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Alternative Basis for the Theory of Complex Spectra*

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A new method is given for deriving the angular factors of energy matrices in l^n atomic configurations, and the need for coefficients of fractional parentage, Racah coefficients, algebraic formulas, and chain calculations is avoided. Instead, matrix elements are obtained directly by a comparatively simple digital counting procedure.

I. INTRODUCTION

Racah's group-theoretical techniques for analyzing complex atomic spectra have seen extensive use and development since their introduction over 20 years ago.[1] The application[2] of Lie-group-representation theory has become a more powerful tool for physicists than the earlier methods of Condon, Shortley, or Slater. For one thing, the mathematics of Racah provided a better labeling, than previously existed, for the plethora of spectral terms that arise in an orbital shell configuration of the pure form l^n. The quantum numbers that gave this labeling corresponded to irreducible representations of various (depending on shell l) chains of Lie groups chosen with their terminal links being the groups $R(3) > R(2)$ of spatial rotations in three and two dimensions (the latter about a "z axis"), respectively. These chain links allowed a simplifying factorization of states and operators with the final two links corresponding to total orbital momentum L and z-component M, and thereby one obtained some additional computational power above that of ordinary angular momentum calculus.

However, physics problems are now arising for which even Racah's methods can become extremely difficult or impractical. For example, exhaustive searches for rare-earth–crystal-field laser systems require optimum use of enormous computing machinery just to get energy matrices by Racah's techniques, leaving little flexibility and time to solve or analyze them. Many other mathematically similar problems in atomic, molecular, or nuclear physics remain untouched apparently because of the complexity of "quantum bookkeeping."

I report here that most of these problems, for orbital l^n configurations at least, vanish if one redoes the angular factor analysis using a relatively new type of mathematics.[3] Furthermore, we expect that similar problems can also experience great simplification since this new approach and mathematics is quite general in scope. The mathematics used is based upon the recent works of Gelfand and Zetlin[4]; Baird, Biedenharn, Louck, and Giovannini[5-8]; Moshinsky and Ciftan[9,10]; and Gilmore,[11] as referenced below. The theory is different from the seniority or quasispin and inter-shell group analysis given by Judd[12,13] and others. However, the following work was motivated by an apparent need in Judd's intriguing theories to deal efficiently with enormous Lie groups,[14] and undoubtedly the two procedures will eventually blend in an interesting way.

I demonstrate the analysis by giving some simple rules (Sec. IV) for obtaining angular matrix elements of orbital 2^k-pole one-body operators and scalar two-body operators. We replace previous expressions or chain calculations involving Racah coefficients, fractional parentage coefficients, Wigner coefficients, phases, sums, and other factors, with comparatively simple counting algorithms. Indeed, the higher angular momentum states for any multiplet from p^n, d^n, f^n, g^n, etc. configuration can have matrix elements evaluated "on the back of an envelope" without extensive numerical or algebraic tables. Lower momenta which, in atoms, generally have higher energy, may require more computation depending on the configuration, but always the procedure is straightforward, and the use of tables or other forms of memory is avoided.

In order to appreciate the motivation for rejecting the Racah scheme, one should be aware of an apparent difficulty in its mathematics. No group chain that ends with $R(3) \supset R(2)$ can guarantee only one state exists for a given set of irreducible representation labels. In fact, Racah's labels fail[15] to delineate several pairs of states in configurations f^5-f^9. This is a serious flaw if one expects the group-mathematical machinery to provide closed-form expressions for operators. In fact, the Racah scheme uses coefficients of fractional parentage which require individual (and often laborious) treatment since no closed form can be written for them. (The Racah recoupling coefficients,

on the other hand, do have a closed, albeit somewhat complicated, formula.)

Another more or less serious objection to the Racah scheme involves the work one must do to make states correspond to the Pauli principle, since this scheme is set up to couple particles one pair at a time. When dealing with two or less particles, comparatively little difficulty arises; but wave functions or operators involving three or more particles must be uncoupled and recoupled repeatedly, using various coefficients and phases to get the right permutational symmetry. Consequently, the procedure becomes grossly inelegant.

The preceding objectionable behaviors do not exist in the new approach. First of all, the orbital states are labeled uniquely by a chain of quantum numbers $\{\lambda_{jm}\}$, $\{\lambda_{j\,m-1}\}$, ..., λ_{11} corresponding to a "canonical" chain of unitary groups $U(m) \supset U(m-1) \supset \cdots \supset U(1)$. The notation for a state is given by a triangular array of these numbers, and called a Gelfand pattern. [An example with $m=5$ is shown in Fig. 1(a).] Secondly, the orbital wave function implied by each Gelfand pattern has a quasidefinite permutational symmetry, so recoupling is unnecessary. The role of box diagrams, which are called "Young Tableaux" [see Fig. 1(b), for example], to define permutational symmetry

