

Abstract

New tableau formulas are derived which allow mixed configuration Russell-Saunders states to be expressed in terms of products of their pure configuration constituents. Using these and other simple tableau formulas, matrix elements for spin- and orbit-dependent operators can be easily evaluated for mixed configurations without the use of recoupling or fractional-parentage coefficients.

Alternative basis for the theory of complex spectra. III

Chris W. Patterson and William G. Harter

Instituto de Física, Departamento de Eletronica Quantica, Universidade Estadual de Campinas, Caixa Postal 1170 Campinas, São Paulo, Brazil

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New tableau formulas are derived which allow mixed configuration Russell-Saunders states to be expressed in terms of products of their pure configuration constituents. Using these and other simple tableau formulas, matrix elements for spin- and orbit-dependent operators can be easily evaluated for mixed configurations without the use of recoupling or fractional-parentage coefficients.

I. INTRODUCTION

To put the present treatment in the proper context we briefly review the progress that has been made in the application of a Gel'fand basis¹ to atomic and molecular problems.

The basic theory and formalism for the unitary group approach to the many-body problem has been laid down by Moshinsky *et al.*,² Biedenharn and co-workers,³ and Louck *et al.*⁴ It was Moshinsky⁵ who first outlined the specific applicability of a Gel'fand basis for atomic and molecular problems, and his ideas were put to use for complex atomic configurations independently by Patera and Sharp,⁶ and Harter.⁷ Although it was realized early that the Gel'fand bases could be used to enumerate the angular momentum states within a multiplet,⁸ the actual construction of orbital angular momentum states out of a Gel'fand basis was tedious for multielectron configurations. This was because of the complicated formulas needed to evaluate unitary operators acting on a Gel'fand basis and the difficulties involved with repeated angular momentum states within a multiplet (the multiplicity problem).

Simplifications of the unitary operator formulas were made by Paldus⁹ and the present authors.¹⁰ These formulas could be easily computer coded and enabled the orbital angular momentum states to be readily constructed from a Gel'fand basis and orbital operators to be easily evaluated. The equivalence of the various formulas used has recently been demonstrated by Paldus.¹¹ The problem of repeated angular momentum states within a multiplet was resolved numerically by Drake, Drake, and Schlesinger.¹²

The evaluation of spin-dependent operators has been carried out by Gouyet, Schrammer, and Seligman¹³ in a second quantization scheme using angular momentum recoupling coefficients. The present authors have developed simple tableau techniques for constructing antisymmetric states from Russell-Saunders states using a Gel'fand basis.¹⁰ The evaluation of spin- and orbit-depen-

dent operators acting on the resulting Slater determinants is then trivial. Our tableau techniques have been computer coded by Caird¹⁴ to find oscillator strengths in rare earths and by Drake, Drake, and Schlesinger¹⁵ to compute spin-orbit parameters in the atomic f shell. Applications of our tableau formulas to atomic jj coupling and more than half-filled shells have also been made.¹⁶ Recently, the Gel'fand basis has been applied to various molecular problems by Matsen,¹⁷ Wormer and Avoird,¹⁸ and Paldus.¹⁹

In this work, we shall give a detailed treatment of mixed configurations in atoms and develop further the tableau techniques introduced in two earlier works.^{7,10} (We shall refer to these as I and II.) We described in II a treatment of pure configurations which represents a significant improvement over the methods developed by Racah,²⁰ since complicated sums over recoupling and fractional-parentage coefficients are avoided. Now we give tableau formulas as promised in II which express mixed-configuration Russell-Saunders states in terms of products of their pure configuration constituents. We can then easily extend all the techniques developed for pure configurations to mixed configurations.

Such an extension is difficult using a Racah basis. Earlier treatments of mixed configurations by Elliot,²¹ Innes, and Ufford²² using the Racah basis led to complicated expressions which made computer matrix calculations for complex atoms impractical. Subsequent improvements have been made by Layzer,²³ Shore,²⁴ and others,²⁵⁻²⁸ but still many matrix calculations are beyond the capability of modern computers. Again, the problem is with expressions involving $3n - j$ and fractional-parentage coefficients, the latter being stored in the computer since no closed-form expressions exist.

In I and II, we already developed methods for evaluating matrix elements of spin- and orbit-dependent operators acting on Gel'fand bases. Our main concern for mixed configurations

$(n_1 l_1)^{p_1} (n_2 l_2)^{p_2} \dots$, is therefore the construction of Gel'fand bases of $U_{[l_1]+[l_2]+\dots}$ ($[l] = 2l + 1$) which are eigenstates of total orbital angular momentum $L_1^2 + L_2^2 + \dots$.

For pure configurations $(nl)^p$ we have constructed Gel'fand bases of $U_{[l]}$ with good total angular momentum L by applying the lowering operator L_- to the highest L state. The highest L state is always a Gel'fand state, and furthermore we may easily expand L_- in terms of the lowering generators $E_{i+1,i}$ of $U_{[l]}$. Since the matrix elements of the $E_{i+1,i}$ are known, the effect of L_- acting on the Gel'fand bases is readily evaluated. For repeated L states lowering does not uniquely specify the bases and one must use projection operators and Gram-Schmidt orthogonalization procedures.^{12,16} It is not difficult to generate Gel'fand bases with good L for pure configurations using lowering operators, and such bases have been constructed by Caird¹⁴ for the p , d , and f shells.

For mixed configurations we can obtain Gel'fand bases with good L by lowering with $L_- = L_{1-} + L_{2-} + \dots$ from the highest L state, as explained in II. However, there are problems with Gel'fand bases for mixed configurations derived with lowering operator techniques. First, the orthogonalization procedures can lead to extremely large numbers which overflow the computer for high multiplicities of L . Second, the bases must be derived independently for each mixed configuration without taking advantage of the fact that we have already derived bases for the separate pure configurations. Finally, the bases generated have no physical significance—they do not represent any partial symmetry of the Hamiltonian.

