarkable classification, valid for all $f^N$, of the $F$ terms. It can be described by first separating all the representations of $G_2$ that contain $F$ terms into three classes, as follows:

I: $(10)F$.

II: $(21)F$, $(31)F$.

III: $(30)F$, $(31)F'$, $(40)F$.

A survey of various tables [5–8] reveals the following:

a) No terms belonging to any one class possess parents or offspring belonging to another class.

b) All matrix elements of $V^{(3)}$ vanish when constructed from a bra and a ket drawn from different classes.

c) All two-electron cfp vanish when a state and its grand-parents belong to different classes, and when, in addition, the two added electrons are coupled to $^3F$.

The existence of class I can be immediately understood in terms of the normal techniques for determining selection rules. It is the division of the remaining $F$ terms into classes II and III that is so remarkable and surprising. Interestingly enough, the separation of the two $F$ terms of (31) into classes II and III corresponds exactly to the apparently arbitrary separation of Racah [1]. The study of the classification thus touches on the inner-multiplicity problem.

The key to the puzzle lies in the fact that, of all the various $L$ terms in $f^N$, it is the $F$ terms that are susceptible of a special classification. These terms can all be produced by the action of a single creation or annihilation operator on an $S$ term; and $S$ terms occur in precisely three irreducible representations of $G_2$, namely (00), (22), and (40). Consider, then, the three possible pairs

$$\left.\begin{matrix} \boldsymbol{a}^\dagger\,|(00)S\rangle \\ \boldsymbol{a}\,|(00)S\rangle \end{matrix}\right\} \quad \left.\begin{matrix} \boldsymbol{a}^\dagger\,|(22)S\rangle \\ \boldsymbol{a}\,|(22)S\rangle \end{matrix}\right\} \quad \left.\begin{matrix} \boldsymbol{a}^\dagger\,|(40)S\rangle \\ \boldsymbol{a}\,|(40)S\rangle \end{matrix}\right\}. \tag{10}$$

The first pair can only produce $F$ states belonging to (10). A consideration of $(22)\times(10)$ reveals that the second pair can only produce $F$ states belonging to (21) or (31) (or to a mixture of these two representations). In a similar way, we find that the third pair can only give rise to $F$ states belonging to (30), (31), or (40) (or to a superposition of these three representations). Since there are just two $F$ states in (31), we can separate them by defining their respective sources as $(22)S$ and $(40)S$. We thus obtain the three classes of $F$ states. Although the states (10) above are the superposition of the several $G_2$ representations belonging to a class, the members of a class are effectively independent. This is because they first appear in configurations $f^N$ of different $N$, where their properties can be studied in an independent manner.

It only remains to show that any operator $\boldsymbol{T}$ that transforms according to (10) of $G_2$ has vanishing matrix elements when it is set between any two of the states (10) coming from different columns. The method is identical for all cases, and we illustrate it for

$$((22)S\,|\,\boldsymbol{a}\,\boldsymbol{T}\,\boldsymbol{a}\,|(40)S)\,. \tag{11}$$

The operator $\boldsymbol{a}\,\boldsymbol{T}\,\boldsymbol{a}$ transforms like $(10)\times(10)\times(10)$. To link two $S$ states, we need an $R_3$ scalar. However, we can easily find, from the tables of Wybourne [3], that

$$(10)^3=(00)+4(10)+2(11)+3(20)+2(21)+(30)\,.$$

Of all the representations of $G_2$ on the right-hand side of this equation, only (00) contains an $S$ state in its reduction [3]. But (00) cannot link (22) to (40); and hence the matrix element (11) vanishes. We can infer that $\boldsymbol{T}$, when set between a bra belonging to class II and a ket belonging to class III, produces a null matrix element.