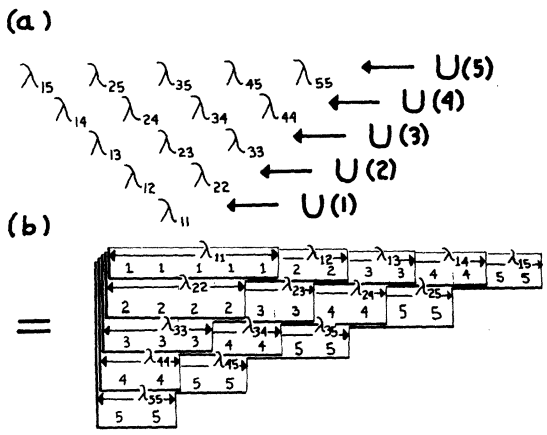

FIG. 1. Conversion from (a) Gelfand pattern notation to (b) "Young tableau" notation for $U(5)$. Gelfand quantum numbers $\lambda_{1n}\lambda_{2n}\cdots\lambda_{nn}$ give the lengths of rows of boxes in a tableau for $U(n)$. Then $\lambda_{1\,n-1}\lambda_{2\,n-1}\cdots\lambda_{n-1\,n-1}$ tell the lengths of a $U(n-1)$ tableau inside the previous tableau, and so on down to $U(1)$, which corresponds to only one row of λ_{11} boxes containing 1's. Each box represents a particle, and the number it holds tells in what state the particle resides. A Young tableau indicates the permutational symmetry of a many-particle state. For example, a tableau state is antisymmetric to permutation of states in a column. (Hence, no two numbers in a column are alike). On the other hand, a tableau state is symmetric to permutation of states in any row that has no boxes above or below it.

happens to be fairly complicated and subject to some choice of convention. However, the basic idea of the "tableaus" is sketched in the figure caption of Fig. 1, and very little more knowledge than this is required to understand and use the theory given in the following.

Gelfand[4] first wrote closed-form expressions for the "elementary operators" $E_{\alpha\beta}$ in terms of rational roots of polynomials in the numbers λ_{ij}. Biedenharn[5] and Louck[8] have elucidated the structure of these results and developed a "Gelfand pattern calculus" to obtain further algebraic formulas.[6] Gilmore[11] has given patterns that produce similar algebraic formulas for all the classical Lie groups.

For applications, it turns out to be convenient to convert the algebraic-pattern formulas to counting algorithms involving the tableaus of Fig. 1(b). These algorithms are generally much simpler to remember and to use when a numerical result is desired. The "Jawbone formula" of Sec. III, is a counting algorithm for matrix elements of elementary operators.

Hall and G. deB. Robinson[16] may have been the first to derive any sort of tableau algorithms when they wrote counting formulas for unitary representation dimension (Fig. 2) and permutation group representation dimension, but until now, this sort of "calculus" has seen little development or application.[17,18]

The elementary operators are components of the more familiar multipole orbital operators V^k_q, as

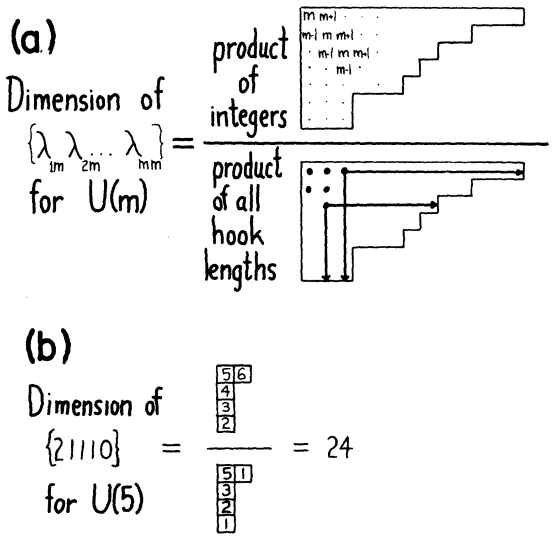

FIG. 2. (a) Hall-Robinson formula for unitary dimension and (b) example for $U(5)$. A "hook length" of a given box in a tableau is the number of boxes in a "hook" which includes the given box and every other box below it and to the right of it. The 24 states predicted by example (b) are displayed in Fig. 6.

explained in Sec. IV. Also, the Gelfand states are related to states of definite total orbital momentum. This last point represents a disadvantage of the new basis. While the new orbital base states have definite total z-component M of orbital momentum and can be assigned to a definite total spin S, they have indefinite total orbital (L) momentum and are, to this extent, unphysical. However, in Sec. II we give a physical interpretation of Gelfand states and compare the level diagrams of p^n configurations (Fig. 3) involving Gelfand states on the one hand, to Racah states on the other. Furthermore, in Sec. IV the procedure for explicitly relating the two types of states is given, as part of a sample calculation for a d^5 configuration.