These difficulties are eliminated by the development of simple formulas which relate the Gel'fand states of $U_{[l_1]+[l_2]+\dots}$ to the Gel'fand product states of $U_{[l_1]} \times U_{[l_2]} \times \dots$. Once Gel'fand bases have been derived for the separate pure configurations $(n_1 l_1)^{p_1}, (n_2 l_2)^{p_2}, \dots$, of $U_{[l_1]}, U_{[l_2]}, \dots$, with good total orbital angular momenta L_1, L_2, \dots , we may use these formulas to couple the angular momenta of the pure configurations and thereby find Gel'fand states of the mixed configuration $(n_1 l_1)^{p_1}, (n_2 l_2)^{p_2}, \dots$, with $L = L_1 + L_2 + \dots$. The treatment of mixed configurations then becomes a relatively simple extension of that for pure configurations.

II. UNITARY STRUCTURE FOR MIXED CONFIGURATIONS

If a single electron can occupy q different orbital subshells $n_1 l_1, n_2 l_2, \dots, n_q l_q$, there will be

$$h = [l_1] + [l_2] + \dots + [l_q]$$

single-electron states possible. We shall restrict our attention for the moment to p electrons occu-

pying only two orbital subshells $n_1 l_1$ and $n_2 l_2$ with $h = [l_1] + [l_2]$, since this special case is easily generalized. For typographical convenience, the α th particle state shall be labeled $|1\rangle^\alpha, |2\rangle^\alpha, \dots, |[l_1]\rangle^\alpha$ corresponding to magnetic quantum numbers $m_1 = -l_1, -l_1 + 1, \dots, l_1$ and $|[l_1] + 1\rangle^\alpha, |[l_1] + 2\rangle^\alpha, \dots, |h\rangle^\alpha$ corresponding to magnetic quantum numbers $m_2 = -l_2, -l_2 + 1, \dots, l_2$. We may consider these α th particle states to form a basis for U_h , the unitary group of dimension h . The single-particle generators operate on the single-particle states such that

$$e_{ij}^\alpha |j'\rangle^{\alpha'} = \delta_{\alpha\alpha'} \delta_{jj'} |i\rangle^\alpha, \quad (1)$$

where $i, j = 1, 2, \dots, h$ and $\alpha = 1, 2, \dots, p$.

The product states of p electrons $(n_1 l_1 + n_2 l_2)^p$ form a reducible basis for U_h with generators

$$E_{ij} = \sum_{\alpha=1}^p e_{ij}^\alpha, \quad (2)$$

where $i, j = 1, 2, \dots, h$. These generators satisfy the well-known unitary commutation relations

$$[E_{ij}, E_{kl}] = \delta_{jk} E_{il} - \delta_{li} E_{kj}. \quad (3)$$

The *intershell* multipole or tensor operators $V_q^k(l_1 l_2)$ can be expressed in terms of these generators using Wigner's $3 - j$ symbols as follows:

$$\begin{aligned} V_q^k(l_1 l_2) &= \sum_{m_1, m_2} \left\langle \begin{matrix} n_1 l_1 \\ m_1 \end{matrix} \middle| v_q^k \middle| \begin{matrix} n_2 l_2 \\ m_2 \end{matrix} \right\rangle E_{m_1 m_2} \\ &= \sum_{m_1, m_2} (-1)^{l_1 - m_1} (2k + 1)^{1/2} \begin{pmatrix} l_1 & k & l_2 \\ -m_1 & q & m_2 \end{pmatrix} E_{m_1 m_2}. \end{aligned} \quad (4)$$

Also,

$$\bar{V}_q^k(l_2 l_1) = (-1)^{l_1 - l_2 + q} \bar{V}_{-q}^k(l_1 l_2),$$

where $\bar{E}_{m_1 m_2} = E_{m_2 m_1}$. The *intrashell* operators $V_q^k(l_1 l_1)$ and $V_q^k(l_2 l_2)$ can also be expressed in terms of the generators E_{ij} as follows:

$$\begin{aligned} V_q^k(l_1 l_1) &= \sum_{m_1, m_1'} \left\langle \begin{matrix} n_1 l_1 \\ m_1 \end{matrix} \middle| v_q^k \middle| \begin{matrix} n_1 l_1 \\ m_1' \end{matrix} \right\rangle E_{m_1 m_1'} \\ &= \sum_{m_1, m_1'} (-1)^{l_1 - m_1} (2k + 1)^{1/2} \begin{pmatrix} l_1 & k & l_1 \\ -m_1 & q & m_1' \end{pmatrix} E_{m_1 m_1'}, \end{aligned} \quad (5)$$

and

$$V_q^k(l_2 l_2) = \sum_{m_2, m_2'} (-1)^{l_2 - m_2} (2k + 1)^{1/2} \begin{pmatrix} l_2 & k & l_2 \\ -m_2 & q & m_2' \end{pmatrix} E_{m_2 m_2'}. \quad (6)$$

Together, the intershell and intrashell tensor operators form a complete set of operators for U_h .

We now consider the mixed configurations subspace $(n_1 l_1)^{p_1} (n_2 l_2)^{p_2}$ of the product space $(n_1 l_1 + n_2 l_2)^p$

where $p = p_1 + p_2$. We shall first analyze the pure configuration factor spaces $(n_1 l_1)^{p_1}$ and $(n_2 l_2)^{p_2}$ separately.

The configuration $(n_1 l_1)^{p_1}$ forms a reducible basis for $U_{[l_1]}$ with generators

$$E_{m_1 m'_1} = \sum_{\alpha=1}^{p_1} e_{m_1 m'_1}^{\alpha} \quad (7)$$

for $m_1, m'_1 = 1, 2, \dots, [l_1]$. We may express the intrashell operators $V_a^k(l_1 l_1)$ in terms of the generators $E_{m_1 m'_1}$ as in Eq. (5). These tensor operators form a complete set of operators for $U_{[l_1]}$. The configuration $(n_2 l_2)^{p_2}$ forms a reducible basis for $U_{[l_2]}$ with generators

$$E_{m_2 m'_2} = \sum_{\alpha=p_1+1}^p e_{m_2 m'_2}^{\alpha} \quad (8)$$

for $m_2, m'_2 = [l_1] + 1, [l_1] + 2, \dots, n$. Again, we may express the intrashell operators $V_a^k(l_2 l_2)$ in terms of the generators $E_{m_2 m'_2}$ as in Eq. (6) and these tensor operators form a complete set of operators for $U_{[l_2]}$.