## 5. Vanishing Isoscalar Factors for $R_7$

The techniques introduced in the preceding section can be adapted to account for the apparently accidental vanishing of a number of single-particle cfp. The tables of Nutter and Nielson [6] indicate that

$$((221)\,(21)\,|(221)\,(20)+(100)\,(10))=0 \tag{12}$$

and also that

$$((221)\,U\,|(211)\,U'+(100)\,(10))=0 \tag{13}$$

for the four pairs

$$U\,U'\equiv(30)\,(20),\;\;(20)\,(10),\;\;(20)\,(30),\;\;(10)\,(20)\,.$$

As an example, consider the last pair. The vanishing isoscalar factor corresponds to

$$(f^{5\,2}(221)\,(10)\,|\,\boldsymbol{a}^\dagger\,|\,f^{4\,3}(211)\,(20))=0\,. \tag{14}$$

The spins $S$ of the electron configurations $f^N$ are represented by the prefixed multiplicities $2S+1$ to the irreducible representations of $R_7$. Although it is not obvious by the traditional techniques why Eq. (14) should hold good, we have only to note that the bra is uniquely defined (to within a multiplicative constant) by

$$\langle f^{6\,1}(222)\,(00)\,|\,\boldsymbol{a}^\dagger\,.$$

To produce a change of 1 in $S$, the two members of the creation pair $\boldsymbol{a}^\dagger \boldsymbol{a}^\dagger$ have to be coupled to the irreducible representations (11) or (10) of $G_2$, for these representations contain the states of $f^2$ for which $S=1$. But neither representation can link (00) of $f^6$ to (20) of $f^4$. The use of the fermion basis thus makes the vanishing of the isoscalar factor quite transparent.

The other examples of Eq. (13), as well as Eq. (12), can be accounted for in a precisely similar way. In all these cases, the representation (10) of $G_2$ belongs to (100) of $R_7$. An examination of the matrix elements of $V^{(3)}$ and the two-particle cfp reveal null isoscalar factors for which (10) belongs to (110). Some can be readily understood in terms of conflicting symmetries [12]. For example, we can deduce, from the tables of Donlan [7] for the cfp of $f^5$, that

$$((111)(10)|(110)(10)+(110)(10))=0\,. \tag{15}$$

To understand this equation, we have only to observe that (111) appears in the symmetric part of $(110)\times(110)$, whereas (10) appears in the antisymmetric part of $(10)\times(10)$.

It is more difficult to account for

$$((111)(10)|(210)(20)+(110)(10))=0\,. \tag{16}$$

This isoscalar factor appears in the two-particle cfp

$$(f^3(210)(20)|(\boldsymbol{a}\,\boldsymbol{a})^{(13)}|f^5(111)(10))\,.$$

It also appears in the matrix element

$$(f^3(210)(20)|(\boldsymbol{a}\,\boldsymbol{a})^{(13)}(\boldsymbol{a}^\dagger\boldsymbol{a})^{(03)}|f^5(111)(00))\,, \tag{17}$$

since the operator $V^{(3)}$, when acting on the ket, yields (111)(10) of $f^5$. Now the commutator

$$[(\boldsymbol{a}\,\boldsymbol{a})^{(13)},(\boldsymbol{a}^\dagger\boldsymbol{a})^{(03)}]$$

can only produce tensors of the type $(\boldsymbol{a}\,\boldsymbol{a})^{(1k)}$, where $k$ is odd. Since the $L$ structure of (20) is $DGI$ – that is, $L$ is even – the commutator cannot connect (20) to (00). Hence (17) is equal to

$$(f^3(210)(20)|(\boldsymbol{a}^\dagger\boldsymbol{a})^{(03)}(\boldsymbol{a}\,\boldsymbol{a})^{(13)}|f^5(111)(00))\,. \tag{18}$$

We now use the fact that $(\boldsymbol{a}^\dagger\boldsymbol{a})^{(03)}$, being proportional to $V^{(3)}$, is a generator of $R_7$. It can therefore only connect (210)(20) to the representations $U$ belonging to (210), namely (11), (20), and (21). We immediately note that (10) does not appear in this list. This is of crucial significance, since the operator $(\boldsymbol{a}\,\boldsymbol{a})^{(13)}$, when acting on (00), can only produce (10). We can deduce that (18) is zero. It only remains for us to work our way back and thus confirm the validity of Eq. (16).