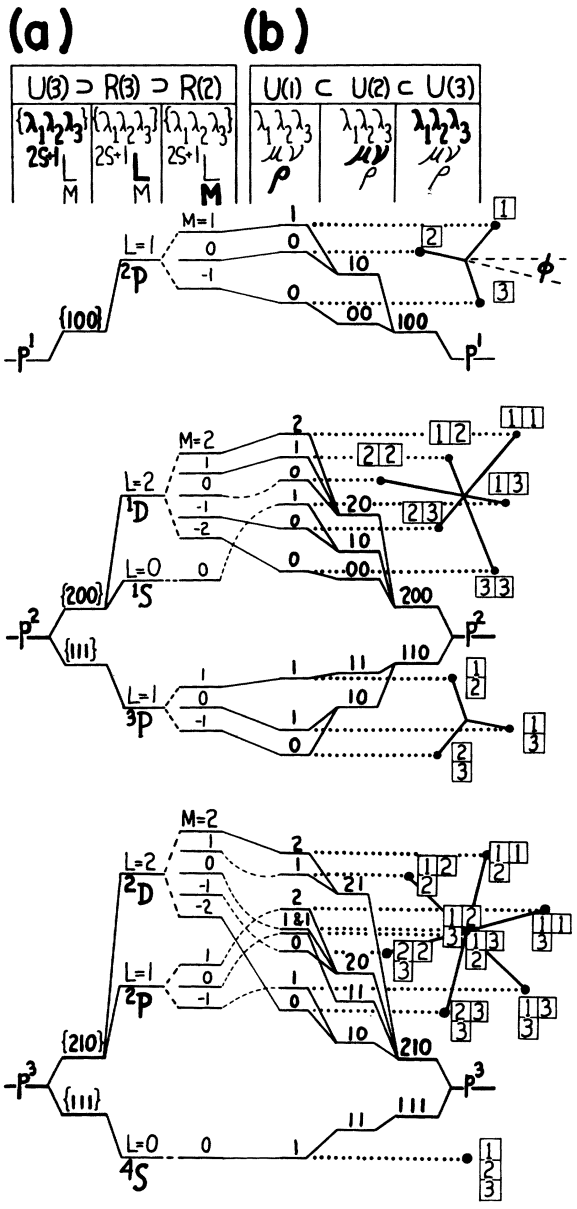

FIG. 3. (a) Racah basis and (b) Gelfand basis of atomic p-shell. Standard angular momentum basis (a) for p^n configurations is compared to the basis (b) arising from a Gelfand chain. Correlation of final levels from each is expressed by dashed or solid lines in the center of the figure. A solid line implies an equality of the two states it connects, while dashed lines imply a linear mixing with some of the other levels connected by dashed lines.

It should be noted now (since the difficulty does not arise in Sec. IV) that one is free to pick whatever combinations of repeated equal-total-angular-momentum states one finds convenient without interfering with the effectiveness of the matrix evaluation. Racah's choice of sharp seniority is one possibility but, outside of nuclear physics, not always a convenient one.

II. COMPARISON OF GELFAND STATES WITH RACAH STATES

The Racah bases for pure configurations were labeled by quantum numbers associated with certain chains of groups depending on what shell was involved. For example, orbital d^n configurations used the chain $U(5)\supset R(5)\supset R(3)\supset R(2)$, corresponding to quantum numbers $[\lambda_1\,\lambda_2\,\lambda_3\,\lambda_4\,\lambda_5]$, $\{\mu_1, \mu_2\}$, L, and M. The new procedure involves one of the so-called canonical bases developed by Gelfand, Zetlin, and others. In the d^n shell, which we shall use as an example, the group chain and the quantum numbers are given by the notations of Fig. 1(a). In this notation the top row is the same as Racah's $U(5)$ ($\lambda_{i5}=\lambda_i$), but otherwise the correspondence is not direct.

To obtain some idea of this correspondence, we examine p^n configurations. The Racah chain for these would be $U(3)\supset R(3)\supset R(2)$, corresponding to quantum numbers $[\lambda_1\,\lambda_2\,\lambda_3]$, L, and M. The Gelfand chain is $U(3)\supset U(2)\supset U(1)$, corresponding to the quantum pattern

$$\begin{matrix}\lambda_1 & \lambda_2 & \lambda_3\\ \mu & \nu & \\ \rho & & \end{matrix}\,. \tag{1}$$

The latter starts with the same triad $[\lambda_1\,\lambda_2\,\lambda_3]$ as the former.

There is a one-to-one correspondence between a given triad and a certain total-spin S or "multiplicity" $2S+1$. This is because a triad denotes a particular tableau of permutational symmetry for the orbital wave function, and the "opposite" tableaus of spin states must be "mated" in order to make a totally antisymmetric (Pauli) state. [A tableau of spin states corresponds to just one total-

spin S, because of the fairly intimate relation between two-dimensional unitary transformation $U(2)$ and ordinary rotation $R(3)$.] The rule for converting orbital tableaus to an S is given by Eqs. (4), in Sec. IV.

The p^n levels as visualized by the Racah scheme are shown in Fig. 3(a). The states correspond to limiting eigenfunctions of strong scalar two-body interactions and weak magnetic field.

The p^n levels as visualized by a Gelfand basis [Fig. 3(b)] can be thought to be limiting eigenfunctions of a strong magnetic (Zeeman) field proportional to one-body multipole operator V_0^1 colinear with a quadratic (Stark) electric field proportional to one-body quadrupole operator V_0^2, and weak two-body interactions. If the proportions of the two one-body components are $\cos\phi : \sin\phi$, then the exact locations of energy levels are given, as in Fig. 3(b), by the projections of triangular or hexagonal "weight-vector" diagrams. $\phi = 0$ gives pure Zeeman splitting while $\phi = \pi/2$ gives pure quadratic Stark splitting.

The weight-vector diagrams were invented by Cartan to display the eigenvalues of commuting operators and show various relationships between states and group operators E_{ij}.

These relationships can be seen quite easily by referring to the tableaus. A given tableau sits on a point in a lattice which supports all possible weight diagrams. (In general several tableaus may share a single point.) In Fig. 3(b) a "1" in a box means a particle with $m = 1$; "2" means $m = 0$; and "3" means $m = -1$. The operator E_{ij} is capable of changing a "j" to an "i" so one of the six operators E_{12}, E_{13}, E_{23}, E_{21}, E_{31}, and E_{32} may change a tableau state in Fig. 3(b) to any other state on any other neighboring lattice point.

