Alternative basis for the theory of complex spectra. II*

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The atomic angular-factor calculation methods given in a previous work are simplified and extended to include a treatment of spin-orbit operators and multiple shell configurations $(ll'\cdots)^n$. A tableau formula is given for the matrix between Slater states and states of definite total spin.

In an earlier work[1] the unitary group representations of Gelfand were used to find orbital angular factors in atomic l^n configurations. In this paper these methods are simplified and extended to include a treatment of spin and orbital operators and multiple-shell configurations $(ll'\cdots)^n$. The description is given in a concise form that requires very little knowledge of unitary mathematics or group theory.

Various suggestions have been made for improving the application of these methods to atomic orbitals by Drake, Drake, and Schlesinger,[2] and to molecular orbitals in Abelian symmetry by Paldus.[3] (Independently, Matsen[4] has discussed the unitary approach to certain molecules.) One conclusion drawn in Refs. 2 and 3 is that the Gelfand framework is more complicated than it needs to be for atomic and molecular spectroscopy analysis.

The Gelfand pattern analysis as developed by Biedenharn *et al.*,[5] Louck,[6] Moshinsky,[7] and others is a very good foundation upon which to base the theory of the mathematics. However, for applications it is apparently more convenient to use some recent developments of the more well-known Young tableau patterns including two very simple formulas which we report here for the first time.

The tableau approach is based on the use of the permutation group as developed by Rutherford,[8] Weyl,[9] Yamanouchi,[10] Robinson,[11] and, more recently, Goddard.[12] The main problem with this approach has been that it usually appears to be an extremely complicated algebra involving many factors containing sums over $n!$ terms. However, now our two very simple graphical formulas permit one to understand and use tableaus very easily, without getting involved in the complex details of multielectron wave-function structure.

The way the tableau notation is used for labeling is sketched in Sec. I. Nothing new is given there except possibly a more concise review. In Sec. II a new orbital tableau formula is introduced and applied to a simple atomic configuration. In Sec. III another tableau formula is shown which involves spin and orbit. In Secs. IV and V we outline various applications of the two tableau formulas in a way which shows some of their structure.

It is hoped that this exposition will make the new formulas available to physicists and quantum chemists who are not necessarily specialists in group theory. Most of the work has been stimulated by the apparent needs of researchers in modern atomic physics who have expressed concern about the computing labor involved in calculating or storing various "group theoretical" coefficients.[13-15] We hope the present work will help reduce this labor without requiring much new knowledge or change.

The extension of this work to the treatment of molecular orbitals will be discussed in a separate work. It is mostly a straightforward application of the methods described in this work.

I. REVIEW OF TABLEAU LABELING

Two groups of operators are useful in the description of a quantum system of n identical particles occupying a shell which has m states $|1\rangle$, $|2\rangle, \ldots |m\rangle$ for each particle. The first is the symmetric group S_n of $n!$ permutations of the n particles. The second is the unitary group U_m of all linear transformations of the m states subject only to the restriction that orthonormality ($\langle i|j\rangle = \delta_{ij}$) is preserved.

The symmetric group S_n is an invariance group or symmetry for a system of n identical particles. In fact, this is one of the apparently perfect symmetries found in nature. The eigenstates of the system must be bases of irreducible representations (IR) of S_n, which are labeled by the Young tableaus. The Pauli principle and other physical considerations tell which IR or tableau of S_n will be used.

For example, if the n particles are electrons or other types of fermions, the Pauli principle demands that the eigenstates be totally antisymmetric under permutations. Total antisymmetry is designated by the Young tableau shown in Fig.

1(a), i.e., by a single vertical column of n boxes. On the other hand, a totally symmetric n-boson state would be labeled by a single horizontal row of n boxes as shown in Fig. 1(b).

The second group of interest, U_m, is generally not an invariance group of the system. (One exception is the m-dimensional harmonic oscillator.[16]) Instead we find that all physical operators of the system can be made by taking linear combinations of U_m elements and all states can be made from combinations of U_m IR bases. In other words, the group U_m may provide a complete labeling for operators and states. This was discussed in Ref. 1.

Each operator U_m transforms all n single-particle states in the same way and all at once. Therefore it commutes with the S_n permutation operators and this leads to a formalism in which the U_m IR may be labeled by a tableau notation also. Operationally, this labeling is accomplished by selecting an integer i_α which stands for a single-particle state ($i_\alpha = 1, 2, \ldots, m$) and writing it in place of the αth box ($\alpha = 1, 2, \ldots, n$) in the appropriate Young tableau. For fermions this just gives a labeling of a Slater determinant wave function as shown below,

$$\langle x_1 x_2 \cdots x_n | S \rangle = \left\langle x_1 x_2 \cdots x_n \left| \begin{bmatrix} i_1 \\ i_2 \\ \vdots \\ i_n \end{bmatrix} \right\rangle = \frac{\det}{\sqrt{(n!)}} \begin{vmatrix} \langle x_1|i_1\rangle & \langle x_2|i_1\rangle & \cdots & \langle x_n|i_1\rangle \\ \langle x_1|i_2\rangle & \langle x_2|i_2\rangle & \cdots & \langle x_n|i_2\rangle \\ \vdots & & & \vdots \\ \langle x_1|i_n\rangle & \langle x_2|i_n\rangle & \cdots & \langle x_n|i_n\rangle \end{vmatrix}, \tag{1a}$$

$$i_1 < i_2 < \cdots < i_n \leq m . \tag{1b}$$

The ordering rule, Eq. (1b), is called a tableau lexicality rule. States with nonlexical tableaus can always be defined but they will just be proportional to one of the $m!/(m-n)!n!$ states which have lexical labeling. (In particular, we recall the exclusion principle: $|S\rangle = 0$ if $i_l = i_k$ for $l \neq k = 1, \ldots, n$.)

An analogous labeling of n-boson states gives what might have been called "Slater-permanent" wave functions if bosons were common in atomic or molecular physics,

$$\langle x_1 x_2 \cdots x_n | S \rangle = \langle x_1 x_2 \cdots x_n | [i_1 i_2 \cdots i_n] \rangle = (n!)^{-1/2} \mathrm{perm} |\langle x_j | i_\alpha \rangle| , \tag{2a}$$

$$i_1 \leq i_2 \leq \cdots \leq i_n \leq m . \tag{2b}$$

There are $(m+n-1)!/(m-1)!n!$ ordered rows of m different integers. (We now allow up to n repeated integers in the row tableau.) Again each tableau labels a state uniquely, and every independent state has a lexical tableau to label it.

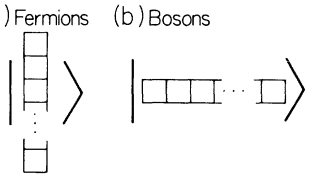


FIG. 1. Young frames for labeling Slater wave functions. (a) A vertical column of n boxes is used to label an n-fermion Slater determinant wave function. (b) A horizontial row of n boxes is used to label an n–boson wave function.

Now the main advantage of a tableau notation is that we may efficiently treat states of particles which have an "internal" structure such as a spin or isospin. We may separate this neatly from the "external" orbital or spatial structure while treating multiparticle states. This is a very useful separation for treating electrons in atoms or molecules when total spin is more or less conserved and when the most important effects are described by orbital operators.

The tableau notation for the states with orbit and spin separated consists of a pair of tableaus. One tableau labels the orbital part, while the other labels the spin or internal part. However, each tableau may now have more complicated shapes than the single columns or single rows that label Slater states.

The shape of the spin tableau for electronic spin-$\frac{1}{2}$ will be, in general, two rows having different lengths. The difference in length between the two rows equals $2S$ where S is the total spin. In order to label multielectron spin-$\frac{1}{2}$ (U_2) states, we write in place of the boxes various integers or arrows which stand for state 1 or spin up ($\uparrow$) and state 2 or spin down ($\downarrow$). We demand lexical ordering in the columns according to Eq. (1b) and in the rows according to Eq. (2b). A tableau such as the example in Eq. (3) is a code for quantum numbers S, S_z, and n; n is the number of boxes, integers, or arrows, S_z equals half the difference between the number of up ($\uparrow$) and down ($\downarrow$) states, and S equals half the difference between the length

of the rows:

$$|n=13, S=\tfrac{5}{2}, S_z=-\tfrac{1}{2}\rangle = \left|\begin{matrix}1\,1\,1\,1\,1\,1\,2\,2\,2\\ 2\,2\,2\,2\end{matrix}\right\rangle$$

$$= \left|\begin{matrix}\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\\ \downarrow\downarrow\downarrow\downarrow\end{matrix}\right\rangle . \tag{3}$$

The shape of the orbital tableau is determined by that of the spin tableau through the Pauli principle. For fermions the orbital tableau must have a shape *conjugate* to that of the spin tableau; i.e., rows are replaced by columns and vice versa, as shown by the examples in Fig. 2. For bosons the orbital tableau must be identical in shape to the spin tableau. Each orbital tableau labels a base state of U_h, where h is the number of orbital states available in the shell for each particle. For electrons the total number of states m must equal twice the number of orbital states ($m=2h$).

Finally, the complete tableau labeling of Pauli states of definite total spin will have the following form:

$$|^{2S+1}T\rangle = |(\text{orbital tableau}), (\text{spin tableau})\rangle . \tag{4}$$

These are unambiguously labeled with respect to separate spin and orbital properties. Each electronic state vector is an IR base of $U_h \times U_2$ which contains only those operators that transform the orbital state without changing the spin state or vice versa. From those one may construct the (Russell Saunders) states $|^{2S+1}L\rangle$ of definite orbital momentum or various molecular states $|^{2S+1}\Gamma\rangle$ of definite spatial point symmetry.

Each of these states are complicated combinations of $n!$ primitive orbit states $|h_1\rangle|h_2\rangle\cdots|h_n\rangle$ multiplied by similar combinations of spin states $|s_1\rangle|s_2\rangle\cdots|s_n\rangle$. Indeed, there would be much less to gain by redoing this factorization if we had not derived simple matrix formulas based on the tableaus which allow one to virtually ignore this complexity. Those formulas are demonstrated in Sec. II and III.

II. ORBITAL TABLEAUS FOR EQUIVALENT ELECTRONS

We now discuss the orbital operators and states associated with the orbital tableau in Eq. (4) for the case of equivalent electrons in a single l-shell. For the time being we ignore the spin tableau since it is not changed by the orbital operators.