## 6. Alternative Bases

The preceding analysis accounts for all the unexpectedly null isoscalar factors of $R_7$ that contain the vector representation (10) of $G_2$ and which, at the same time, involve only those irreducible representations of $R_7$ that occur in the electronic configurations $f^N$. As for the $G_2$ isoscalar factors, most of the apparently accidental zeros are examples of Eq. (7) or of the special $F$ classification described in Section 4. A few remain to be treated, however. The two $F$ terms of the irreducible representation (31) of $G_2$ (belonging to class II and class III respectively) appear in the three vanishing isoscalar factors specified by

$$((21)H|(31)F+(10)F)=0, \tag{19a}$$

$$((40)H|(31)F+(10)F)=0, \tag{19b}$$

$$((22)H|(31)F'+(10)F)=0. \tag{19c}$$

All these equations can be accounted for in a similar way, and we shall consider only the first in detail. We visualize the isoscalar factor of Eq. (19a) as being derived from the matrix element

$$((21)H|\boldsymbol{a}|(31)F). \tag{20}$$

Now, for electronic states, $(31)F$ can be regarded as being produced by either $\boldsymbol{a}^\dagger|(22)S\rangle$ or $\boldsymbol{a}|(22)S\rangle$. The other $F$ state that has $(22)S$ as its source, namely $(21)F$, plays no role in the analysis owing to Eq. (7). So the matrix element (20) is proportional to

$$((21)H|\boldsymbol{Y}|(22)S),$$

where $\boldsymbol{Y}$ is an operator transforming according to $(10)\times(10)$. By reducing this product, we find that a tensor of rank 5 (which is needed to connect $H$ to $S$) belongs to the irreducible representation (11) of $G_2$; and, for this, $(11)\times(22)$ does not contain (21). Thus (20) is zero and so is the corresponding isoscalar factor. The product $(11)\times(22)$ does not contain (40) either, and so Eq. (19b) is readily understood. By similar arguments, Eq. (19c) follows from the fact that (22) does not occur in the reduction of $(11)\times(40)$.

One null isoscalar factor cannot be so easily explained. From Nielson and Koster's tables [5], we can deduce that

$$((40)H|(40)H+(10)F)=0. \tag{21}$$

All efforts to account for this equation using a fermion basis for the states have failed. However, because all the irreducible representations of $G_2$

that appear in the isoscalar factor are of the type $(u0)$, we can consider the possibility of using a boson basis. We first note that the isoscalar factor arises in the consideration of the matrix element

$$((40)H\,|\,(\boldsymbol{b}^\dagger\,\boldsymbol{b})^{(3)}\,|\,(40)H)\,.$$

Since $(\boldsymbol{b}^\dagger\,\boldsymbol{b})^{(5)}$ is a generator of $G_2$, the matrix element above can be thought of as being derived from

$$((40)S\,|\,\boldsymbol{Z}\,|\,(40)S)\,, \tag{22}$$

where

$$\boldsymbol{Z}=(\boldsymbol{b}^\dagger\,\boldsymbol{b})^{(5)}\,(\boldsymbol{b}^\dagger\,\boldsymbol{b})^{(3)}\,(\boldsymbol{b}^\dagger\,\boldsymbol{b})^{(5)}\,.$$

The operator $\boldsymbol{Z}$ transforms according to $(11)\times(10)\times(11)$, for which we find [3]

$$(11)\times(10)\times(11)=3(10)+(11)+3(20)+4(21)+2(30)+2(31)+(32)+(40)\,.$$

Of all the irreducible representations of $G_2$ on the right-hand side of this equation, only (40) contains an $S$ state under the reduction $G_2\to R_3$. This, then, describes how the effective part of $\boldsymbol{Z}$ transforms under the operations of $G_2$.