The general derivation and analysis of diagrams like Fig. 3, is given in Sec. IV, along with a more complicated example shown by Fig. 6.

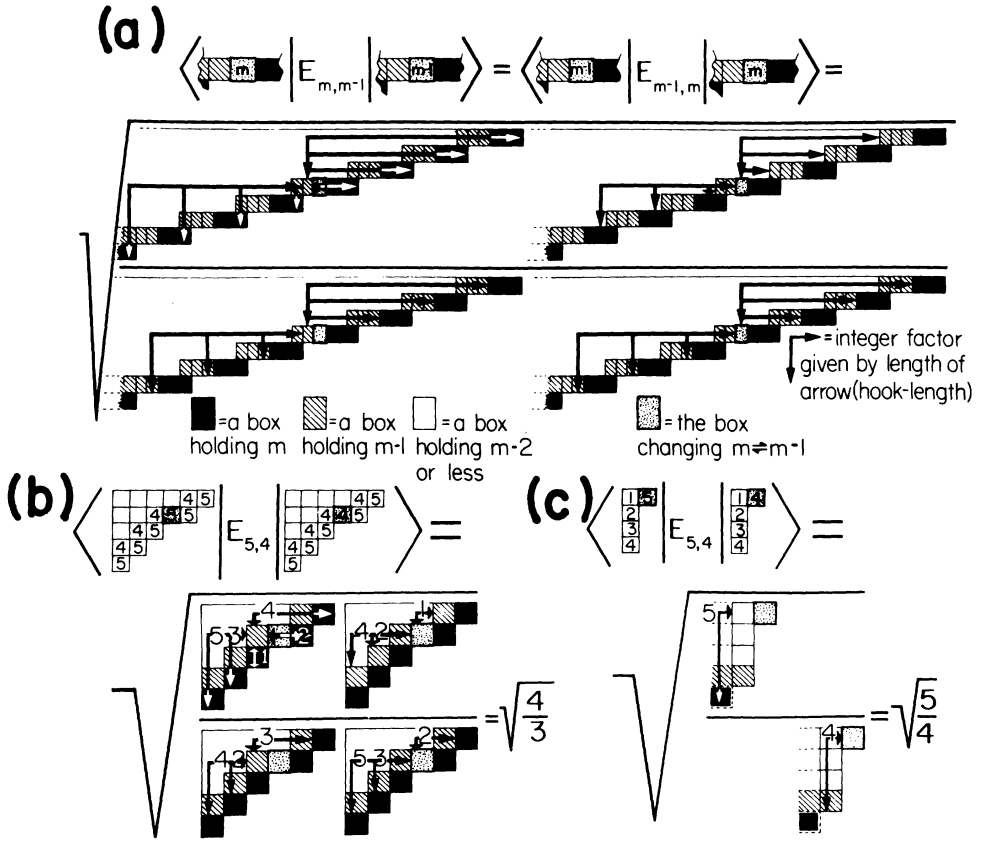

FIG. 4. Jawbone counting formula for elementary operator matrix elements. (a), (b) Matrix element is a positive square root of a rational fraction made of products of hook lengths, as shown. When applying formula to a general tableau, only those boxes containing m or less will be involved, so the rest can be shaved off. (c) An example involving five-particle atomic orbital states appearing in Fig. 6.

III. THE JAWBONE FORMULA

The elementary operator $E_{m,m-1}$ can change one particle from state $m-1$ into state m. In other words $E_{m,m-1}$ can change any number $m-1$ in a tableau into an m, provided another m was not already in its column. The jawbone counting formula of Fig. 4(a) gives the matrix element for this change, and a reverse change. The figure explains the algorithm, although it should be pointed out that it sometimes helps to add m-box columns to tableaus lacking them [viz., Fig. 4(c)] in order to visualize all factors. (An m-box column is scalar to $E_{m,m-1}$.) Also, manifestly cancelling factors in Fig. 4(c) are not drawn.

Still simpler algorithms can be derived for special applications. However, Fig. 4(a) is convenient to remember (with practice) and has the advantage of being completely general, and in quite direct correspondence to algebraic results of Refs. 2–9.

Finally, elementary operators $E_{m,m}$ are diagonal with eigenvalues given simply by the number of boxes containing m's.

IV. EXAMPLE OF APPLICATION

Some matrix elements involving quartet ($S=\frac{3}{2}$) states of definite orbital momentum L in a five-particle $l=2$ configuration (d^5) are evaluated below