The single-particle states $|^l_m\rangle$ shall be numbered $|^l_l\rangle = |1\rangle$, $|^l_{l-1}\rangle = |2\rangle, \ldots, |^l_{-l}\rangle = |2l+1\rangle$ for typographical convenience. The single-particle unit or elementary operators are the following:

$$e_{ij} = |i\rangle\langle j| . \tag{5}$$

Let an operator $e_{ij}(\alpha)$ be defined for each of n electrons $\alpha = 1, 2, \ldots, n$ so that the following holds:

$$e_{ij}(\alpha)|j_1\rangle|j_2\rangle\cdots|j_\alpha\rangle\cdots|j_n\rangle = \delta_{jj_\alpha}|j_1\rangle|j_2\rangle\cdots|i\rangle\cdots|j_n\rangle, \tag{6a}$$

$$e_{ij}(\alpha)e_{kl}(\alpha) = \delta_{jk}e_{il}(\alpha), \tag{6b}$$

$$e_{ij}(\alpha)e_{kl}(\beta) = e_{kl}(\beta)e_{ij}(\alpha), \quad \text{for } \alpha \neq \beta. \tag{6c}$$

The unitary group U_{2l+1} is generated by the elementary one-body operators

$$E_{ij} = \sum_{\alpha=1}^{n} e_{ij}(\alpha) \tag{7}$$

which satisfy the well-known unitary commutation relations

$$[E_{ij}, E_{kl}] = \delta_{jk}E_{il} - \delta_{li}E_{kj} . \tag{8}$$

The unit multipole or tensor operators v^k_q can be expressed in terms of the elementary operators and vice versa. For a single particle we have

$$v^k_q = \sum_{m,m'=-l}^{l} \left|\begin{matrix} l \\ m\end{matrix}\right\rangle\left\langle\begin{matrix} l \\ m\end{matrix}\right| v^k_q \left|\begin{matrix} l \\ m'\end{matrix}\right\rangle\left\langle\begin{matrix} l \\ m'\end{matrix}\right| \tag{9a}$$

$$= \sum \left\langle\begin{matrix} l \\ m\end{matrix}\right| v^k_q \left|\begin{matrix} l \\ m'\end{matrix}\right\rangle e_{(m)(m')} \tag{9b}$$

$$= \sum \begin{pmatrix} k \\ (m)\ (m')\end{pmatrix} e_{(m)(m')} , \tag{9c}$$

where the coefficients $\binom{k}{ij}$ are defined as follows in terms of Wigner's 3-j symbol:

$$\begin{pmatrix} k \\ (m)\ (m')\end{pmatrix} = (-1)^{l-m}(2k+1)^{1/2}\begin{pmatrix} l\ k\ l \\ -m\ q\ m'\end{pmatrix} . \tag{10}$$

[We use parentheses, (m), to indicate the typo-

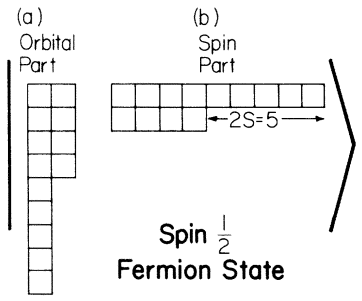


FIG. 2. Young frames for labeling separate orbit and spin wave functions for spin-$\frac{1}{2}$ fermions. (a) A frame of 13 boxes would be used to label the 13-particle orbital states (^6L) of spin multiplicity $2S+1=6$. (b) A frame conjugate to (a), obtained by converting rows to columns, corresponds to spin states of total spin $S=5/2$ since only five of the spin boxes are "unpaired."

graphical index $i = 1, 2, \ldots,$ that goes with the magnetic quantum number $m = l, l-1, \ldots, -l.$] These coefficients are tabulated (Table I) in a form which allows one to quickly locate them for $l = \frac{1}{2}$, 1, $\frac{3}{2}$, 2, $\frac{5}{2}$, 3, and 4. Such a format is useful for a number of applications.

The corresponding n-particle one-body multiple operators V_q^k are the same combination of the one-body elementary operators E_{ij},

$$V_q^k = \sum_{\alpha=1}^{n} v_q^k(\alpha) = \sum_{m,m'} \begin{pmatrix} k \\ (m)\ (m') \end{pmatrix} E_{(m)(m')} . \qquad (11)$$

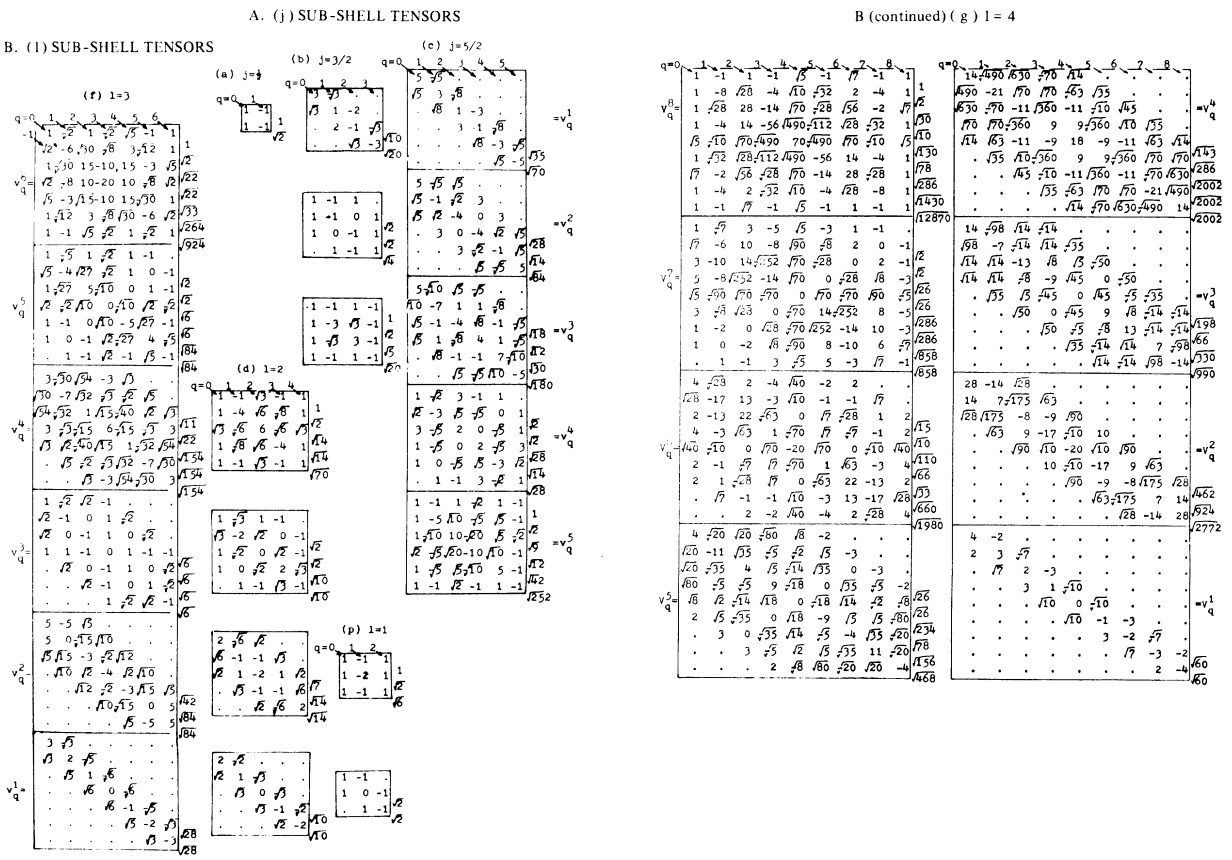
One may think of the E_{ij} operator as a product $a_i^\dagger a_j$ of a destruction operator for state j followed by a creation operator for state i, and of E_{jj} as a number operator for the jth state. However, the creation operators should not be confused with electronic creation operators. We are dealing here with just the orbital part of the electronic states, and the rules are therefore quite different. A self-consistent creation operator approach to U_m representations using boson operators has been developed by Biedenharn, Louck,[17] and others to give algebraic formulas for operators.

It is now possible to avoid the algebra of creation operators and derive matrix elements directly from the tableau. The general jawbone counting formula discussed in Refs. 1 and 2 will now be given in a simpler form that is valid for all orbital tableaus associated with particles of spin $\frac{1}{2}$. (Such tableaus have, at most, two columns.) We now discuss the formula given by Fig. 3.

The "number operators" E_{ii} give only diagonal matrix elements as shown in Fig. 3(a). The matrix for E_{ij} is simply the transpose of the matrix for E_{ji} according to Fig. 3(b). The rest of Fig. 3 deals with operators of the form $E_{12}, E_{23}, E_{34}, \ldots, E_{i-1,i}, \ldots,$ which change an i into an $i-1$.

The result of applying $E_{i-1,i}$ to a lexical tableau is nonzero if and only if there is an i in a column which does not already have an $i-1$. (The tableau that results from converting an i to $i-1$ must be lexical.)

TABLE I. Unit tensor matrices representing unit tensor operators V_q^k tabulated according to the convention of Eq. (9). All tensors with different q but with the same k are drawn together into one matrix. The superdiagonal belonging to each q is indicated at the top. The normalization denominator for a superdiagonal is located at its lower end on the right-hand side of each matrix.



The most complicated case occurs when the initial or final tableau has an i and $i-1$ in different columns, as given in Figs. 3(c) and 3(d), but the result is easily remembered. The matrix element is a function only of the "city block" distance d between the i and $i-1$. d is an integer equal to the minimum number of streets or lines one must cross in going from one block to the other. The matrix element is equal to $[(d-1)/d]^{1/2}$ if $i-1$ is above i in the initial or final side of the matrix element and equal to $[(d+1)/d]^{1/2}$ if i is above $i-1$. This makes a very nice mnemonic coincidence which is due partly to our choice of numbering. Note that the maximum value for a matrix element of $E_{i-1,i}$ is $\sqrt{2}$, which occurs when $d=0$ [see Fig. 3(f)], while the smallest nonzero value is 1, which occurs for the remaining cases in Figs. 3(g) and 3(h) or when $d \to \infty$.

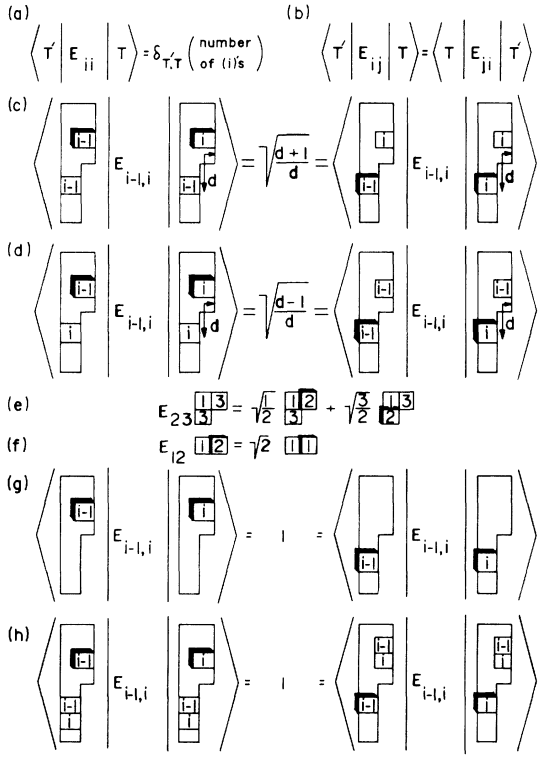


FIG. 3. Simplified jawbone formula for electronic orbital operators. (a) Number operators E_{ii} are diagonal. (The only eigenvalues for orbital states are 0, 1, and 2.). (b) Raising and lowering operators are simply transposes of each other. (c)–(h) $E_{i-1,i}$ acting on a tableau state gives zero unless 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) involved the "city block" distance d which is the denominator of the matrix element. The numerator is one larger $(d+1)$ or smaller $(d-1)$, depending on whether the involved tableaus favor the larger or smaller state number (i or $i-1$) with a higher position. The 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.