Turning now to the representations of $R_7$, we observe that $\boldsymbol{Z}$ transforms according to the triple Kronecker product

$$(110)\times(110)\times(110)\,.$$

Wybourne's tables [3] can be used to reduce this to its irreducible parts: we can then select those that contain (40) of $G_2$. It turns out that there are only two, namely (311) and (321). Thus the effective part of $\boldsymbol{Z}$ is a superposition of two operators whose $WUL$ descriptions are $(311)\,(40)S$ and $(321)\,(40)S$.

The representation (40) also appears in the bra and the ket of the matrix element (22). For boson states, all irreducible representations of $R_7$ are of the type $(w00)$; and (40) can only belong to (400). Putting in the group labels, we see that the matrix element (22) becomes

$$((400)\,(40)S\,|\,[(311),(321)]\,(40)S\,|\,(400)\,(40)S)\,.$$

The final step is to work out the Kronecker products $(311)\times(400)$ and $(321)\times(400)$. In both cases, (400) does not appear. It follows that the matrix element vanishes and Eq. (21) is accounted for.

Strictly speaking, one subsidiary point has to be checked. This is that not all matrix elements of $(10)F$ vanish between the boson states $(40)L$. This is easy to do, since the maximum value of $L$ and its projection $M_L$ correspond to the symmetrized state $\{ffff\}$, for which every $f$ boson has its maximum component. The fact that the CG coefficient

$(33\,|\,30, 33)$ of $R_3$ is non-zero guarantees that the state $(40)Q$ has a non-vanishing matrix element of $(\boldsymbol{b}^\dagger \boldsymbol{b})^{(3)}_0$. Thus the fact that the matrix element (22) is zero implies the validity of Eq. (21) and not the vanishing of some special isoscalar factor of $R_7$.

## 7. Separation of Duplicated Terms

In the classification of the states of the electronic $f$ shell, the two irreducible representations (31) and (40) of $G_2$ each contain several pairs of terms with the same $L$. It has already been mentioned that the $F$-term separation of Section 4 coincides with the separation that Racah adopted in his classic work on the $f$ shell. It is natural to ask whether his other separations can be given a similar kind of theoretical basis. This is too large a question to be completely answered here: but the frequent appearance of $H$ terms in such isoscalar factors as those appearing in Eqs. (7) and (19) suggests that perhaps analogous equations could be used to separate the two $H$ states of (31). For example, we can ask whether we can consistently define the two states $(31)H\alpha$ and $(31)H\beta$ by means of the equations

$$((31)H\alpha\,|\,(31)F + (10)F) = 0\,, \tag{23a}$$

$$((31)H\alpha\,|\,(21)F + (10)F) = 0\,, \tag{23b}$$

$$((31)H\beta\,|\,(31)F' + (10)F) = 0\,, \tag{23c}$$

$$((31)H\beta\,|\,(30)F + (10)F) = 0\,, \tag{23d}$$

$$((31)H\beta\,|\,(40)F + (10)F) = 0\,. \tag{23e}$$

The arguments that were used to explain Eq. (19) can be readily adapted to confirm that this is indeed possible. In fact, we can show that equivalent definitions of $H\alpha$ and $H\beta$ are provided by the equations

$$((31)H\alpha\,|\,(22)S + (11)H) = 0\,,$$
$$((31)H\beta\,|\,(40)S + (11)H) = 0\,.$$