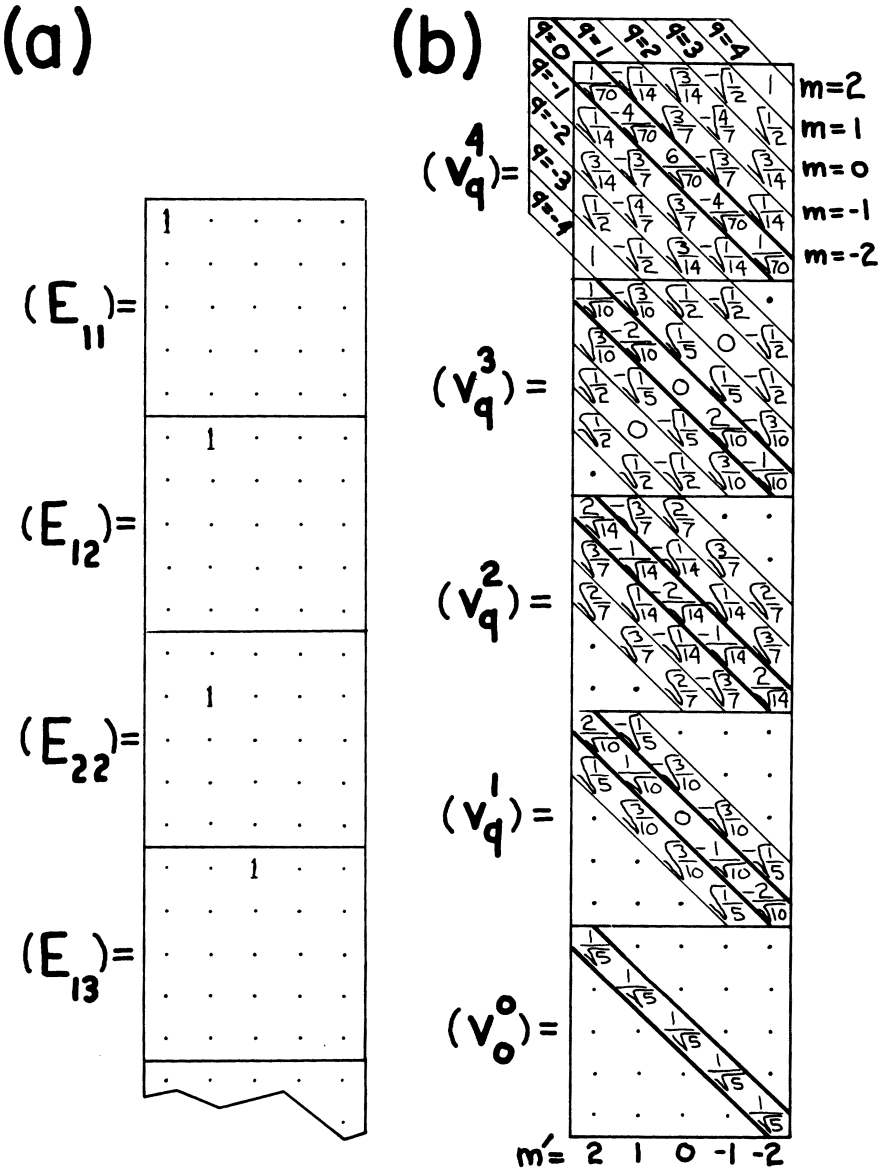

FIG. 5. Fundamental (one-particle) representation of $U(5)$. (a) Elementary operators E_{ij} and (b) Wigner unit-tensor operators v_q^k.

to show the procedure.

All operators in d shell are constructed from the unit tensors given by Eq. (2) and displayed in Fig. 5(b):

$$\left(\begin{matrix} l \\ m \end{matrix}\middle| V_q^k \middle| \begin{matrix} l \\ m' \end{matrix}\right) = (-1)^{l-m}(2k+1)^{1/2}\begin{pmatrix} l & k & l \\ -m & q & m' \end{pmatrix}. \tag{2}$$

A d orbiting particle can take on five values of magnetic quantum number, and these are numbered: 1, $m=2$; 2, $m=1$; 3, $m=0$; 4, $m=-1$; and 5, $m=-2$. The operators $E_{n,m}$ are related to the V_q^k through their fundamental (one-particle) representations, which are given in Fig. 5. Equation (3) is one such relation:

$$V_1^1 = (-1/\sqrt{10})(\sqrt{2}E_{12} + \sqrt{3}E_{23} + \sqrt{3}E_{34} + \sqrt{2}E_{45}). \tag{3}$$

An n-particle l-shell spin-S multiplet belongs to a particular set of Racah's λ_j labels defined by (4), with the understanding that 1's appear exactly $2S$ times:

$$[\lambda_1 \lambda_2 \cdots \lambda_{2l+1}] = [22\cdots 211\cdots 10\cdots 0], \tag{4a}$$

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{2l+1} = n. \tag{4b}$$

As previously mentioned, this set is the first row of the Gelfand pattern defining all those orbital states. For example, each orbital state in the five-particle d-shell spin-$\frac{3}{2}$ quartet belongs to a Gelfand pattern having the top row $[\lambda_1 \lambda_2 \lambda_3 \lambda_4 \lambda_5] = [2\ 1\ 1\ 1\ 0]$.

The example calculation is now given as a series of steps which apply in general.

Step 1. Filling out the Gelfand pattern so that every integer is between the two integers above it (the "betweenness" condition[19]) gives all states, as shown in Fig. 6(a). It is helpful to lexically order the states (211 > 210 > 111 > 110 etc.) Robinson's formula (Fig. 2) can check the number at any level.

Step 2. Converting each pattern to a tableau determines the z component M of angular momentum of the state represented, since the M for a tableau is the sum of its numbers less a constant.

It is convenient to reorder, where necessary, the tableau into groups of equal M, as in Fig. 6(b). This dictates the allowed ^{2S+1}L terms, which for the example of Fig. 6(b) are 4_G, 4_F, 4_D, and 4_P.