As has been discussed in II, the irreducible representations (IR) of $U_{[l_1]}$ for configuration $(n_1 l_1)^{p_1}$ are labeled by Young frames $[u_1]$ with $[l_1]$ rows and p_1 boxes. Similarly, the IR of $U_{[l_2]}$ for configuration $(n_2 l_2)^{p_2}$ are labeled by Young frames $[u_2]$ with $[l_2]$ rows and p_2 boxes. The canonical irreducible bases or Gel'fand bases for $U_{[l_1]}$ or $U_{[l_2]}$ may be enumerated using Gel'fand tableaux. For example, for the pure configuration $(n_1 l_1)^{p_1} = (nd)^2$ we have the Gel'fand tableaux

$$|\frac{1}{2}\rangle : |\frac{1}{3}\rangle : |\frac{1}{4}\rangle |\frac{2}{3}\rangle : |\frac{1}{5}\rangle |\frac{2}{4}\rangle : |\frac{2}{5}\rangle |\frac{3}{4}\rangle : |\frac{3}{5}\rangle : |\frac{4}{5}\rangle$$

corresponding to IR $[u_1] = [11]$. Similarly, for the pure "configuration" $(n_2 l_2)^{p_2} = (np)$ we have the Gel'fand tableaux $|\frac{6}{7}\rangle : |\frac{7}{8}\rangle$ corresponding to IR $[u_2] = [1]$.

For the case where the Gel'fand bases of $[u_1]$ or $[u_2]$ have two columns or less, we may easily evaluate the effect of operators $E_{m_1 m'_1}$ and $E_{m_2 m'_2}$ on the bases as shown in II. (We reproduce these results in Fig. 1 to make our presentation reasonably self-contained.) In particular, we note that the Gel'fand bases are eigenstates of the "number operators" E_{ii} . Thus, the above states of d^2 and p are eigenstates of the angular momentum projection operators L_{1z} and L_{2z} given below:

$$L_{1z} = \sqrt{10} V_0^1(dd) = 2E_{11} + E_{22} - E_{44} - 2E_{55}, \quad (9)$$

$$L_{2z} = \sqrt{2} V_0^1(pp) = E_{66} - E_{88}.$$

To find the linear combination of Gel'fand states in $(n_1 l_1)^{p_1}$ or $(n_2 l_2)^{p_2}$ which have good orbital angular momentum we simply lower the highest L state using the lowering operators L_{1-} or L_{2-} . In our case

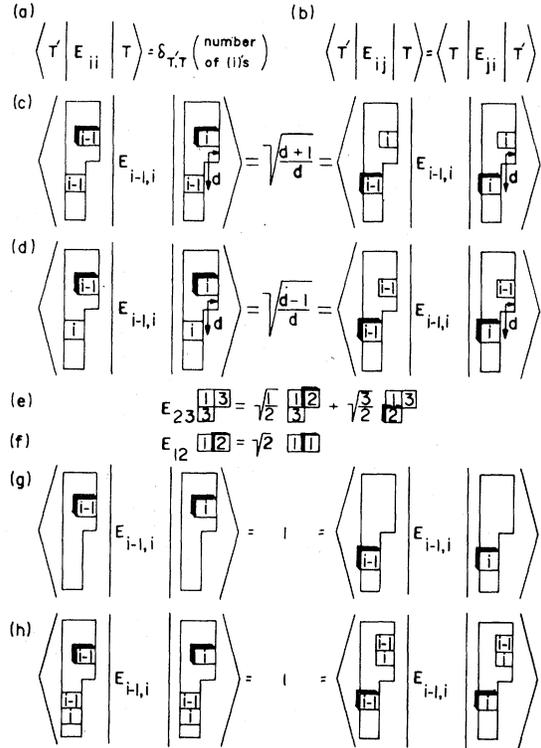


Fig. 1. Simplified jawbone formula for electronic orbital operators. (a) Number operators E_{ii} are diagonal. (The only eigenvalues for orbital states are 0, 1, and 2.) (b) Raising and lowering operators and simply transposes of each other. (c)-(h) $E_{i-1,i}$ acting on a tableau state gives zero unless there is an i in a column of the tableau that doesn't already have an $i-1$, too. Then it gives back a new state with the (i) changed to $(i-1)$ and a factor (matrix element) that depends on where the other (i) 's and $(i-1)$'s are located. (Boxes not outlined in the figure contain numbers not equal to i or $i-1$.) Cases (c) and (d) involve the "city block" distance d which is the denominator of the matrix element. Numerator is one larger $(d+1)$ or smaller $(d-1)$, depending on whether the involved tableaux favor the larger or smaller state number $(i$ or $i-1)$ with a higher position. Special cases of $(d=1)$ shown in (f) always pick the larger (and nonzero) choice of $d+1=2$. All other nonzero matrix elements are equal to unity.

$$L_{1-} = \sqrt{20} V_{-1}^1(dd) = 2E_{21} + \sqrt{6} E_{32} + \sqrt{6} E_{43} + 2E_{54},$$

$$L_{2-} = 2V_{-1}^1(pp) = \sqrt{2} E_{76} + \sqrt{2} E_{87}. \quad (10)$$

Applying Eqs. (9) and (10) to the d^2 configuration we find the $|L_1 M_1\rangle$ states below:

$$|d^2 F3\rangle = |\frac{1}{2}\rangle,$$

$$|d^2 F2\rangle = |\frac{1}{3}\rangle,$$

$$|d^2 F1\rangle = (L_{1-}/\sqrt{10})|\frac{1}{3}\rangle$$

$$= (1/\sqrt{10})(2E_{21} + \sqrt{6} E_{32} + \sqrt{6} E_{43} + 2E_{54})|\frac{1}{3}\rangle$$

$$= (2|\frac{2}{3}\rangle + \sqrt{6} |\frac{1}{4}\rangle)/\sqrt{10}.$$

Orthogonalizing, we find

$$|d^2 P1\rangle = (\sqrt{6} |^2_3\rangle - 2|^1_4\rangle) / \sqrt{10}.$$

Similarly,

$$|d^2 F0\rangle = (4|^2_4\rangle + 2|^1_5\rangle) / \sqrt{20}, \tag{11}$$

$$|d^2 P0\rangle = (2|^2_4\rangle - 4|^1_5\rangle) / \sqrt{20}.$$

For the trivial p "configuration" we find the $|L_2 M_2\rangle$ states below:

$$|p P1\rangle = |6\rangle, \quad |p P0\rangle = |7\rangle, \quad |p P-1\rangle = |8\rangle. \tag{12}$$

Later, we shall use the results in Eqs. (11) and (12) to derive Gel'fand states of $(d^2 p)$ with good $L = L_1 + L_2$ which can be readily coupled to spin states to form an antisymmetric basis.