The matrices of other operators such as $E_{i-2,i}$, $E_{i-3,i}$, ... may be found using the commutation relations [Eq. (8)] as follows:

$$E_{i-2,i}=[E_{i-2,i-1},E_{i-1,i}],$$
$$E_{i-3,i}=[E_{i-3,i-2},E_{i-2,i}], \tag{12}$$
$$\vdots$$

A more direct procedure suitable for high-speed electronic computation applications has been developed by Paldus.[18]

The tableau treatment of the $(p)^3$ configuration will be given now since the whole manifold can be displayed in a limited space and related easily to other more standard treatments.

The operators V_q^k are given by Eqs. (13) and (14) or Table I (p). The V_0^k are the following combinations of the diagonal E_{ii}:

$$\sqrt{3}\,V_0^0=E_{11}+E_{22}+E_{33}$$
$$\sqrt{2}\,V_0^1=E_{11}\qquad -E_{33}\equiv L_z. \tag{13}$$
$$\sqrt{6}\,V_0^2=E_{11}-2E_{22}+E_{33}$$

The remaining tensor operators are combinations of various raising and lowering operators E_{ij} $(i\neq j)$,

$$V_2^2=E_{13},\quad -2V_1^2=\sqrt{2}(E_{12}-E_{23}),$$
$$-2V_1^1=\sqrt{2}(E_{12}+E_{23})\equiv L_+,\quad 2V_{-1}^1=\sqrt{2}(E_{21}+E_{32})\equiv L_-,$$
$$2V_{-1}^2=\sqrt{2}(E_{21}-E_{32}),\quad V_{-2}^2=E_{31}. \tag{14}$$

The shape of the orbital tableaus for $(p)^3$ depends on which spin tableaus or multiplets are being considered. With three particles there are only two choices: the doublet ($|\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\downarrow\rangle$) with $S=\frac{1}{2}$ and the quartet ($|\uparrow\uparrow\uparrow\rangle$, $|\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\downarrow\rangle$, $|\downarrow\downarrow\downarrow\rangle$) with $S=\frac{3}{2}$. Now the orbital states are labeled by tableaus conjugate to these. For each conjugate shape we find a lexical tableau with the largest L_z eigenvalue [see Eq. (13)]. This corresponds to a $|^{2S+1}L,M=L\rangle$ state as in the examples shown by Eqs. (15),

$$|p^3\,{}^2D,M=2\rangle=\left|\begin{matrix}1&1\\2\end{matrix}\right\rangle, \tag{15a}$$

$$|p^3\,{}^4S,M=0\rangle=\left|\begin{matrix}1\\2\\3\end{matrix}\right\rangle. \tag{15b}$$

In general, such "highest tableaus" must label states of definite total orbital momentum L and, of course, spin S. The remaining states can be generated by applying L_- from Eq. (14) using the "jawbone" formula and the following:

$$|^{2S+1}LM-1\rangle = L_-|^{2S+1}LM\rangle/[(L+M)(L-M+1)]^{1/2}. \tag{16}$$

For example we use Figs. 2(g) and 2(h) in the following:

$$|^2D\,1\rangle = \tfrac{1}{2}L_-|^2D\,2\rangle = \tfrac{1}{2}\sqrt{2}(E_{21}+E_{32})\left|\begin{matrix}1&1\\2&\end{matrix}\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{matrix}1&2\\2&\end{matrix}\right\rangle + \left|\begin{matrix}1&1\\3&\end{matrix}\right\rangle\right). \tag{17}$$

We then obtain the highest ^2P state by orthogonalization,

$$|^2P\,1\rangle = \frac{1}{\sqrt{2}}\left(\left|\begin{matrix}1&2\\2&\end{matrix}\right\rangle - \left|\begin{matrix}1&1\\3&\end{matrix}\right\rangle\right). \tag{18}$$

Now one-body multipole matrix elements are obtained quite directly, as seen in the following example: Note that all k moments V^k_q for fixed q are given by one expression involving the modified Wigner coefficients $(\,{}_i{}^k{}_{j+q})$. These are tabulated along the qth superdiagonal of each V^k matrix in Table I,

$$\begin{aligned}\langle {}^2P\,1|V^k_0|{}^2D\,1\rangle &= \frac{1}{\sqrt{2}}\left(\left\langle\begin{matrix}1&2\\2&\end{matrix}\right| - \left\langle\begin{matrix}1&1\\3&\end{matrix}\right|\right)\left[\begin{pmatrix}k\\1&1\end{pmatrix}E_{11}+\begin{pmatrix}k\\2&2\end{pmatrix}E_{22}+\begin{pmatrix}k\\3&3\end{pmatrix}E_{33}\right]\left(\left|\begin{matrix}1&2\\2&\end{matrix}\right\rangle + \left|\begin{matrix}1&1\\3&\end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}}\\ &= \frac{1}{2}\left[-\begin{pmatrix}k\\1&1\end{pmatrix}+2\begin{pmatrix}k\\2&2\end{pmatrix}-\begin{pmatrix}k\\3&3\end{pmatrix}\right] = -\sqrt{\tfrac{3}{2}} \quad \text{for } k=2\\ &= 0 \quad \text{for } k=1\\ &= 0 \quad \text{for } k=0.\end{aligned} \tag{19}$$

In contrast, the usual Racah approach uses more complicated expressions involving coefficients which are more numerous and more difficult to obtain, such as the $6-j$ (Ref. 19) or fractional-parentage coefficients,[20]

$$\langle p^3\,{}^2P\,1|V^2_0|p^3\,{}^2D\,1\rangle = C^{221}_{011}\left[(p^2D\|p^3D)(p^2D\|p^3P)\sqrt{(15)}\begin{Bmatrix}1&2&1\\2&2&1\end{Bmatrix} - (p^2P\|p^3D)(p^2P\|p^3P)\sqrt{(15)}\begin{Bmatrix}1&2&1\\2&1&1\end{Bmatrix}\right]\langle 1||2||1\rangle$$

$$= -\sqrt{\tfrac{3}{2}}. \tag{20}$$

Equation (21) gives all of the matrix elements for the remaining $S=\frac{1}{2}$ or doublet states. The superscript $^{(ij)}$ above each matrix element in this equation indicates which operator E_{ij} was responsible, and which coefficient $(\,{}_i{}^k{}_j)$ is to be multiplied when evaluating a V^k_q (no more than one (ij) can occupy an off-diagonal position when $i\neq j$):

	$\left\|\begin{matrix}1&1\\2&\end{matrix}\right\rangle$	$\left\|\begin{matrix}1&2\\2&\end{matrix}\right\rangle$	$\left\|\begin{matrix}1&1\\3&\end{matrix}\right\rangle$	$\left\|\begin{matrix}1&2\\3&\end{matrix}\right\rangle$	$\left\|\begin{matrix}1&3\\2&\end{matrix}\right\rangle$	$\left\|\begin{matrix}1&3\\3&\end{matrix}\right\rangle$	$\left\|\begin{matrix}2&2\\3&\end{matrix}\right\rangle$	$\left\|\begin{matrix}2&3\\3&\end{matrix}\right\rangle$
	$M=2$	$M=1$		$M=0$		$M=-1$		$M=-2$
$\left\langle\begin{matrix}1&1\\2&\end{matrix}\right\|$	$2^{(11)}+1^{(22)}$	$1^{(12)}$	$1^{(23)}$	$-\sqrt{\frac{1}{2}}{}^{(13)}$	$\sqrt{\frac{3}{2}}{}^{(13)}$			
$\left\langle\begin{matrix}1&2\\2&\end{matrix}\right\|$		$1^{(11)}+2^{(22)}$		$\sqrt{\frac{1}{2}}{}^{(23)}$	$\sqrt{\frac{3}{2}}{}^{(23)}$		$-1^{(13)}$	
$\left\langle\begin{matrix}1&1\\3&\end{matrix}\right\|$			$2^{(11)}+1^{(33)}$	$\sqrt{2}{}^{(12)}$		$1^{(13)}$		
$\left\langle\begin{matrix}1&2\\3&\end{matrix}\right\|$				$1^{(11)}+1^{(22)}+1^{(33)}$		$\sqrt{\frac{1}{2}}{}^{(23)}$	$\sqrt{2}{}^{(12)}$	$\sqrt{\frac{1}{2}}{}^{(13)}$
$\left\langle\begin{matrix}1&3\\2&\end{matrix}\right\|$					$1^{(11)}+1^{(22)}+1^{(33)}$	$\sqrt{\frac{3}{2}}{}^{(23)}$		$\sqrt{\frac{3}{2}}{}^{(13)}$
$\left\langle\begin{matrix}1&3\\3&\end{matrix}\right\|$						$1^{(11)}+2^{(33)}$		$1^{(12)}$
$\left\langle\begin{matrix}2&2\\3&\end{matrix}\right\|$							$2^{(22)}+1^{(33)}$	$1^{(23)}$
$\left\langle\begin{matrix}2&3\\3&\end{matrix}\right\|$								$1^{(22)}+2^{(33)}$

$= \langle E_{ij}\rangle$,

for $i\leq j = 1,\ 2,$ or 3. (21)

For the quartet terms ($S=\frac{3}{2}$) there is only one allowed orbital tableau [Eq. 15(b)] and for it only the V_0^0 matrix is nonzero.