Step 3. Evaluation of relevant submatrices of V_1^1 [Eq. (6a)] by jawbone formula and by Eq. (3)

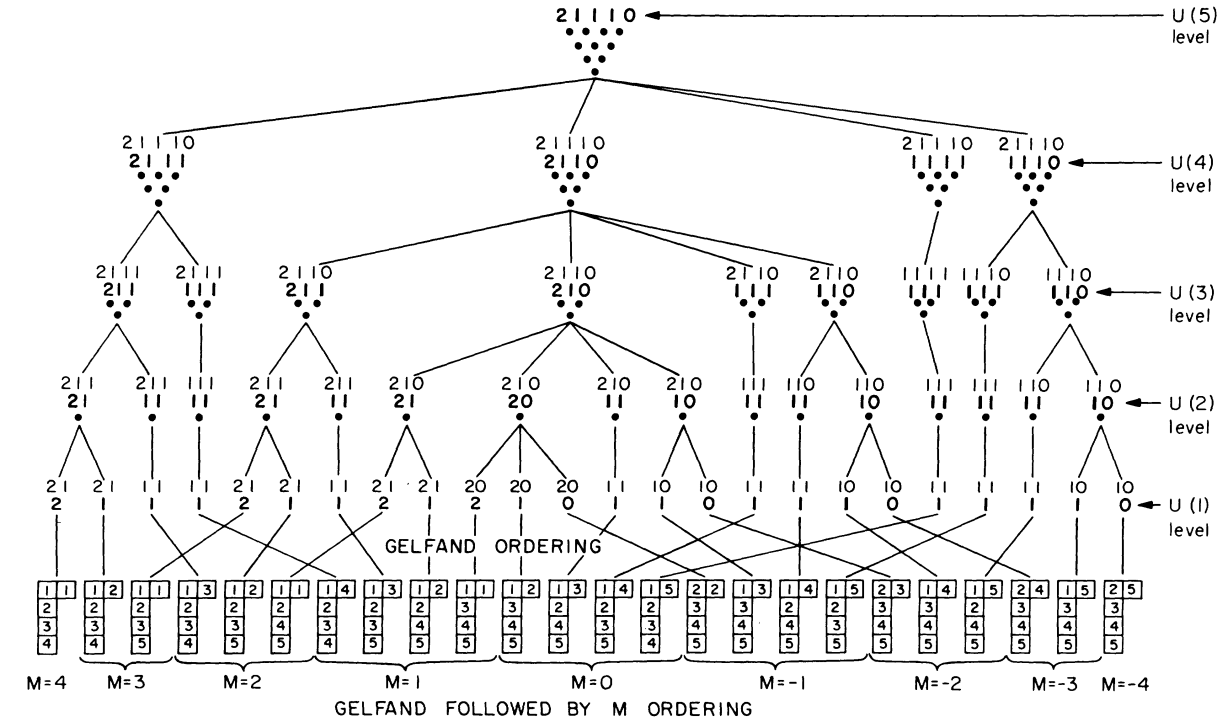

FIG. 6. Display of $(d^5\,{}^4L)$ states. (a) States are first Gelfand ordered, and then (b) reordered according to total z-component M of angular momentum.

leads directly to a block diagonal total-angular-momentum matrix [Eq. (6b)]. [For the d shell, total angular momentum operator is Eq. (5)]:

$$L^2 = 10\{V_0^1 V_0^1 - V_1^1 V_{-1}^1 - V_{-1}^1 V_1^1\}. \tag{5}$$

Since V_{-1}^1 is the negative transpose of V_1^1, the products $V_{-1}^1 V_1^1$ and $V_1^1 V_{-1}^1$ are formed by making a few select row and column intersections in V_1^1 submatrices. $V_0^1 V_0^1$ contributes diagonal M^2:

$$-V_1^1 = \frac{1}{\sqrt{10}}$$

1 1	1 2	1 1	1 3	1 2	1 1	1 4	1 3	1 2	1 1	⋯
2	2	2	2	2	2	2	2	2	3	
3	3	3	3	3	4	3	3	4	4	
4	4	5	5	5	5	4	5	5	5	
·	$\sqrt{2}$	$\sqrt{2}$								
	·	·	$\sqrt{3}$	$\sqrt{2}$	0					
			0	$\sqrt{2}$	$\sqrt{3}$					
			·	·	·	$\sqrt{3}$	$\sqrt{2}$	0	0	
			·	·	·	0	$\sqrt{3}$	$\sqrt{3}$	0	
			·	·	·	0	0	$\sqrt{2}$	$\sqrt{3}$	
						·	·	·	·	

, (6a)

$$(L)^2 =$$

1 1	1 2	1 1	1 3	1 2	1 1	⋯
2	2	2	2	2	2	
3	3	3	3	3	4	
4	4	5	4	5	5	
20						
	16	4				
	4	16				
			12	$2\sqrt{6}$	0	
			$2\sqrt{6}$	14	$2\sqrt{6}$	
			0	$2\sqrt{6}$	12	

, (6b)