It is now clear that the mixed configuration $(n_1 l_1)^{p_1} (n_2 l_2)^{p_2}$ forms a reducible basis for $U_{[l_1]} \times U_{[l_2]}$ with IR $[u_1] \times [u_2]$ and with generators $E_{m_1 m_1}, E_{m_2 m_2}$, and is a subspace of the product space $(n_1 l_1 + n_2 l_2)^p$ of U_h . The IR of U_h are labeled by Young frames $[u]$ with h rows and p boxes.

It is much more convenient to deal with the Gel'fand bases of U_h than the product Gel'fand bases of $U_{[l_1]} \times U_{[l_2]}$. This is because orbital operators may be evaluated without introducing spin states. For each IR $[u]$ of U_h there are associated spin states corresponding to an IR of U_2 conjugate to $[u]$ with rows and columns exchanged. The orbital states of U_h and the spin states of U_2 may be coupled using the assembly formula in II to produce antisymmetric states with good orbit and spin-quantum numbers. We reproduce this formula in Fig. 2.

Since spin states of U_2 are limited to frames with two rows or less, the orbital states of U_h must be limited to frames with two columns or less. This limitation enables us to calculate matrix elements for any intershell or intrashell operators E_{ij} with $i, j = 1, 2, \dots, h$ between orbital Gel'fand states of U_h using the formulas in Fig. 1. It would therefore be helpful if we could find the orbital states of U_h for configuration $(n_1 l_1 + n_2 l_2)^p$ in terms of the orbital product states of $U_{[l_1]} \times U_{[l_2]}$ for mixed configurations $(n_1 l_1)^{p_1} (n_2 l_2)^{p_2}$. First, let us specify which IR $[u_1] \times [u_2]$ of the subgroup $U_{[l_1]} \times U_{[l_2]}$ are contained in the IR $[u]$ of group U_h . That is, we first find the subduction series

$$[u] \uparrow U_{[l_1]} \times U_{[l_2]} = \sum_{u_1, u_2} g_{u_1 u_2 u} [u_1] \times [u_2]. \tag{13}$$

The series expansion coefficients $g_{u_1 u_2 u}$ may be evaluated using the simple methods developed by Littlewood.²⁹ When $[u]$ is restricted to frames with no more than two columns, it is found that $g_{u_1 u_2 u} = 0$ unless both $[u_1]$ and $[u_2]$ are frames with no more than two columns. Thus, $[u_1]$ and $[u_2]$

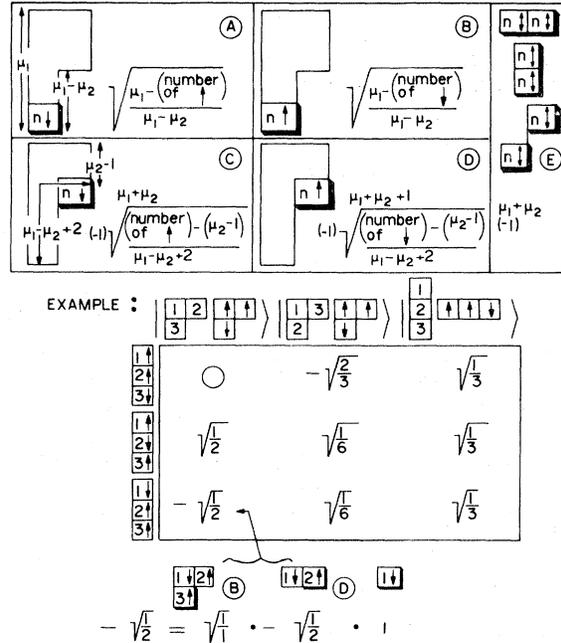


FIG. 2. Assembly formula for combining orbital and spin states. Each column state (Slater determinant) on the left-hand side of the sample table has a definite spin (arrow) on each orbital state (number). Formulas will give the overlap of this Slater state with a given orbital tableau state if we first write the spins within this orbital tableau in exactly the same way. Then we proceed to remove boxes with numbered spins starting with the highest number(s). Each "removal" gives a factor depending on what is being removed and where (cases A-E). All of the numbers in the formulas refer to the condition of the tableau just before the box outlined in the figure is removed.

must correspond to IR which are allowable for the pure configurations $(n_1 l_1)^{p_1}$ and $(n_2 l_2)^{p_2}$. Let S_1, S_2 , and S be the total spin angular momentum for the spin states conjugate to the frames $[u_1], [u_2]$, and $[u]$, respectively. Then we find that for a given $[u_1]$ and $[u_2]$, $g_{u_1 u_2 u}$ is zero unless

$$|S_1 - S_2| \leq S \leq S_1 + S_2. \tag{14}$$

The allowable frames $[u]$ for a given $[u_1]$ and $[u_2]$ are found by coupling the conjugate spin states such that $S = S_1 \times S_2$. Thus, the inequality Eq. (14) and the fact that $[u]$ must have p boxes uniquely determine the possible $[u]$.