Isotropic interaction operators such as electrostatic repulsion are combinations of products $\tilde{E}_{ij}E_{ij}$ of elementary operators or tensor operators $\tilde{V}_q^k V_q^k$. For the pure l^n configuration we obtain the following formula in the appendix:

$$\tfrac{1}{2}\langle l^n T|\sum_{\alpha\neq\beta}\frac{1}{r_{\alpha\beta}}|l^n T'\rangle=\sum_k A^k(l)\langle l^n T|(k)|l^n T'\rangle, \tag{22}$$

where the angular part is given in terms of tableau (T) matrices of V^k operators,

$$2\langle l^n T|(k)|l^n T'\rangle=\langle T|V_0^k V_0^k+\sum_{q=1}^{k}(\tilde{V}_q^k V_q^k+V_q^k\tilde{V}_q^k)|T'\rangle - \frac{n(2k+1)}{2l+1}, \tag{23}$$

and where the radial part contains the standard Slater integral F^k,

$$A^k(l)=F^k(l\,l\,l\,l)\begin{pmatrix} l & k & l\\ 0 & 0 & 0\end{pmatrix}^2\frac{(2l+1)^2}{2k+1}. \tag{24}$$

We may conveniently find the matrix elements of $V_0^k V_0^k$, $\tilde{V}_q^k V_q^k$, and $V_q^k\tilde{V}_q^k$ between the tableaux T and T' from the corresponding rows and columns in a $E-V$ matrix such as Eq. (21). The first term $\langle T|(V_0^k)^2|T'\rangle$ is just the square of the (T,T) element of the $E-V$ matrix if $T=T'$, and zero otherwise. To obtain $\sum\langle T|\tilde{V}_q^k V_q^k|T'\rangle$ (or $\sum\langle T|V_q^k\tilde{V}_q^k|T'\rangle$) we find the scalar product of the Tth row (column) with the T'th row (column) in the $E-V$ matrix. For example, the resulting sums of the three terms are given below for the tableaux $\begin{smallmatrix}1&1\\2\end{smallmatrix}$, $\begin{smallmatrix}1&2\\2\end{smallmatrix}$, and $\begin{smallmatrix}1&1\\3\end{smallmatrix}$,

$$\left\langle\begin{matrix}1&1\\2\end{matrix}\middle|V^k\cdot V^k\middle|\begin{matrix}1&1\\2\end{matrix}\right\rangle=\left[2\binom{k}{1\,1}+\binom{k}{2\,2}\right]^2+\binom{k}{1\,2}^2+\binom{k}{2\,3}^2+2\binom{k}{1\,3}^2,$$

$$\left\langle\begin{matrix}1&2\\2\end{matrix}\middle|V^k\cdot V^k\middle|\begin{matrix}1&2\\2\end{matrix}\right\rangle=\left[\binom{k}{1\,1}+2\binom{k}{2\,2}\right]^2+\binom{k}{1\,2}^2+2\binom{k}{2\,3}^2+\binom{k}{1\,3}^2,$$

$$\left\langle\begin{matrix}1&2\\2\end{matrix}\middle|V^k\cdot V^k\middle|\begin{matrix}1&1\\3\end{matrix}\right\rangle=2\binom{k}{1\,2}\binom{k}{2\,3}, \tag{25}$$

$$\left\langle\begin{matrix}1&1\\3\end{matrix}\middle|V^k\cdot V^k\middle|\begin{matrix}1&1\\3\end{matrix}\right\rangle=\left[2\binom{k}{1\,1}+\binom{k}{3\,3}\right]^2+2\binom{k}{1\,2}^2+\binom{k}{2\,3}^2+\binom{k}{1\,3}^2.$$

Substituting the values for $k=2$, which is the only nonscalar k to give finite A^k, we find the following submatrix:

$$\langle V^2\cdot V^2\rangle=\begin{array}{c|ccc} & \left|\begin{matrix}1&1\\2\end{matrix}\right\rangle & \left|\begin{matrix}1&2\\2\end{matrix}\right\rangle & \left|\begin{matrix}1&1\\3\end{matrix}\right\rangle\\ \hline \left\langle\begin{matrix}1&1\\2\end{matrix}\right| & 3 & & \\ \left\langle\begin{matrix}1&2\\2\end{matrix}\right| & & 4 & -1\\ \left\langle\begin{matrix}1&1\\3\end{matrix}\right| & & -1 & 4\end{array}. \tag{26}$$

The eigenvalues of this matrix are 3 for ^2D [Eq. (17)] and 5 for ^2P [Eq. (18)], and together these numbers give the well-known elementary predictions for the relative spacing between the three lowest levels of nitrogen. (The eigenvalue of $V^2\cdot V^2$ for ^4S is identically zero.)

It may be instructive to see a display of all of the orbital tableaus in the p subshell. These are drawn in Fig. 4 in a Cartesian coordinate system $(x_1x_2x_3)$ where x_j is the eigenvalue of E_{jj}, i.e., the number of j's in the orbital tableau. At the same time we see a display of the eigenvalues of the moment operators V_0^2 and V_0^1 given by Eq. (13). The V_0^2 and V_0^1 coordinate axes are explicitly labeled in p^1 in Fig. 4. The "trigonal" axis V_0^0 determines the number n for each p^n system and would be perpendicular to the plane of the figure if it could be shown.

Another thing that is evident is the symmetry between less-than-half-filled-shell (LHF) states and more-than-half-filled (MHF) ones. It should be evident that the tableau formalism is no more difficult to manage for MHF "multihole" states than it was for the LHF states. In addition, it turns out to be quite easy to derive general relations for spin or orbital operators between corresponding MHF and LHF structures. These will be studied in a future work.

III. SPIN AND ORBIT TABLEAUS AND OPERATORS

As reviewed in Sec. I, a Pauli antisymmetric basis can be made from Slater states labeled by Young columns, or else from states labeled by orbit and spin pairs of tableaus of mutually conjugate shapes. It is much easier to obtain a basis of definite L, M, S, and M_s using the tableau-pair labeled states. For example, we give some examples for p^3 below, where the orbital parts follow from Eqs. (15)–(18):

$$
\left|{}^4S\ \begin{matrix}L=0 & S=\frac{3}{2}\\ M=0 & M_s=\frac{3}{2}\end{matrix}\right\rangle = \left|\begin{matrix}1\uparrow\uparrow\uparrow\\ 2\\ 3\end{matrix}\right\rangle,
$$

$$
\left|{}^4S\ \begin{matrix}0 & \frac{3}{2}\\ 0 & \frac{1}{2}\end{matrix}\right\rangle = \left|\begin{matrix}1\uparrow\uparrow\downarrow\\ 2\\ 3\end{matrix}\right\rangle,
$$

$$
\vdots
$$

$$
\left|{}^2P\ \begin{matrix}1 & \frac{1}{2}\\ 1 & \frac{1}{2}\end{matrix}\right\rangle = \frac{1}{\sqrt{2}}\left[\left|\begin{matrix}1\,2\uparrow\uparrow\\ 2\ \downarrow\end{matrix}\right\rangle - \left|\begin{matrix}1\,1\uparrow\uparrow\\ 3\ \downarrow\end{matrix}\right\rangle\right],
$$

$$
\left|{}^2P\ \begin{matrix}1 & \frac{1}{2}\\ 1 & -\frac{1}{2}\end{matrix}\right\rangle = \frac{1}{\sqrt{2}}\left[\left|\begin{matrix}1\,2\uparrow\downarrow\\ 2\ \downarrow\end{matrix}\right\rangle - \left|\begin{matrix}1\,1\uparrow\downarrow\\ 3\ \downarrow\end{matrix}\right\rangle\right], \qquad (27)
$$

$$
\left|{}^2P\ \begin{matrix}1 & \frac{1}{2}\\ 0 & \frac{1}{2}\end{matrix}\right\rangle = \frac{1}{2}\left[-\left|\begin{matrix}1\,2\uparrow\downarrow\\ 3\ \downarrow\end{matrix}\right\rangle + \sqrt{3}\left|\begin{matrix}1\,3\uparrow\downarrow\\ 2\ \downarrow\end{matrix}\right\rangle\right],
$$

$$
\vdots
$$

$$
\left|{}^2D\ \begin{matrix}2 & \frac{1}{2}\\ 2 & \frac{1}{2}\end{matrix}\right\rangle = \left|\begin{matrix}1\,1\uparrow\uparrow\\ 2\ \downarrow\end{matrix}\right\rangle.
$$

$$
\vdots\ .
$$

When dealing with spin- and orbit-dependent operators, it may be convenient to expand the tableau-pair states in terms of Slater states and vice versa. This can be done directly by a tableau formula we call the *assembly* formula. This formula is given in Fig. 5 along with an explanation of its use and a p^3 example.

It may help to see the simplest possible example of its application using two-particle states:

$$
\begin{array}{c|cc}
 & \left|\begin{matrix}1\,2\uparrow\\ \ \ \downarrow\end{matrix}\right\rangle & \left|\begin{matrix}1\\ 2\uparrow\downarrow\end{matrix}\right\rangle \\
\left\langle\begin{matrix}1\uparrow\\ 2\downarrow\end{matrix}\right| & \sqrt{\tfrac{1}{2}} & \sqrt{\tfrac{1}{2}} \\
\left\langle\begin{matrix}1\downarrow\\ 2\uparrow\end{matrix}\right| & -\sqrt{\tfrac{1}{2}} & \sqrt{\tfrac{1}{2}}
\end{array}. \qquad (28)
$$

The preceding two-particle matrix is easily derived without the assembly formula. However, one can appreciate that derivation of similar matrices for $n=3,4,\ldots$ becomes very laborious without it.

Now we shall label the six p-shell states $\left|{}^{l}_{(m_l)}{}^{1/2}_{(m_s)}\right\rangle$ as follows: $|a\rangle=|1\uparrow\rangle$, $|b\rangle=|1\downarrow\rangle$, $|c\rangle=|2\uparrow\rangle$, $|d\rangle=|2\downarrow\rangle$, $|e\rangle=|3\uparrow\rangle$, and $|f\rangle=|3\downarrow\rangle$. We use the letters $a,b,\ldots$ for typographical convenience and to avoid confusion with the orbit numbers defined in Sec. II. Along with these states come 36 U_6 operators $E_{aa},E_{ab},\ldots,E_{ff}$, or Racah's double tensor operators V^k_q defined as follows:

$$
\left\langle\begin{matrix}l & \frac{1}{2}\\ m_l' & m_s'\end{matrix}\right| V^{k\lambda}_{q\sigma} \left|\begin{matrix}l & \frac{1}{2}\\ m_l & m_s\end{matrix}\right\rangle = \left\langle\begin{matrix}l\\ m_l'\end{matrix}\right| V^k_q \left|\begin{matrix}l\\ m_l\end{matrix}\right\rangle \left\langle\begin{matrix}\frac{1}{2}\\ m_s'\end{matrix}\right| V^{\lambda}_{\sigma} \left|\begin{matrix}\frac{1}{2}\\ m_s\end{matrix}\right\rangle. \qquad (29)
$$

Two examples of those are given:

$$
V^{1\,1}_{1\,-1} = -\sqrt{\tfrac{1}{2}}\begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} = -\sqrt{\tfrac{1}{2}}(E_{bc}+E_{de}),
$$

$$
V^{1\,1}_{0\,0} = \frac{1}{2}\begin{bmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{bmatrix} = \tfrac{1}{2}(E_{aa}-E_{bb}-E_{ee}+E_{ff}). \qquad (30)
$$

Note that these matrices are derived from outer products of Table I(a) with Table I(p).