Unfortunately, the two states $(31)H\alpha$ and $(31)H\beta$ are not orthogonal to each other. As they stand, they are unsuitable as replacements for Racah's pair. We can nevertheless improve on Racah's separation by taking $(31)H\alpha$ and its orthogonal companion $(31)H\alpha'$. In place of the single equation

$$((31)H\,|\,(30)I + (10)F) = 0\,,$$

which Racah used to define the first $H$ state of his pair, we have the two Eqs. (23a) and (23b). Moreover, it turns out (for reasons that need not be discussed here) that

$$((31)H\alpha'|(22)H+(10)F)=0\,,$$
$$((31)H\alpha'|(22)L+(10)F)=0\,.$$

Thus the state $(31)H\alpha'$ is also involved in a pair of unexpectedly null isoscalar factors, since the product $(22)\times(10)$ contains (31) in its reduction [3]. By reducing the number of parents that the two $H$ states possess, we facilitate the calculation of the matrix elements of operators of physical interest. Of course, Racah's separation has become so well established that it is now too late to make changes of this kind; but it is interesting to see that alternative separations, had they been considered, would have simplified the analysis somewhat.

More systematic methods are available for separating duplicated terms. Perhaps the most obvious one is to diagonalize an operator $X$ formed from the generators of $G_2$. This topic is beyond the scope of the present article, but it is worth noting that the separation of the two $F$ terms of (31) into class II and class III ensures that several operators have vanishing matrix elements between the two. For example, it is easy to see that

$$((31)F|V^{(k)}|(31)F')=0 \qquad (k=1,5)\,.$$

It is often convenient to take, for $X$, operators that are scalar with respect to $R_3$; for then their diagonalization automatically restricts attention to one value of $L$ at a time. To separate the duplicated terms of (31) and (40), it is necessary to consider multiple products of the type $V^n$, where $n$ is at least 4, and $V$ stands for either $V^{(1)}$ or $V^{(5)}$. One particular linear combination of the products $VVVV$ transforms according to $(44)S$, and it turns out that the diagonalization of this operator within the $F$ states of the irreducible representation (31) yields precisely the pair $(31)F$ and $(31)F'$. A correspondingly simple result does not obtain for the $H$ states, however. It is hoped to pursue this subject in a subsequent article.

## 8. Concluding Remarks

The analysis presented above provides reasonably direct explanations for all the unexpectedly null isoscalar factors that involve the vector representation (10) of $G_2$ and that, at the same time, implicitly appear in the various tables [5–7] of spectroscopic coefficients for the electronic $f$ shell. This restriction to $f$ electrons has limited our attention to the simpler irreducible representations of $G_2$. As we proceed to representations of higher dimensionality, we might expect to find analogues of such Eqs. as (7) or (12). A natural way to extend the analysis would be to consider the bases provided by the nuclear $f$ shell. The existence of both spin and isospin considerably enlarges the range of the representations $W$ and $U$. For $f^{12}$, for example, we find such representations as $W=(444)$ and $U=(80)$. Extensions to configurations as complex as $f^{12}$ make it much more important to have a satisfactory way of resolving the multiplicity problem, for we cannot hope to progress very far with the properties of the CG coefficients if the states themselves are not well defined.

It should be stressed that the apparently accidental vanishing of CG coefficients involving the representation (10) of $G_2$ constitutes only a fraction of all such cases. The result of our analysis for just one species of zeros suggests that the techniques at present at our disposal are adequate for the purposes we have put them to. All the null coefficients can be understood without preambles of too elaborate a kind. However, we cannot completely rule out the possibility that some structure in the $f$ shell remains to be discovered. For example, we might ask whether the three classes of $F$ terms, introduced in Section 4, correspond to three irreducible representations of some group. If we actually count the states in each class (including the spin multiplicities), we find that the dimensions of these hypothetical representations are 144, 76, and 56. These numbers do not suggest any very useful group, although we could formally construct trivial direct products such as the unitary triple product $U_{144} \times U_{76} \times U_{56}$, of course. Such groups add nothing to our understanding of the $f$ shell. Whether more fruitful groups exist is a matter for speculation.

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Communicated by W. Hunziker

B. R. Judd
Physics Department
The Johns Hopkins University
Baltimore 21218, Maryland, USA