Let us continue with our example to illustrate these results. For the configuration d^2 or U_5 we found orbital terms P and F for the frame $[u_1] = [11]$ with conjugate total spin $S_1 = 1$. For the p "configuration" of U_3 we have a P term for the frame $[u_2] = [1]$ with conjugate total spin $S_2 = \frac{1}{2}$. Finally, for the mixed configuration $d^2 p$, the IR $[11] \times [1]$ of $U_5 \times U_3$ give rise to the terms

$$(P+F) \times P = G+F+2(D)+P+S$$

with total spins $1 \times \frac{1}{2} = \frac{3}{2} + \frac{1}{2}$. The frames of U_8 conjugate to the quartet $S = \frac{3}{2}$ and the doublet $S = \frac{1}{2}$ are [111] and [21], respectively, each containing the same angular momentum terms above. Of course, the coupling of the total angular momenta of spin S_1, S_2, \dots , and orbit L_1, L_2, \dots , of pure configurations $(n_1 l_1)^{p_1}, (n_2 l_2)^{p_2}, \dots$, to determine the orbital terms L and total spin S of the mixed configuration $(n_1 l_1)^{p_1} (n_2 l_2)^{p_2} \dots$, is well known. It is a result of the fact that the Pauli exclusion principle makes no restrictions on product states arising from different pure configurations with different parentage.

We would like to find the coupled orbital states of $U_5 \times U_3$ above in terms of the Gel'fand bases of [111] and [21] of U_8 . In Sec. III we show that this may be accomplished in two ways.

III. GEL'FAND BASES FOR MIXED CONFIGURATIONS

A. Lowering operators for Gel'fand bases

We begin by finding the total angular momentum states for the d^2p configuration in terms of the Gel'fand bases of U_8 with conjugate total spin $S = \frac{1}{2}$. We shall use the lowering operator methods described in II. Operating with $L_- = L_{1-} + L_{2-}$ on the highest L state $|^2_2^{16}\rangle$ with the proper parentage, we find the $|^{2S+1}LM\rangle$ states below:

$$|d^2p^2G4\rangle = |^2_2^{16}\rangle,$$

$$|d^2p^2G3\rangle = (L_-/\sqrt{8})|^2_2^{16}\rangle = \frac{1}{2}(\sqrt{3}|^2_3^{16}\rangle + |^2_2^{17}\rangle).$$

The $|^2F3\rangle$ state must be orthogonal to $|^2G3\rangle$. Hence,

$$|d^2p^2F3\rangle = \frac{1}{2}(|^2_3^{16}\rangle - \sqrt{3}|^2_2^{17}\rangle).$$

Similarly, we find

$$\begin{aligned} &|^2_3^{26}\rangle \quad |^2_4^{16}\rangle \quad |^2_3^{17}\rangle \quad |^2_2^{18}\rangle \\ |d^2p^2G2\rangle &= (2\sqrt{3} \quad 3\sqrt{2} \quad 2\sqrt{6} \quad \sqrt{2})/2\sqrt{14}, \quad (15) \\ |d^2p^2F2\rangle &= (2 \quad \sqrt{6} \quad -2\sqrt{2} \quad -\sqrt{6})/2\sqrt{6}. \end{aligned}$$

The repeated $|^2D2\rangle$ states may be found by Gram-Schmidt orthogonalizing the columns of the projection operator

$$\hat{P} = \hat{1} - |^2G2\rangle\langle^2G2| - |^2F2\rangle\langle^2F2|. \quad (16)$$

we find

$$\begin{aligned} &|^2_3^{26}\rangle \quad |^2_4^{16}\rangle \quad |^2_3^{17}\rangle \quad |^2_2^{18}\rangle \\ |d^2p^2D2\rangle_1 &= (13 \quad -4\sqrt{6} \quad -\sqrt{2} \quad \sqrt{6})/(3 \times 7 \times 13)^{1/2}, \\ |d^2p^2D2\rangle_2 &= (0 \quad 1 \quad -\sqrt{3} \quad 3)/\sqrt{13}. \quad (17) \end{aligned}$$

There are several disadvantages in using a Gel'fand bases in a mixed configuration derived from lowering and projection operator orthogonalization. From a computational standpoint, the

numbers involved in expansions such as Eq. (17) can be extremely large, and lead to computer overflow—especially when dealing with the many repeated L terms which arise for complex configurations. Also, we must separately treat the Gel'fand bases conjugate to different total spins S without making use of the Gel'fand bases already derived for the pure configurations such as in Eqs. (11) and (12). From a physical standpoint, the Gel'fand bases generated do not correspond to any group-theoretical scheme representing partial symmetries of the Hamiltonian. In particular, the $|^2D2\rangle_1$ and $|^2D2\rangle_2$ states are always mixed by the Coulomb electrostatic energy operator. The Gel'fand bases that we now construct have none of these disadvantages.

B. Subduction coefficients for Gel'fand bases

The subduction coefficients $S_{i_1 i_2 i}^{[u_1] [u_2] [u]}$ are used to transform the Gel'fand bases

$$| \begin{smallmatrix} [u] \\ i \end{smallmatrix} \rangle \text{ of } U_h$$

into linear combinations of product Gel'fand bases

$$| \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \rangle \times | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \rangle$$

of the subgroup $U_{[i_1]} \times U_{[i_2]}$ as shown below:

$$| \begin{smallmatrix} [u] \\ i \end{smallmatrix} \rangle = \sum_{\substack{i_1, i_2 \\ [u_1], [u_2]}} S_{i_1 i_2 i}^{[u_1] [u_2] [u]} | \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \rangle \times | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \rangle. \quad (18)$$

Since the subduction coefficients are elements of an orthogonal matrix, we have the following conditions:

$$\sum_i S_{i_1 i_2 i}^{[u_1] [u_2] [u]} S_{i_1' i_2' i'}^{[u_1'] [u_2'] [u']} = \delta_{i_1 i_1'} \delta_{i_2 i_2'} \delta_{[u_1] [u_1']} \delta_{[u_2] [u_2']}, \quad (19a)$$

$$\sum_{\substack{i_1, i_2 \\ [u_1], [u_2]}} S_{i_1 i_2 i}^{[u_1] [u_2] [u]} S_{i_1 i_2 i'}^{[u_1] [u_2] [u']} = \delta_{ii'}. \quad (19b)$$