We consider now the treatment of the spin-orbit (SO) operator in the p^3 configuration:

$$
\begin{aligned}
\mathrm{SO} &= \xi\sum_{\alpha=1}^{n} \vec{s}(\text{electron }\alpha)\cdot\vec{l}\ (\text{electron }\alpha)\\
&= \xi(V^{1\,1}_{0\,0} - V^{1\,1}_{1\,-1} - V^{1\,1}_{-1\,1})\\
&= \xi[\tfrac{1}{2}(E_{aa}-E_{bb}-E_{ee}+E_{ff})\\
&\quad +\sqrt{\tfrac{1}{2}}(E_{bc}+E_{de}+E_{cb}+E_{ed})]. \qquad (31)
\end{aligned}
$$

Since this operator is invariant to rigid rotations of both spin and orbit, it is convenient to deal with the states of definite total angular momentum J, given as follows:

$$
|^{2S+1}L_J\,M_J\rangle = \sum_{M,M_S} C^{L\ S\ J}_{M\,M_S\,M_J}|L\,M\rangle|S\,M_S\rangle. \qquad (32)
$$

The maximum M_J examples of the $^{2S+1}L_J$ states for the p^3 configuration are the following:

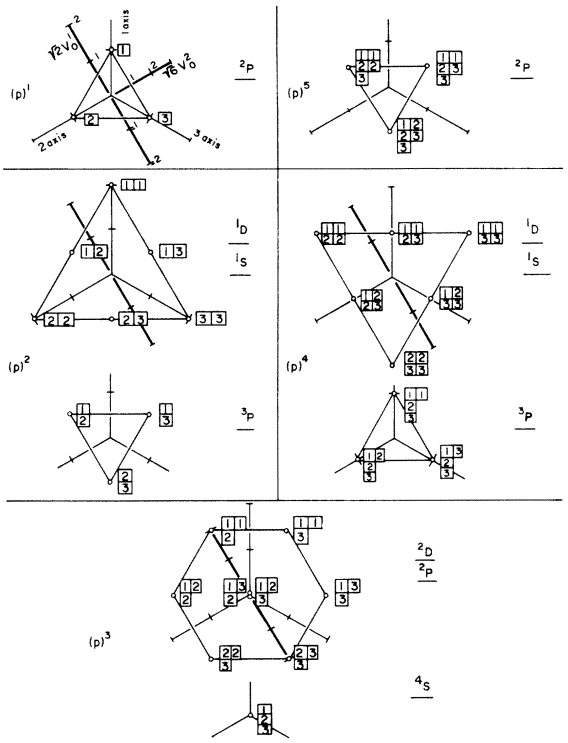


FIG. 4. Weight or moment diagrams of atomic $(p)^n$ states. Each tableau is located at point $(x_1x_2x_3)$ in a cartesian coordinate system for which x_n is the number of n in the tableau. An alternative coordinate system is (v_0^2, v_0^1, v_0^0) defined by Eq. 13, which gives the zz quadrupole moment, z magnetic dipole moment, and number of particles, respectively. The last axis (v_0^0) would be pointing straight out of the figure, and each family of states lies in a plane perpendicular to it.

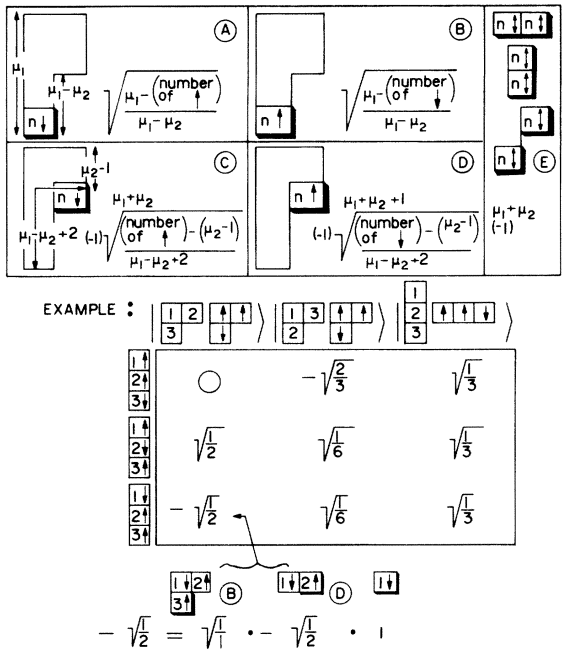


FIG. 5. Assembly formula for combining orbital and spin states. Each column state (Slater determinant) on the left-hand side of the sample table has a definite spin (arrow)on each orbital state (number). The formulas will give the overlap of this Slater state with a given orbital tableau state if we 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.

$$|^2D_{5/2}\,\tfrac{5}{2}\rangle = \left|\begin{matrix}a\\b\\c\end{matrix}\right\rangle, \qquad |^2D_{3/2}\,\tfrac{3}{2}\rangle = \sqrt{\tfrac{4}{5}}\left|\begin{matrix}a\\b\\d\end{matrix}\right\rangle + \sqrt{\tfrac{1}{10}}\left(\left|\begin{matrix}a\\c\\d\end{matrix}\right\rangle - \left|\begin{matrix}b\\c\\e\end{matrix}\right\rangle\right),$$

$$|^2P_{1/2}\,\tfrac{1}{2}\rangle = -\sqrt{\tfrac{1}{3}}\left|\begin{matrix}b\\c\\d\end{matrix}\right\rangle - \sqrt{\tfrac{1}{3}}\left|\begin{matrix}a\\b\\f\end{matrix}\right\rangle - \sqrt{\tfrac{1}{6}}\left|\begin{matrix}a\\c\\f\end{matrix}\right\rangle + \sqrt{\tfrac{1}{6}}\left|\begin{matrix}b\\c\\e\end{matrix}\right\rangle, \qquad |^2P_{3/2}\,\tfrac{3}{2}\rangle = -\sqrt{\tfrac{1}{2}}\left(\left|\begin{matrix}a\\c\\d\end{matrix}\right\rangle + \left|\begin{matrix}a\\b\\e\end{matrix}\right\rangle\right), \qquad |^4S_{3/2}\,\tfrac{3}{2}\rangle = \left|\begin{matrix}a\\c\\e\end{matrix}\right\rangle. \tag{33}$$

The matrix elements of the SO operator are now easily made according to the standard determinant rules. Examples of this are given by the following:

$$\langle {}^2P_{3/2}|\mathrm{SO}|{}^4S_{3/2}\rangle = -\frac{1}{\sqrt{2}}\left(\left\langle\begin{matrix}a\\c\\d\end{matrix}\right| + \left\langle\begin{matrix}a\\b\\e\end{matrix}\right|\right)(\mathrm{SO})\left|\begin{matrix}a\\c\\e\end{matrix}\right\rangle = -\frac{1}{\sqrt{2}}\,\xi\left(\left\langle\begin{matrix}a\\c\\d\end{matrix}\right| + \left\langle\begin{matrix}a\\b\\e\end{matrix}\right|\right)\cdot\left(\left|\begin{matrix}a\\b\\e\end{matrix}\right\rangle + \left|\begin{matrix}a\\c\\d\end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = -\xi, \tag{34a}$$

$$\mathrm{SO}=\xi\begin{array}{c|cccc} & {}^2D_{5/2} & {}^2D_{3/2} & {}^2P_{3/2} & {}^4S_{3/2}\ \ {}^2P_{1/2} \\ \hline {}^2D_{5/2} & 0 & & & \\ {}^2D_{3/2} & & 0 & -\sqrt{\tfrac{5}{4}} & 0 \\ {}^2P_{3/2} & & -\sqrt{\tfrac{5}{4}} & 0 & -1 \\ {}^4S_{3/2} & & 0 & -1 & 0 \\ {}^2P_{1/2} & & & & 0 \end{array} . \quad (34b)$$

There is probably a convenient way to derive spin- and orbit-dependent operators directly using the tableau pairs that label bases of $U_{2l+1}\times U_2$. However, since the general SO operator can connect different IR of $U_{2l+1}\times U_2$, a theory of unitary tensor operators, more general than the E's, will probably be needed to accomplish this. The theory of such operators is still being developed.[21]

IV. RELATING TABLEAU AND SENIORITY DEFINED STATES

We consider now the doublet orbitals of a d^3 configuration, since this is the simplest example in which there is more than one state for a particular L and S.

As pointed out by Drake, Drake, and Schlesinger,[22] a complete tableau angular momentum basis is obtained using lowering operators and orthogonal projection operators for any number of repeated ${}^{2S+1}L$ terms. Algorithms exist for efficiently evaluating the energy matrices.

For the d^3 example these procedures give two ${}^2D$ states which are written below along with the ${}^2F$, ${}^2G$, and ${}^2H$ states obtained by lowering,

$$\begin{array}{l|ccccc} & \left|{}^{1\,3}_{3}\right\rangle & \left|{}^{1\,4}_{2}\right\rangle & \left|{}^{2\,2}_{3}\right\rangle & \left|{}^{1\,2}_{4}\right\rangle & \left|{}^{1\,1}_{5}\right\rangle \\ \hline |d^3\,{}^2D\,2\rangle_1 = & (5\sqrt{2} & -5\sqrt{3} & -2\sqrt{3} & -1 & +\sqrt{2})\,/\sqrt{140}, \\ |d^3\,{}^2D\,2\rangle_2 = & (\ 0 & +0 & +\sqrt{6} & -2\sqrt{2} & +4)\ /\sqrt{30}, \\ |d^3\,{}^2F\,2\rangle = & (\ 0 & +\sqrt{3} & -2\sqrt{3} & +1 & +2\sqrt{2})\,/2\sqrt{6}, \\ |d^3\,{}^2G\,2\rangle = & (4\sqrt{6} & +9 & -2 & -5\sqrt{3} & -2\sqrt{6})/2\sqrt{70}, \\ |d^3\,{}^2H\,2\rangle = & (\ 6 & +\sqrt{6} & +2\sqrt{6} & +5\sqrt{2} & +2)\ /2\sqrt{30}. \end{array} \quad (35)$$

The repeated states found in this way do not have definite seniority in general. For nuclear applications the pairing or seniority operator can often be used effectively as a model short-range interaction. However, for atomic physics seniority is probably of only mathematical interest since it is not a good quantum number in the presence of the long-range electrostatic repulsion.