Step 4. Desired sharp L and M states [Eq. (7)] are obtained by applying Sylvester's theorem or the row-minor method to submatrices of L^2. [Given the eigenvalues $L(L+1)$ of submatrices, one finds eigenvectors]:

$$\left|\begin{matrix}G\\4\end\right\rangle = \begin{matrix}1&1\\2&\\3&\\4&\end{matrix}, \quad \left|\begin{matrix}G\\3\end\right\rangle = \frac{1}{\sqrt{2}}\begin{matrix}1&2\\2&\\3&\\4&\end{matrix} + \frac{1}{\sqrt{2}}\begin{matrix}1&2\\2&\\3&\\5&\end{matrix}, \quad \left|\begin{matrix}G\\2\end\right\rangle = \sqrt{\tfrac{3}{14}}\begin{matrix}1&3\\2&\\3&\\4&\end{matrix} + \sqrt{\tfrac{4}{7}}\begin{matrix}1&2\\2&\\3&\\5&\end{matrix} + \sqrt{\tfrac{3}{14}}\begin{matrix}1&1\\2&\\4&\\5&\end{matrix},$$

$$\left|\begin{matrix}F\\3\end\right\rangle = \frac{1}{\sqrt{2}}\begin{matrix}1&2\\2&\\3&\\4&\end{matrix} - \frac{1}{\sqrt{2}}\begin{matrix}1&2\\2&\\3&\\5&\end{matrix}, \quad \left|\begin{matrix}F\\2\end\right\rangle = \frac{1}{\sqrt{2}}\begin{matrix}1&3\\2&\\3&\\4&\end{matrix} + 0 - \frac{1}{\sqrt{2}}\begin{matrix}1&2\\2&\\4&\\5&\end{matrix}, \tag{7}$$

$$\left|\begin{matrix}D\\2\end\right\rangle = \sqrt{\tfrac{2}{7}}\begin{matrix}1&3\\2&\\3&\\4&\end{matrix} - \sqrt{\tfrac{3}{7}}\begin{matrix}1&2\\2&\\3&\\5&\end{matrix} + \sqrt{\tfrac{2}{7}}\begin{matrix}1&1\\2&\\4&\\5&\end{matrix}.$$

This allows the determination of all one-body (crystal-field) operators of Eq. (8), where the α are given in Fig. 5(b):

$$V_0^k = \alpha_1 E_{11} + \alpha_2 E_{22} + \alpha_3 E_{33} + \alpha_4 E_{44} + \alpha_5 E_{55}. \tag{8}$$

In examples (9) we note that even-k diagonal components are zero, as expected in center shell:

$$\left\langle \begin{matrix} G \\ 4 \end{matrix} \middle| V_0^k \middle| \begin{matrix} G \\ 4 \end{matrix} \right\rangle = \begin{matrix} 1\,1 & 1\,1 \\ 2 & \\ 3 & V_0^k \\ 4 & \end{matrix} \begin{matrix} & 2 \\ & 3 \\ & 4 \end{matrix}$$

$$= 2\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + 0\alpha_5$$

$$= 4/\sqrt{10} \quad \text{for } k=1$$

$$= 0 \qquad \text{for } k=2, \tag{9}$$

$$\left\langle \begin{matrix} F \\ 3 \end{matrix} \middle| V_0^k \middle| \begin{matrix} G \\ 3 \end{matrix} \right\rangle = \begin{matrix} 1\,2 & 1\,1 & 1\,2 & 1\,1 \\ 2 & 2 & 2 & 2 \\ 3 & -3 & 3 & -3 \\ 4 & 5 & 4 & 5 \end{matrix} \frac{}{\sqrt{2}} V_0^k \frac{}{\sqrt{2}}$$

$$= -\tfrac{1}{2}\alpha_1 - \tfrac{1}{2}\alpha_2 + \tfrac{1}{2}\alpha_4 - \tfrac{1}{2}\alpha_5 .$$

Step 5. Scalar two-body operators are found using the same procedure as for Eq. (6), with one additional thing. For example, to find the quadrupole-quadrupole operator in Eq. (10),

$$(V^2 \cdot V^2) = V_2^2 V_{-2}^2 + V_{-2}^2 V_2^2 - V_1^2 V_{-1}^2 - V_{-1}^2 V_1^2 + V_0^2 V_0^2 , \tag{10}$$

one needs the $E_{n,\,n-2}$ to evaluate (11) (the V_1^2 are taken care of by $E_{n,\,n-1}$):

$$V_2^2 = \frac{1}{\sqrt{14}}(2E_{13} + \sqrt{6}E_{24} + 2E_{35}) . \tag{11}$$

The jawbone formula applied in sequence using commutation relations (12) gives all components needed, as seen, for example, in (13):

$$E_{13} = [E_{12}, E_{23}], \quad E_{24} = [E_{23}, E_{34}], \quad E_{35} = [E_{34}, E_{45}], \tag{12}$$

$$E_{13} \begin{matrix} 2\,3 \\ 3 \\ 4 \\ 5 \end{matrix} = E_{12} \begin{matrix} 2\,2 \\ 3 \\ 4 \\ 5 \end{matrix} - E_{23} \begin{matrix} 1\,3 \\ 3 \\ 4 \\ 5 \end{matrix} = \sqrt{2} \begin{matrix} 1\,2 \\ 3 \\ 4 \\ 5 \end{matrix} - \frac{1}{\sqrt{2}} \begin{matrix} 1\,2 \\ 3 \\ 4 \\ 5 \end{matrix} - \sqrt{\tfrac{3}{2}} \begin{matrix} 1\,3 \\ 2 \\ 4 \\ 5 \end{matrix}$$

$$= \frac{1}{\sqrt{2}} \begin{matrix} 1\,2 \\ 3 \\ 4 \\ 5 \end{matrix} - \sqrt{\tfrac{3}{2}} \begin{matrix} 1\,3 \\ 2 \\ 4 \\ 5 \end{matrix} . \tag{13}$$