We may use Eqs. (19a) and (18) to express the Gel'fand bases of $U_{[i_1]} \times U_{[i_2]}$ in terms of the bases of U_h as follows:

$$| \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \rangle \times | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \rangle = \sum_i S_{i_1 i_2 i}^{[u_1] [u_2] [u]} | \begin{smallmatrix} [u] \\ i \end{smallmatrix} \rangle. \quad (20)$$

To find these subduction coefficients, we shall first couple the Gel'fand states

$$| \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \rangle \text{ and } | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \rangle$$

of $U_{[i_1]}$ and $U_{[i_2]}$ to arbitrary conjugate spin states

$$| \begin{smallmatrix} S_1 \\ a_1 \end{smallmatrix} \rangle \text{ and } | \begin{smallmatrix} S_2 \\ a_2 \end{smallmatrix} \rangle$$

of U_2 using the assembly formula. In this manner, we find the direct product states

$$| \begin{smallmatrix} [u_1] \otimes S_1 \\ i_1 a_1 \end{smallmatrix} \rangle \text{ and } | \begin{smallmatrix} [u_2] \otimes S_2 \\ i_2 a_2 \end{smallmatrix} \rangle$$

of $U_{[i_1]} \otimes U_2$ and $U_{[i_2]} \otimes U_2$ in terms of antisymmetric states of $U_{2[i_1]}$ and $U_{2[i_2]}$. We use \otimes to denote direct products and \times to denote simple products. In the following example, we expand Gel'fand direct product states of $U_5 \otimes U_2$ and $U_3 \otimes U_2$ in terms of antisymmetric states of U_{10} and U_6 using the assembly formula.

$$|\frac{1}{2} \otimes \uparrow\uparrow\rangle = \sqrt{\frac{1}{2}} (|\frac{1}{2} \uparrow\rangle + |\frac{1}{2} \downarrow\rangle), \tag{21a}$$

$$|\frac{6}{7} \otimes \uparrow\uparrow\rangle = |\frac{6}{7} \uparrow\rangle. \tag{21b}$$

It is now a simple matter to generate antisymmetric states of U_{2h} from the antisymmetric product states of $U_{2[i_1]} \times U_{2[i_2]}$ as shown below. Using the assembly formula once more, the antisymmetric states of U_{2h} may be decoupled from spin to form the direct Gel'fand states

$$| \begin{smallmatrix} [u] \\ i \end{smallmatrix} \otimes_q^S \rangle \text{ of } U_h \otimes U_2.$$

The final result is an expansion of states

$$| \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \otimes_{q_1}^{S_1} \rangle \times | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \otimes_{q_2}^{S_2} \rangle$$

of $(U_{[i_1]} \otimes U_2) \times (U_{[i_2]} \otimes U_2)$ in terms of states

$$| \begin{smallmatrix} [u] \\ i \end{smallmatrix} \otimes_q^S \rangle \text{ of } U_h \otimes U_2.$$

For our example, we have

$$\begin{aligned} |\frac{1}{2} \otimes \uparrow\uparrow\rangle \times |\frac{6}{7} \otimes \uparrow\uparrow\rangle &= \sqrt{\frac{1}{2}} (|\frac{1}{2} \uparrow\rangle + |\frac{1}{2} \downarrow\rangle) \times |\frac{6}{7} \uparrow\rangle \\ &= \sqrt{\frac{1}{2}} \left(\left| \begin{smallmatrix} \frac{1}{2} \uparrow \\ \frac{6}{7} \uparrow \end{smallmatrix} \right\rangle + \left| \begin{smallmatrix} \frac{1}{2} \downarrow \\ \frac{6}{7} \uparrow \end{smallmatrix} \right\rangle \right). \end{aligned}$$

Decoupling gives

$$\begin{aligned} |\frac{1}{2} \otimes \uparrow\uparrow\rangle \times |\frac{6}{7} \otimes \uparrow\uparrow\rangle &= -\sqrt{\frac{1}{2}} \left(\sqrt{\frac{1}{3}} \left| \begin{smallmatrix} \frac{1}{2} \uparrow \\ \frac{6}{7} \uparrow \end{smallmatrix} \right\rangle + \sqrt{\frac{2}{3}} \left| \begin{smallmatrix} \frac{1}{2} \downarrow \\ \frac{6}{7} \uparrow \end{smallmatrix} \right\rangle \right) \\ &\quad + \sqrt{\frac{1}{2}} \left(\left| \begin{smallmatrix} \frac{1}{2} \uparrow \\ \frac{6}{7} \downarrow \end{smallmatrix} \right\rangle + \left| \begin{smallmatrix} \frac{1}{2} \downarrow \\ \frac{6}{7} \downarrow \end{smallmatrix} \right\rangle \right). \end{aligned} \tag{22}$$

Using the identity

$$(U_{[i_1]} \otimes U_2) \times (U_{[i_2]} \otimes U_2) = (U_{[i_1]} \times U_{[i_2]}) \otimes (U_2 \times U_2),$$

we have

$$\begin{aligned} | \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \otimes_{q_1}^{S_1} \rangle \times | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \otimes_{q_2}^{S_2} \rangle \\ &= | (\begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \otimes_{q_1}^{S_1}) \times (\begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \otimes_{q_2}^{S_2}) \rangle \\ &= | (\begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \times \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix}) \otimes (\begin{smallmatrix} S_1 \\ q_1 \end{smallmatrix} \times \begin{smallmatrix} S_2 \\ q_2 \end{smallmatrix}) \rangle \\ &= \sum_{[u], i} | \begin{smallmatrix} [u] \\ i \end{smallmatrix} \otimes_q^S \rangle \langle \begin{smallmatrix} [u] \\ i \end{smallmatrix} \otimes_q^S | (\begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \times \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix}) \otimes (\begin{smallmatrix} S_1 \\ q_1 \end{smallmatrix} \times \begin{smallmatrix} S_2 \\ q_2 \end{smallmatrix}) \rangle. \end{aligned}$$