Nevertheless, we shall derive a d^3 pair state with the help of the assembly formula in order to demonstrate more of the structure of the tableau labeling. First, we write the two-particle state of a pair. This is the d^2 orbital scalar shown below,

$$\begin{aligned} |\mathrm{pair}\rangle &= |d^{2\,1}S\rangle \\ &= \frac{|1\rangle|5\rangle+|5\rangle|1\rangle-|2\rangle|4\rangle-|4\rangle|2\rangle+|3\rangle|3\rangle}{\sqrt{5}} \\ &\quad\times\frac{|\uparrow\rangle|\downarrow\rangle-|\downarrow\rangle|\uparrow\rangle}{\sqrt{2}} \\ &= \frac{\sqrt{2}\ \left|1\,5\,{}^{\uparrow}_{\downarrow}\right\rangle-\sqrt{2}\ \left|2\,4\,{}^{\uparrow}_{\downarrow}\right\rangle+\left|3\,3\,{}^{\uparrow}_{\downarrow}\right\rangle}{\sqrt{5}} . \end{aligned} \quad (36)$$

In the last line above, the double tableau notation is used. This is now converted to a combination of Slater tableau states by the assembly formulas or Eq. (28),

$$|\mathrm{pair}\rangle=\left(\left|\begin{matrix}1\uparrow\\5\downarrow\end{matrix}\right\rangle-\left|\begin{matrix}1\downarrow\\5\uparrow\end{matrix}\right\rangle-\left|\begin{matrix}2\uparrow\\4\downarrow\end{matrix}\right\rangle+\left|\begin{matrix}2\downarrow\\4\uparrow\end{matrix}\right\rangle+\left|\begin{matrix}3\uparrow\\3\downarrow\end{matrix}\right\rangle\right)\Big/\sqrt{5} . \quad (37)$$

The state with lowest seniority ($\nu=1$) is the pair state plus one more d particle all properly antisymmetrized. This is constructed below by attaching a $(1\uparrow)$ to the pair state. In the first line below we may drop the zero state written in brackets. The second or third lines are obtained by applying the assembly formula again.

$$\begin{aligned} |\mathrm{pair}+1\uparrow\rangle &= \frac{1}{2}\left(\left[\begin{matrix}1\uparrow\\1\uparrow\\5\downarrow\end{matrix}\right]-\left|\begin{matrix}1\uparrow\\1\downarrow\\5\uparrow\end{matrix}\right\rangle-\left|\begin{matrix}1\uparrow\\2\uparrow\\4\downarrow\end{matrix}\right\rangle+\left|\begin{matrix}1\uparrow\\2\downarrow\\4\uparrow\end{matrix}\right\rangle+\left|\begin{matrix}1\uparrow\\3\uparrow\\3\downarrow\end{matrix}\right\rangle\right) \\ &= \frac{1}{2}\left[-\left|\begin{matrix}1\,1\uparrow\uparrow\\5\ \downarrow\end{matrix}\right\rangle+\sqrt{\tfrac{2}{3}}\left|\begin{matrix}1\,4\uparrow\uparrow\\2\ \downarrow\end{matrix}\right\rangle+\left(\sqrt{\tfrac{1}{2}}\left|\begin{matrix}1\,2\uparrow\uparrow\\4\ \downarrow\end{matrix}\right\rangle+\sqrt{\tfrac{1}{6}}\left|\begin{matrix}1\,4\uparrow\uparrow\\2\ \downarrow\end{matrix}\right\rangle\right)-\left|\begin{matrix}1\,3\uparrow\uparrow\\3\ \downarrow\end{matrix}\right\rangle\right] \\ &= \left(-\sqrt{6}\left|\begin{matrix}1\,1\\5\end{matrix}\right\rangle+3\left|\begin{matrix}1\,4\\2\end{matrix}\right\rangle+\sqrt{3}\left|\begin{matrix}1\,2\\4\end{matrix}\right\rangle-\sqrt{6}\left|\begin{matrix}1\,3\\3\end{matrix}\right\rangle\right)\left(\left|\begin{matrix}\uparrow\uparrow\\\downarrow\end{matrix}\right\rangle\right)\Big/\ 2\sqrt{6} . \end{aligned} \quad (38)$$

One may verify that the preceding state vector and its orthogonal ($\nu=3$) state below,

$$|d^3\,{}^2D\,2\,(\nu=3)\rangle=\left(-5\sqrt{2}\begin{vmatrix}1&1\\5\end{vmatrix}\rangle-3\sqrt{3}\begin{vmatrix}1&4\\2\end{vmatrix}\rangle-4\sqrt{3}\begin{vmatrix}2&2\\3\end{vmatrix}\rangle+5\begin{vmatrix}1&2\\4\end{vmatrix}\rangle+3\sqrt{2}\begin{vmatrix}1&3\\3\end{vmatrix}\rangle\right)\Big/\ 2\sqrt{42}\ , \tag{39}$$

are eigenvectors of $V^3\cdot V^3$. This must be the case for the general seniority state, since in the d shell the operator $V^3\cdot V^3$ is the following combination:

$$V^3\cdot V^3=\tfrac{1}{2}(M-P)-V^1\cdot V^1\ , \tag{40a}$$

where P is the pairing operator and M is the Majorana exchange operator which is a U_5 invariant here,

$$P=\sum_{k=1}^{4}(-1)^k V^k\cdot V^k\ ,\quad M=\sum_{k=1}^{4}V^k\cdot V^k\ . \tag{40b}$$

The preceding indicates some of the ways to relate tableaus to the more conventional Racah states. A more general analysis of these relations will be given in a future paper.[23]

V. MULTIPLE SHELL CONFIGURATIONS

If a single electron can occupy several orbital subshells nl_1, $n'l_2$, ... there will be $h=(2l_1+1)+(2l_2+1)+\ldots$ orbital states and h^2 one-body operators $V^k_q(l_il_j)$. To use the tableau formulas in such problems, one must first express the V operators in terms of the U_h elementary operators $E_{(l_im_i)(l_jm_j)}$ as follows:

$$V^k_q(l_1l_2)=\sum_{m_1=-l_1}^{l_1}\sum_{m_2=-l_2}^{l_2}\left\langle\begin{matrix}l_1\\m_1\end{matrix}\middle|V^k_q(l_1l_2)\middle|\begin{matrix}l_2\\m_2\end{matrix}\right\rangle E_{(l_1m_1)(l_2m_2)}\ , \tag{41}$$

$$\left\langle\begin{matrix}l_1\\m_1\end{matrix}\middle|V^k_q(l_1l_2)\middle|\begin{matrix}l_2\\m_2\end{matrix}\right\rangle=(-1)^{l_1-m_1}(2k+1)^{1/2}\begin{pmatrix}l_1&k&l_2\\-m_1&q&m_2\end{pmatrix}.$$

As an example we consider an $(ndn'p)^3$ configuration. We shall number the states 1–5 for the d orbitals and 6–8 for the p orbitals. We will assume the p states have a higher energy than the d states. (It is usually convenient to number the lowest-energy states first because of the tableau ordering.)

Now the operators in Eq. (41) which we have not discussed are the intershell operators which have a nonzero shift $\Delta=l_i-l_j$. The matrices of these are rectangular as shown in Table II or in the following examples:

$$\sqrt{10}\ V^1_1(pd)=\begin{bmatrix}\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\sqrt{3}&\cdot\\\cdot&\cdot&\cdot&\cdot&\sqrt{6}\end{bmatrix}$$

$$=E_{63}+\sqrt{3}\ E_{74}+\sqrt{6}\ E_{85}\ , \tag{42}$$

$$\sqrt{10}\ V^1_{-1}(dp)=\begin{bmatrix}\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot\\1&\cdot&\cdot\\\cdot&\sqrt{3}&\cdot\\\cdot&\cdot&\sqrt{6}\end{bmatrix}$$

$$=E_{36}+\sqrt{3}\ E_{47}+\sqrt{6}\ E_{58}\ .$$

The tables give the matrices for $\Delta>0$, and the others are found using the following transpose relation:

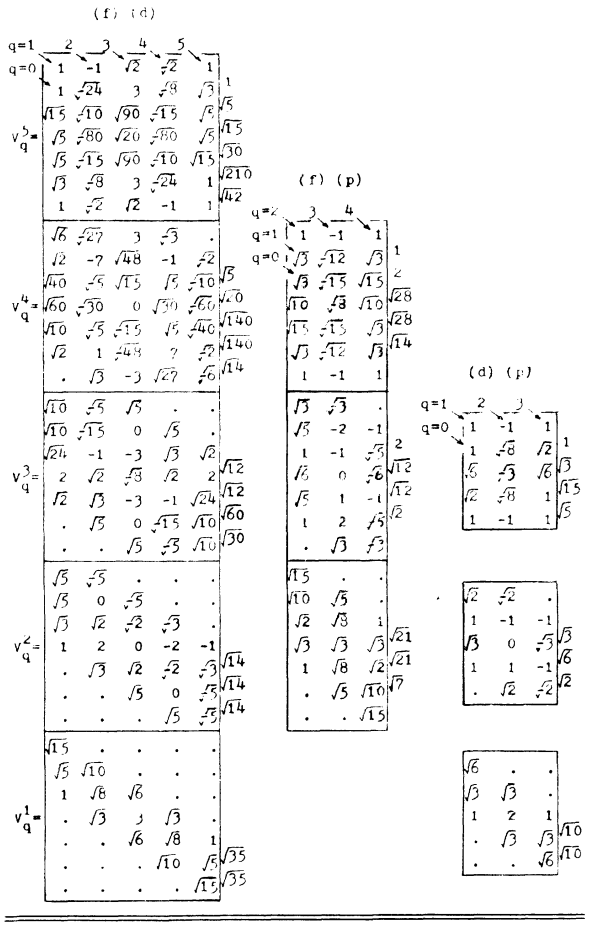
$$V^k_q(l_2l_1)=(-1)^{\Delta+q}\,\tilde{V}^k_{-q}(l_1l_2)\ . \tag{43}$$

To see the implied physical distinction between operators with $\Delta=0$ on the one hand and those with $\Delta\neq0$ on the other, we may compare the two types of vector operators ($k=1$) which we will be using shortly. The $\Delta=0$ operators $V^1_q(pp)$ or $V^1_q(dd)$ correspond to components of the angular momentum operator L_q or some other axial vector operators such as those of magnetic dipole. The $\Delta=\pm1$ operators $V^1_q(pd)$ or $V^1_q(dp)$ correspond to the electric dipole or some other polar vector operator.

We consider as an example the doublet terms (^2L) that arise from the configuration $(dp)^3$. The tableau shape is the same (two boxes over one box) as has appeared in the previous sections, but now it belongs to an IR of U_8, whose dimension (see Fig. 2 of Ref. 1) is the following:

$$\begin{matrix}8&9\\7\\3&1\\1\end{matrix}=168. \tag{44}$$

TABLE II. Unit tensor matrices representing unit tensor operators V^k_q tabulated according to the convention of Eq. (41). All tensors with different q but with the same k are drawn together into one matrix. The superdiagonal belonging to each q is indicated at the top. The normalization denominator for a superdiagonal is located at its lower end on the right-hand side of each matrix.