Some resulting V_2^2 and two-body quadrupole submatrices are shown in Eqs. (14). One uses the vectors produced in Step 4 to obtain the energy matrices or, in this case, the energy eigenvalues (14b) (this process is repeated for higher multipole terms where desired):

$$\begin{matrix} 1\,1 & 1\,2 & 1\,1 & 1\,3 & 1\,2 & 1\,1 & 1\,4 & 1\,3 & 1\,2 & 1\,1 & 1\,2 & 1\,3 & 1\,4 & 1\,5 \\ 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 3 & 3 & 2 & 2 & 2 & \\ 3 & 3 & 3 & 3 & 3 & 4 & 3 & 3 & 4 & 4 & 4 & 4 & 3 & 3 \\ 4 & 4 & 5 & 4 & 5 & 5 & 4 & 5 & 5 & 5 & 5 & 5 & 5 & 4 \end{matrix} \quad \cdots$$

$$V_2^2 = \begin{vmatrix} \cdot & \cdot & \cdot & 2 & 0 & -2 & & & & & & & & \\ & & & \cdot & \cdot & \cdot & \sqrt{6} & 0 & -2 & 0 & & & & \\ & & & \cdot & \cdot & \cdot & 0 & 2 & 0 & -\sqrt{6} & & & & \\ & & & & & & \cdot & \cdot & \cdot & \cdot & 0 & -\sqrt{\tfrac{8}{3}} & -\sqrt{\tfrac{1}{3}} & \sqrt{5} \\ & & & & & & \cdot & \cdot & \cdot & \cdot & -\sqrt{3} & -1 & \sqrt{8} & 0 \\ & & & & & & \cdot & \cdot & \cdot & \cdot & -\sqrt{2} & \sqrt{6} & 0 & 0 \end{vmatrix} , \tag{14a}$$

$$\begin{matrix} 1\,1 & 1\,2 & 1\,1 & 1\,3 & 1\,2 & 1\,1 \\ 2 & 2 & 2 & 2 & 2 & 2 \\ 3 & 3 & 3 & 3 & 3 & 4 \\ 4 & 4 & 5 & 4 & 5 & 5 \end{matrix} \quad \cdots$$

$$14(V^2 \cdot V^2) = \begin{vmatrix} 20 & & & & & \\ & 32 & -12 & & & \\ & -12 & 32 & & & \\ & & & 36 & -2\sqrt{6} & -8 \\ & & & -2\sqrt{6} & 26 & -2\sqrt{6} \\ & & & -8 & -2\sqrt{6} & 36 \end{vmatrix} , \tag{14b}$$

[Eigenvalues for the three internal matrices in (14b) are: 20; 20, 44; 20, 44, 34.]

For most applications, one is interested in matrix elements or eigenvalues of a two-body *interaction* operator like (14c):

$$V^0(k \cdot k) = \tfrac{1}{2} \sum_{\substack{\text{particle} \\ a \neq b}} (-1)^{k-q} v_{-q}^k(a)\, v_q^k(b) . \tag{14c}$$

However, operators like (10) differ from this by only a constant "self-energy" term, as shown by the expansion (15), since the canonical scheme automatically sums over all particles:

$$V^k \cdot V^k = \sum_{\substack{\text{particles} \\ a,\, b}} (-1)^{k-q} v^k_{-q}(a)\, v^k_q(b)$$

$$= \sum_{\substack{\text{particles} \\ a \neq b}} (-1)^{k-q} v^k_{-q}(a)\, v^k_q(b)$$

$$+ \sum_a (-1)^{k-q} v^k_{-q}(a)\, v^k_q(a). \qquad (15)$$

For example, in an n-particle d configuration one has the following matrix relation (16) for interaction operators [the self-energy term in (15) is proportional to the unit operator, as can be seen by examining Fig. 5]:

$$\langle \gamma L | V^0(k \cdot k) | \gamma' L \rangle = \tfrac{1}{2} \langle \gamma L | V^k \cdot V^k | \gamma L \rangle - \tfrac{1}{2} n \frac{2k+1}{5} \delta_{\gamma\gamma'}. \qquad (16)$$

Then, for example (16), (14), and (7) give desired matrix elements, like (17):

$$\langle d^5 G | V^0(2 \cdot 2) | d^5 G \rangle = -25/14. \qquad (17)$$

All further results of the type seen in Eqs. (9) and (17) are straightforward applications of the preceding steps, so this completes the description of the canonical formulation of orbital states and operators.

V. CONCLUSION

The preceding methods are immediately applicable for studies involving an orbital shell model, including searches for potentially viable solid-state lasers,[20] and probably represent a significant advance in the state of the art. Generalizations that include effects of spin-dependent and n-body operators will be reported later.

We suggest that these advances are just the beginning of a much larger subject, and encourage the mathematical study of canonical operators, which is not yet complete.[21] The physical meaning of canonical versus angular momentum bases should be investigated more.[22] A general theory of transformations like our Eq. (7) probably exists.[23]

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