Note that q is determined by q_1 and q_2 , and S is determined by $[u]$. Finally, as a result of the factorization lemma,³⁰

$$\langle \begin{smallmatrix} [u] \\ i \end{smallmatrix} \otimes_q^S | (\begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \times \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix}) \otimes (\begin{smallmatrix} S_1 \\ q_1 \end{smallmatrix} \times \begin{smallmatrix} S_2 \\ q_2 \end{smallmatrix}) \rangle = C_{q_1 q_2 q}^{S_1 S_2 S} S_{i_1 i_2 i}^{[u_1] [u_2] [u]}, \tag{23}$$

we have

$$\begin{aligned} | \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \otimes_{q_1}^{S_1} \rangle \times | \begin{smallmatrix} [u_2] \\ i_2 \end{smallmatrix} \otimes_{q_2}^{S_2} \rangle \\ &= \sum_{[u]} C_{q_1 q_2 q}^{S_1 S_2 S} \sum_i S_{i_1 i_2 i}^{[u_1] [u_2] [u]} | \begin{smallmatrix} [u] \\ i \end{smallmatrix} \otimes_q^S \rangle, \end{aligned} \tag{24}$$

where the $C_{q_1 q_2 q}^{S_1 S_2 S}$ are Clebsch-Gordan coefficients of $U_2 \times U_2$.

Applying Eq. (24) to our example, we see that the factors outside the parentheses in Eq. (22) are just the Clebsch-Gordan coefficients

$$\begin{aligned} \langle \uparrow\uparrow \times \uparrow\uparrow | \uparrow\uparrow \rangle &= C_{0111}^{111} = -\sqrt{\frac{1}{2}}, \\ \langle \uparrow\uparrow \times \uparrow\uparrow | \uparrow\uparrow\uparrow \rangle &= C_{0111}^{112} = \sqrt{\frac{1}{2}}. \end{aligned}$$

The factors inside the parentheses in Eq. (22) give us the expansions [Eq. (20)] which we desire:

$$\begin{aligned} |\frac{1}{2}\rangle \times |\frac{6}{7}\rangle &= \sqrt{\frac{1}{3}} \left| \begin{smallmatrix} \frac{1}{2} \\ \frac{6}{7} \end{smallmatrix} \right\rangle - \sqrt{\frac{2}{3}} \left| \begin{smallmatrix} \frac{1}{2} \\ \frac{6}{7} \end{smallmatrix} \right\rangle, \\ |\frac{1}{2}\rangle \times |\frac{6}{7}\rangle &= \left| \begin{smallmatrix} \frac{1}{2} \\ \frac{6}{7} \end{smallmatrix} \right\rangle. \end{aligned} \tag{25}$$

Using the assembly formula, it is a straightforward task to evaluate the matrix expression on the left of Eq. (23). Since the Clebsch-Gordan coefficients $C_{q_1 q_2 q}^{S_1 S_2 S}$ for $U_2 \times U_2$ are known, we may use Eq. (23) to find closed-form expressions for the subduction coefficients $S_{i_1 i_2 i}^{[u_1] [u_2] [u]}$ as shown in Fig. 3. We see that we obtain results using these formulas that agree with Eq. (25). Since we are using a *canonical* unitary basis, the subduction coefficients $S_{i_1 i_2 i}^{[u_1] [u_2] [u]}$ are nonzero only if removing boxes containing $U_{[i_2]}$ states from the Gel'fand tableau

$$| \begin{smallmatrix} [u] \\ i \end{smallmatrix} \rangle \text{ of } U_h$$

results in the Gel'fand tableau

$$| \begin{smallmatrix} [u_1] \\ i_1 \end{smallmatrix} \rangle \text{ of } U_{[i_1]}.$$

Thus, the sums over $[u_1]$ and i_1 in Eqs. (18) and (19b) are superfluous as are the Kronecker δ functions of $[u_1]$ and i_1 in Eq. (19a).

With the aid of Fig. 3, we may now derive two $|^2D 2\rangle$ states of d^2p having *different parentage* with respect to pure configurations d^2 and p . Coupling the states in Eqs. (11) and (12), we derive the doublet states (where $S_1=1, S_2=\frac{1}{2}, S=\frac{1}{2}$ in Fig. 3),

$$\begin{aligned} |(d^2 {}^3P) p {}^2D 2\rangle &= |d^2 P 1\rangle \times |p P 1\rangle \\ &= \sqrt{\frac{1}{10}} (\sqrt{6} | \begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \rangle - 2 | \begin{smallmatrix} 1 \\ 4 \end{smallmatrix} \rangle) \times |6\rangle \\ &= \sqrt{\frac{1}{10}} (-\sqrt{6} | \begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \rangle + 2 | \begin{smallmatrix} 1 \\ 4 \end{smallmatrix} \rangle), \\ |(d^2 {}^3F) p {}^2D 2\rangle &= \sqrt{\frac{5}{7}} |d^2 F 3\rangle \times |p P -1\rangle \\ &\quad - \sqrt{\frac{5}{21}} |d^2 F 2\rangle \times |p P 0\rangle \\ &\quad + \sqrt{\frac{1}{21}} |d^2 F 1\rangle \times |p P 1\rangle \\ &= -\sqrt{\frac{5}{7}} | \begin{smallmatrix} 1 \\ 2 \end{smallmatrix} \rangle + \sqrt{\frac{5}{21}} | \begin{smallmatrix} 1 \\ 3 \end{smallmatrix} \rangle \\ &\quad - (\frac{1}{21} \cdot \frac{1}{10})^{1/2} (2 | \begin{smallmatrix} 2 \\ 3 \end{smallmatrix} \rangle + \sqrt{6} | \begin{smallmatrix} 1 \\ 4 \end{smallmatrix} \rangle), \end{aligned}$$