Fortunately, we may deal individually with smaller subsets of this manifold. First, there are 40 states belonging to the pure configuration (d^3p^0) which was briefly discussed in Sec. IV. After this come 128 "excited" states arising from configurations (d^2p), (dp^2), and (d^0p^3); however, these can be broken up into subsets according to their tableau and angular momentum structure.

The states and terms of a mixed configuration like d^2p may be found systematically by lowering from highest tableaus in a way that is very similar to the one described in Sec. II. The lowering is accomplished by operators $E_{n,n-1}$ which are not intershell operators. Those are the operators that appear in L_-,

$$\begin{aligned} L_- &= \sqrt{20}\; V^1_{-1}(dd) + 2V^1_{-1}(pp) \\ &= 2E_{21} + \sqrt{6}\; E_{32} + \sqrt{6}\; E_{43} + 2E_{54} \\ &\quad + \sqrt{2}\; E_{76} + \sqrt{2}\; E_{87}\ . \end{aligned} \tag{45}$$

Note that the intershell operator E_{65} is absent in Eq. (45).

Consequently several "highest tableaus," i.e., lexical tableaus that cannot be raised by any intrashell $E_{n,n+1}$, may exist in each configuration. For (d^2p) there are two highest tableaus $\begin{smallmatrix}1&1\\6\end{smallmatrix}$ and $\begin{smallmatrix}1&6\\2\end{smallmatrix}$. A separate set of states are obtained from each by lowering with intrashell $E_{n,n-1}$ or L_-. In Eq. (46) the matrices for these operators are partially shown for the states arising from $\begin{smallmatrix}1&1\\6\end{smallmatrix}$. The upper diagonal gives the intrashell E_{ij} in the same form as Eq. (21), Sec. II. The two numbers below the diagonal are the components of L_- which give the ^2L term states written in Eq. (46).

$$\left\langle L_- \middle\backslash E_{mn} \right\rangle = \begin{array}{c} H \quad G \quad F\ F \quad D \quad P\ P \\ \begin{smallmatrix} 11:12 & 11:22 & 13 & 12 & 11:23 & 22 & 14 & 13 & 12:33 & 24 & 23 & 22 & 15 & 14 & 13:34 & 33 & 25 & 24 & 23 & 15 & 14: \\ 6:6 & 7:6 & 6 & 7 & 8:6 & 7 & 6 & 7 & 8:6 & 6 & 7 & 8 & 6 & 7 & 8:6 & 7 & 6 & 7 & 8 & 7 & 8: \end{smallmatrix} \\ \begin{array}{|ccccccccccccccccccccc|} \hline \sqrt{2}^{12}\,1^{67} & & \sqrt{2}^{13} & & 1^{68} & & \sqrt{2}^{14} & & & & & & \sqrt{2}^{15} & & & & & & & & \\ 2\sqrt{2} & & \sqrt{2}^{12} & 1^{23} & 1^{67} & & 1^{13} & 1^{24} & & 1^{68} & 1^{14} & & 1^{25} & & & & & 1^{15} & & \\ \sqrt{2} & & & & \sqrt{2}^{12}\,1^{78} & & & & \sqrt{2}^{13} & & & & & \sqrt{2}^{14} & & & & & & \sqrt{2}^{15} \\ \hline \end{array} \end{array}, \tag{46}$$

$$|^2H,5\rangle = \left|\begin{smallmatrix}1&1\\6\end{smallmatrix}\right\rangle\ , \qquad |^2H,4\rangle = (2\left|\begin{smallmatrix}1&2\\6\end{smallmatrix}\right\rangle + \left|\begin{smallmatrix}1&1\\7\end{smallmatrix}\right\rangle)/\sqrt{5}\ , \qquad |^2G,4\rangle = (\left|\begin{smallmatrix}1&2\\6\end{smallmatrix}\right\rangle - 2\left|\begin{smallmatrix}1&1\\7\end{smallmatrix}\right\rangle)/\sqrt{5}\ .$$

A similar calculation is done for the states arising from $\begin{smallmatrix}1&6\\2\end{smallmatrix}$ in Eq. (47) below,

$$\left\langle \begin{matrix} E_{mn} \\ L_- \end{matrix} \right\rangle = \begin{array}{c} \begin{matrix} G & & F & & & D\ D & & & & P & & & & S \end{matrix} \\ \begin{matrix} 16 & : 16 & 17 : & 26 & 16 & 17 & 18 : & 26 & 27 & 16 & 17 & 18 : & 36 & 26 & 27 & 28 & 17 & 18 : \\ 2 & : 3 & 2 : & 3 & 4 & 3 & 2 : & 4 & 3 & 5 & 4 & 3 : & 4 & 5 & 4 & 3 & 5 & 4 : \end{matrix} \\ \begin{vmatrix} 1^{23}\,1^{67} & -1^{13}\,1^{24} & 1^{68} & -1^{14} & 1^{25} & & -1^{15} & & & & & & & & & & & \\ \sqrt{6} & 1^{12}\,1^{34}\,1^{67} & & & 1^{35} & 1^{68} & -1^{14} & & & & & & & & & & & \\ \sqrt{2} & & 1^{23}\,1^{78} & -1^{13} & 1^{24} & & & -1^{14} & 1^{25} & & & & & & & & & \end{vmatrix} \end{array}, \tag{47}$$

$$|^2G,4\rangle = \left|\begin{matrix}1&6\\2\end{matrix}\right\rangle , \qquad |^2G,3\rangle = \tfrac{1}{2}(\sqrt{3}\left|\begin{matrix}1&6\\3\end{matrix}\right\rangle + \left|\begin{matrix}1&7\\2\end{matrix}\right\rangle) .$$

From the form of the tableau, we may easily see the "parentages" of the states in the preceding two equations. Clearly, $\left|\begin{matrix}1&1\\6\end{matrix}\right\rangle$ arises from a product of p with a singlet d^2 state, namely, ^1G. On the other hand, $\left|\begin{matrix}1&6\\2\end{matrix}\right\rangle$ arises from the triplet d^2 state ^3F. Several of these states are schematized in Fig. 6 along with some of the other levels in the manifold. In the limit of small electrostatic and spin-orbit integrals we may assume the lowest five states indicated in Fig. 6 are eigenstates, and calculate the relative electric dipole strengths between them using the jawbone formula and Eq. (42). This is done in the following:

$$\langle (d^{2\,1}Gp)\,^2G,4\,|V^1_{-1}(pd)|\,d^{3\,2}H,5\rangle$$

$$= \frac{\langle \begin{matrix}1&2\\6\end{matrix}| - 2\langle \begin{matrix}1&1\\7\end{matrix}|}{\sqrt{5}} \; \frac{\sqrt{6}\;E_{61}+\sqrt{3}\;E_{72}+E_{83}\left|\begin{matrix}1&1\\2\end{matrix}\right\rangle}{\sqrt{10}}$$

$$= \frac{(\sqrt{6}\;\langle \begin{matrix}1&2\\6\end{matrix}|E_{61}\left|\begin{matrix}1&1\\2\end{matrix}\right\rangle - 2\sqrt{3}\;\langle \begin{matrix}1&1\\7\end{matrix}|E_{72}\left|\begin{matrix}1&1\\2\end{matrix}\right\rangle)}{\sqrt{50}}$$

$$= \frac{-\sqrt{6}\;\sqrt{\tfrac{1}{2}} - 2\sqrt{3}}{\sqrt{50}}$$

$$= -3\sqrt{3/50} ,$$

$$\langle d^{3\,2}G,4\,|V^1_{-1}(dp)|\,(d^{2\,1}Gp)\,^2H,5\rangle = -\tfrac{2}{10}\,\langle \begin{matrix}1&1\\3\end{matrix}|E_{36}\left|\begin{matrix}1&1\\6\end{matrix}\right\rangle$$

$$= -\tfrac{2}{10} ,$$

$$\langle (d^{2\,3}Fp)\,^2G,4\,|V^1_{-1}(pd)|\,d^{3\,2}H,5\rangle = \left\langle \begin{matrix}1&6\\2\end{matrix}\left|\frac{\sqrt{6}\;E_{61}}{\sqrt{10}}\right|\begin{matrix}1&1\\2\end{matrix}\right\rangle$$

$$= \frac{3}{\sqrt{10}} . \tag{48}$$

All of the states of a given multiplet such as the doublets in Fig. 6 of any multiple-shell manifold belong to one IR of the orbital unitary group U_h. Therefore all transition and energy matrices can be made through the elementary E_{ij} using basically the same formulas and methods that were established in the preceding sections. The additional complications associated with the electrostatic interaction are involved mainly with the appearance of different kinds of radial integers, as shown in the Appendix. Furthermore, the assembly formula connects $U_h \times U_2$ states with U_{2h} states for either single- or multiple-shell problems; thus the treatment of spin-orbit operators is basically unchanged.

We close this section by considering the ordering and parentage structure associated with multiply excited configurations such as p^2d. For the orbital-state ordering we have chosen, there is just one highest tableau $\begin{matrix}1&6\\6\end{matrix}$. Applying the intrashell lowering operators L_- and $E_{n,n-1}$ we would obtain terms ^2G, ^2F, ^2F, ^2D, ^2D, ^2D, ^2P, ^2P, and ^2S arising from 45 tableaus which are partially listed below,

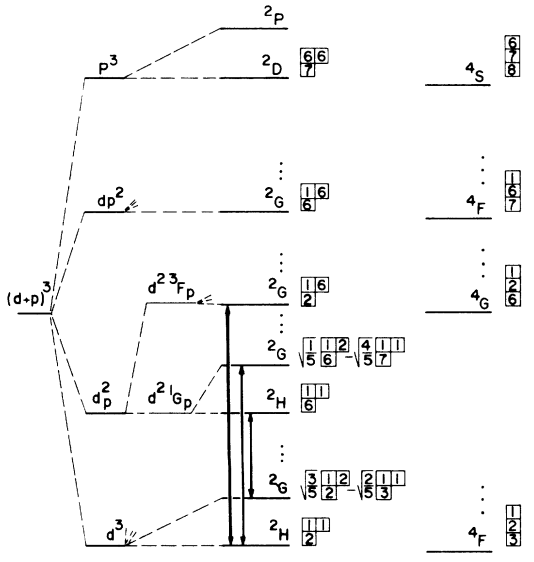


FIG. 6. Example of unitary tableau notation for multiple-shell states. The calculation of the dipole operator using the jawbone formula between states of definite spin and orbit as shown is given in Eq. (48).