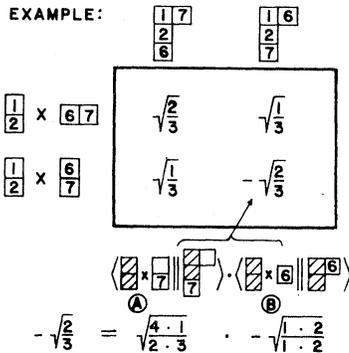
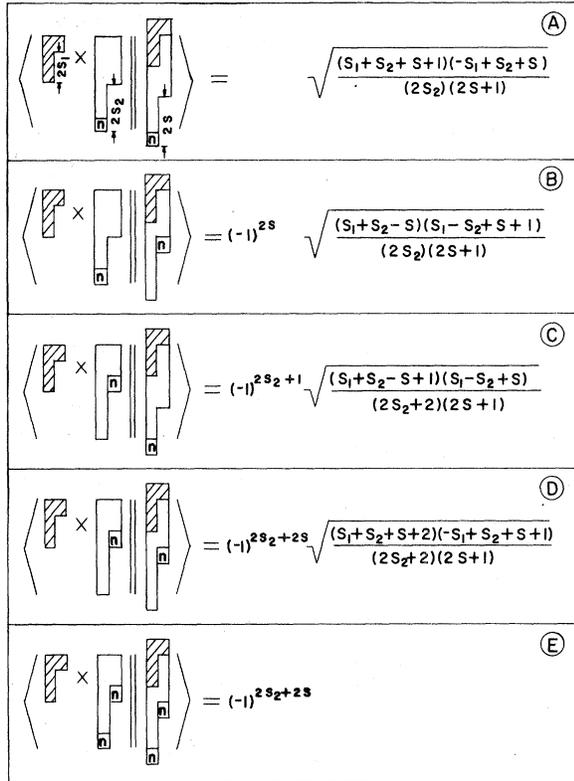


FIG. 3. Subduction coefficients for $[u] \downarrow [u_1] \times [u_2]$ are found by successive removal of boxes with highest state numbers from Gel'fand tableaux $[u_2]$ and $[u]$. Each "removal" gives a factor in terms of conjugate total spins S_1 , S_2 , and S , depending on where the highest states n are located (Cases A-E). All of the numbers in the formulas refer to the condition of the tableaux just before the boxes containing n are removed. Subduction coefficient is zero unless the tableau of $[u]$ contains the tableau of $[u_1]$ as indicated by the shaded area.

or

$$\begin{aligned}
 |(d^2 \ ^3P)p \ ^2D \ 2\rangle &= (-\sqrt{3} \ \sqrt{2} \ 0 \ 0) / \sqrt{5}, \\
 |(d^2 \ ^3F)p \ ^2D \ 2\rangle &= (-\sqrt{2} \ -\sqrt{3} \ 5 \ -5\sqrt{3}) / (3 \times 5 \times 7)^{1/2}.
 \end{aligned}
 \tag{26}$$

Furthermore, we may simultaneously derive the quartet states (where $S_1=1$, $S_2=\frac{1}{2}$, $S=\frac{3}{2}$ in Fig. 3),

$$\begin{aligned}
 & \begin{vmatrix} 2 \\ 3 \\ 6 \end{vmatrix} \quad \begin{vmatrix} 1 \\ 4 \\ 6 \end{vmatrix} \quad \begin{vmatrix} 1 \\ 3 \\ 7 \end{vmatrix} \quad \begin{vmatrix} 1 \\ 2 \\ 8 \end{vmatrix} \\
 |(d^2 \ ^3P)p \ ^4D \ 2\rangle &= (\sqrt{3} \ -\sqrt{2} \ 0 \ 0) / \sqrt{5} \\
 |(d^2 \ ^3F)p \ ^4D \ 2\rangle &= (\sqrt{2} \ \sqrt{3} \ -5 \ 5\sqrt{3}) / (3 \times 5 \times 7)^{1/2}.
 \end{aligned}
 \tag{27}$$

When there are no Coulomb electrostatic interactions between shells (no intershell operators $E_{m_1 m_2}$ or $E_{m_2 m_1}$), the states in Eqs. (26) and (27) will be eigenstates of the Coulomb operator since they have parentage traceable to simple products of d^2 and p states. Hence, in the limit of small electrostatic exchange integrals, there will be little mixing of states with different parentage and the states in Eqs. (26) and (27) become good approximations to the exact eigenstates. This occurs in $J_1 l$ coupling in the rare earths, for example.³¹

For mixed configurations with q subshells

$$(n_1 l_1)^{p_1} (n_2 l_2)^{p_2} \cdots (n_q l_q)^{p_q},$$

where $p = p_1 + p_2 + \cdots + p_q$, we couple the Gel'fand states for each pure configuration iteratively using Fig. 3. We can then easily form Gel'fand states of U_h from the product bases of

$$\{\cdots [(U_{[l_1]} \times U_{[l_2]}) \times U_{[l_3]}] \times \cdots \times U_{[l_q]}\}.$$

Generating Gel'fand states with good L in pure states is a relatively easy task. In fact, Racah states have been generated for the p , d , and f subshells in terms of Gel'fand states by Caird. For computer calculations in pure configurations, the suitable Gel'fand states may be stored. Gel'fand states may then be generated for mixed configurations using Fig. 3. Finally, spin- and orbit-dependent tensor operators may be readily evaluated using Figs. 1 and 2 as has been thoroughly discussed in II.

IV. CONCLUSIONS

We have now completely solved the problem of evaluating matrix elements of spin- and orbit-dependent operators in pure and mixed atomic configurations using a Gel'fand basis. The essential parts of our treatment are the formulas illustrated in Figs. 1-3.

Our fourth and final paper will concern more than half-filled subshells in both pure and mixed configurations. Using Figs. 1-3, we derive new matrix relations for spin- and orbit-dependent operators between configurations with more than half-filled subshells and those with less than half-filled subshells. Thus we relate matrix elements

which involve "hole" states to those involving only "particle" states in both pure and mixed configurations.

Although our techniques have only been applied to atomic subshells, they readily extend to nuclear subshells using the jj -coupling scheme. The orbital states of $(nl)^p$ in the atomic case become spin-orbit coupled states of $(nj)^p$ in the nuclear case

with $j = l \pm \frac{1}{2}$. The conjugate spin states for atoms then corresponds to the conjugate isospin states for nuclei. Configurations such as $(n_1 j_1)^{p_1} (n_2 j_2)^{p_2} \dots$, may be treated as in the atomic case using Fig. 3. Spin-, orbit-, and iso-spin-dependent operators may then be evaluated when operating on a nuclear Gel'fand basis using Figs. 1 and 2. We hope to clarify this in a later paper.

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