$$\begin{array}{cccccccccccccccccccc} G & & F & F & & & D & D & D & & & & P & P & & & & S & & \\ 16 & : & 26 & 17 & 16 & : & 36 & 27 & 26 & 18 & 17 & 16 & : & 46 & 37 & 36 & 28 & 27 & 26 & 18 & 17 & : & 56 & 47 & 46 & 38 & 37 & 36 & 28 & 27 & 18 & : \\ 6 & \cdot & 6 & 6 & 7 & \cdot & 6 & 6 & 7 & 6 & 7 & 8 & \cdot & 6 & 6 & 7 & 6 & 7 & 8 & 7 & 8 & \cdot & 6 & 6 & 7 & 6 & 7 & 8 & 7 & 8 & 8 & \cdot \end{array} \tag{49}$$

Now for some applications it may be convenient to express such tableaus in a way that manifests their orbital parentage. Suppose we order the orbital states so that p states 6, 7, and 8 come first before the d states $1, 2, \ldots, 5$. (We will keep the same number assignment to avoid confusion.) Now p^2d gives rise to the same number of states as came from dp^2, but they come in two separate families as shown in Eqs. (50) and (51), respectively:

$$\left\langle L_- \middle\backslash E_{mn} \middle\rangle = \begin{array}{c} \begin{array}{cccccccccccccccccccc} G & & F & & D & D & & & P & & & S & & & & & & & & \\ 66 & : & 67 & 66 & : & 77 & 68 & 67 & 66 & : & 78 & 77 & 68 & 67 & 66 & : & 88 & 78 & 77 & 68 & 67 & 66 & : \\ 1 & \cdot & 1 & 2 & \cdot & 1 & 1 & 2 & 3 & \cdot & 1 & 2 & 2 & 3 & 4 & \cdot & 1 & 2 & 3 & 3 & 4 & 5 & \cdot \end{array} \\ \hline \begin{array}{cc} \sqrt{2} & 1 \\ 2 & \\ 2 & \end{array} \end{array}, \tag{50}$$

$$|(p^2\,{}^1D)d\,{}^2G, 4\rangle = \left|{}^{66}_{1}\right\rangle, \qquad |(p^2\,{}^1D)d\,{}^2F, 3\rangle = \left(\left|{}^{67}_{1}\right\rangle - \left|{}^{66}_{2}\right\rangle\right)/\sqrt{2}\ ;$$

$$\left\langle L_- \middle\backslash E_{mn} \middle\rangle = \begin{array}{c} \begin{array}{ccccccccccc} F & & D & & P & & & & & & \\ 61 & . & 61 & 62 & . & 71 & 62 & 63 & . & 72 & 63 & 64 & : \\ 7 & \cdot & 8 & 7 & \cdot & 8 & 8 & 7 & \cdot & 8 & 8 & 7 & \cdot \end{array} \\ \hline \begin{array}{cc} 1 & 1 \\ 2 & \\ 2 & \end{array} \end{array}, \qquad |(p^2\,{}^3L)d\,{}^2F, 3\rangle = \left|{}^{61}_{7}\right\rangle. \tag{51}$$

The tableau states in the preceding equations can easily be related to the tableau having the original ordering using the assembly formula. The results are as follows for the first three states:

$$\begin{aligned} &|(p^2\,{}^1D)d\,{}^2G, 4\rangle = \left|{}^{66}_{1}\right\rangle = -\left|{}^{16}_{6}\right\rangle\ , \\ &|(p^2\,{}^3P)d\,{}^2F, 3\rangle = \left|{}^{61}_{7}\right\rangle = \tfrac{1}{2}\left(-\left|{}^{17}_{6}\right\rangle + \sqrt{3}\ \left|{}^{16}_{7}\right\rangle\right), \\ &|(p^2\,{}^1D)d\,{}^2F, 3\rangle = \left(\left|{}^{67}_{1}\right\rangle - \left|{}^{66}_{2}\right\rangle\right)/\sqrt{2} \\ &\qquad = \left(2\left|{}^{26}_{6}\right\rangle - \sqrt{3}\ \left|{}^{17}_{6}\right\rangle - \left|{}^{16}_{7}\right\rangle\right)/\sqrt{8}\ . \end{aligned} \tag{52}$$

The states whose parentage is traceable to simple products of p^2 and d configurations would become eigenstates if the electrostatic exchange integrals approached zero. A more general discussion of the parentage structure will be given in a future paper, where a general method for deriving transformations between $U(l_1 + l_2 + \cdots)$ bases and $U(l_1) \times U(l_2) \times \cdots$ bases will be explained. This theory is useful for calculations that employ a truncated basis.

In addition it is possible to derive transformations between $U(h \cdot s \cdot \cdots)$ based and $U(h) \times U(s) \times \cdots$ bases. This amounts to a generalization of the transformations found by the assembly formula. It is possible to use these transformations in the treatment of wave functions for nuclear supermultiplets, quarks, or relativistic models of electrons.

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APPENDIX: ELEMENTARY EXPRESSIONS FOR ISOTROPIC TWO-BODY INTERACTIONS

We give now the relation between the standard Racah expressions for isotropic two-body operators and products of the one-body elementary (E_{ij}) or (V_q^k) operators. We use the addition theorem to write the interaction between each pair (α, β) of electrons.

$$\frac{1}{|\boldsymbol{r}_{\alpha\beta}|} = \sum_k \sum_q (-1)^q \frac{r_<^k}{r_>^{k+1}} C_{-q}^k(\alpha) C_q^k(\beta)\ , \tag{A1}$$

where the C_q^k are the standard multipole functions

$$C_q^k(\alpha) = [4\pi/(2k+1)]^{1/2}\, Y_q^k(\theta_\alpha, \phi_\alpha)\ . \tag{A2}$$

For a single pair (α, β) one obtains an expression involving the single-particle elementary operators e_{ij}

$$\frac{1}{|r_{\alpha\beta}|} \to \sum_{\substack{l_1 l_2 l_1' l_2' \\ m_1 m_2 m_1' m_2'}} \left|\begin{matrix} l_1' & l_2' \\ m_1' & m_2' \end{matrix}\right\rangle \left\langle \begin{matrix} l_1' & l_2' \\ m_1' & m_2' \end{matrix}\right| \frac{1}{|r_{\alpha\beta}|} \left|\begin{matrix} l_1 & l_2 \\ m_1 & m_2 \end{matrix}\right\rangle \left\langle \begin{matrix} l_1 & l_2 \\ m_1 & m_2 \end{matrix}\right|$$

$$= \sum_{\substack{l_1 l_2 l_1' l_2' \\ m_1 m_2 m_1' m_2'}} e_{\substack{l_1' l_1 \\ m_1' m_1}}(\alpha)\, e_{\substack{l_2' l_2 \\ m_2' m_2}}(\beta) \sum_k F^k(l_1' l_2' l_1 l_2) \left(\sum_q (-1)^q \left\langle \begin{matrix} l_1' \\ m_1' \end{matrix}\right| C^k_{-q}(\alpha) \left|\begin{matrix} l_1 \\ m_1 \end{matrix}\right\rangle \left\langle \begin{matrix} l_2' \\ m_2' \end{matrix}\right| C^k_q(\beta) \left|\begin{matrix} l_2 \\ m_2 \end{matrix}\right\rangle \right) \tag{A3}$$

and the Slater radial integral F^k,

$$F^k(l_1' l_2' l_1 l_2) = \int r_1^2\, dr_1 \int r_2^2\, dr_2\, R_{l_1'}(r_1) R_{l_2'}(r_2) \frac{r_<^k}{r_>^{k+1}} R_{l_1}(r_1) R_{l_2}(r_2)\ . \tag{A4}$$

The summations are over all sub-shells that one is considering in a configuration.

The inclusion of all electron pairs yields an expression involving the one-body elementary operators (see Eqs. (6)–(8) in Sec. II)

$$\frac{1}{2} \sum_{\alpha \neq \beta} \frac{1}{|r_{\alpha\beta}|} \to \frac{1}{2} \sum_{l_1' l_2' l_1 l_2} \sum_k A^k(l_1' l_2' l_1 l_2) \left(\sum_{\substack{q \\ m_1 m_2}} (-1)^{q+\Delta} \begin{pmatrix} k \\ 1' & 1 \end{pmatrix} E_{1' 1} \begin{pmatrix} k \\ 2' & 2 \end{pmatrix} E_{2' 2} \right.$$

$$\left. - \sum_{\substack{q \\ m_1 m_2}} (-1)^{q+\Delta} \begin{pmatrix} k \\ 1' & 1 \end{pmatrix} \begin{pmatrix} k \\ 2' & 2 \end{pmatrix} \delta_{2' 1} E_{1' 2} \right), \tag{A5}$$

in terms of the modified Wigner coefficients [see Eqs. (9), (10), and (41)]

$$\begin{pmatrix} k \\ 1' & 1 \end{pmatrix} = C^{k\ l_1 l_1'}_{-q\ m_1 m_1'} [(2k+1)/(2l_1'+1)]^{1/2}$$

as

$$1' \to {}^{l_1'}_{m_1'}, \quad 1 \to {}^{l_1}_{m_1} \tag{A6}$$

and modified Slater integrals A^k,

$$A^k(l_1' l_2' l_1 l_2) = F^k(l_1' l_2' l_1 l_2) \begin{pmatrix} l_1' & k & l_1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_2' & k & l_2 \\ 0 & 0 & 0 \end{pmatrix} \frac{[(2l_1+1)(2l_2+1)(2l_1'+1)(2l_2'+1)]^{1/2}}{2k+1}. \tag{A7}$$

Note that the A^k are zero unless the following "parity" restrictions are satisfied:

$$(-1)^{l_1'+k+l_1} = 1 = (-1)^{l_2'+k+l_2}\ , \quad (-1)^{\Delta} = (-1)^{l_1 - l_1'} = (-1)^{l_2 - l_2'}. \tag{A8}$$

For deriving matrices such as Eqs. (25) and (26) in Sec. II, it may be convenient to use the following form:

$$\frac{1}{2} \sum_{\alpha \neq \beta} \frac{1}{|r_{\alpha\beta}|} \to \frac{1}{2} \sum_{l_1' l_2' l_1 l_2} \sum_k A^k(l_1' l_2' l_1 l_2) \sum_q \tilde{V}^k_q(l_1 l_1') V^k_q(l_2' l_2) - \frac{1}{2} \sum_{l_1 l_2} \sum_k A^k(l_1 l_2 l_2 l_1) \frac{2k+1}{2l_1+1} \sum_{m_1} E_{\substack{l_1 l_1 \\ m_1 m_1}}\ . \tag{A9}$$

The last term in Eq. (A9) becomes the familiar "self-energy" for pure configurations ($l_1 = l_2 = l_1' = l_2'$) or the "exchange energy" for certain mixed configurations.

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