Selection Rules in the Atomic f Shell from Quarklike Substructures

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Four quarklike eight-dimensional spinors are used to generate the states of the atomic f shell. The automorphisms of SO(8) are put to work through the three SO(7) subgroups of Labarthe. As an example, selection rules are derived for two three-electron operators used in rare-earth and actinide spectroscopy.

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Over the years, a variety of tables for the atomic f shell have become available for the matrix elements of operators of physical interest. The Coulomb interaction, the single-electron spin-orbit interaction, the single-electron spherical tensors $\mathbf{U}^{(k)}$ that arise in crystal-field work, and the one-electron coefficients of fractional parentage (cfp) were tabulated almost thirty years ago by Nielson and Koster [1]. Comparable tables for the two-electron cfp [2], the electronic spin-spin and spin-other-orbit interactions [3,4], and the single-electron double tensors [5] have now become available. Individual workers have also derived the matrix elements of the particular operators they are interested in; thus Carnall has used a program of Hannah Crosswhite to calculate the matrix elements of the three-electron scalar operators that take into account some effects of configuration interaction on the spectroscopic (LS) terms occurring in the rare-earth and actinide configurations f^N [6].

A casual scan of these tables reveals an unusual number of zeros. Many can be understood by applying the Wigner-Eckart theorem to the Lie groups SO(7) and G_2 that are used to define the states, following the scheme of Racah [7]. Special reasons can often be adduced to explain others. However, an uncomfortably large residue remains. More recently, many unexpected proportionalities between blocks of matrix elements of the operators $\mathbf{U}^{(k)}$ have been revealed [8], a fact that has led us to examine the tables of two-electron and three-electron operators. A comparable number of surprising simplifications have been found to occur [9]. The elementary approach that we used [8] to account for the proportionalities involving the $\mathbf{U}^{(k)}$ (an approach based on commutation techniques that was only partially successful) becomes unwieldly for more complex operators, and it is impossible not to feel that some underlying structure of the f shell needs to be brought into play. Towards this end, we report in this Letter some preliminary results based on a quarklike model of the atomic f shell.

To explain the nature of our quarks, we first introduce the creation and annihilation operators, $a_p^\dagger$ and a_p, for the components p (given by m_s and m_l) of an electron with azimuthal quantum number l. With their aid we can write the components $\theta_m^\dagger$ of four mutually anticommuting quasiparticle tensors $\boldsymbol{\theta}^\dagger$ in the form [10]

$$\begin{aligned}\lambda_m^\dagger &= (\tfrac{1}{2})^{1/2}[a_{1/2,m}^\dagger + (-1)^{l-m} a_{1/2,-m}]\,,\\ \mu_m^\dagger &= (\tfrac{1}{2})^{1/2}[a_{1/2,m}^\dagger - (-1)^{l-m} a_{1/2,-m}]\,,\\ \nu_m^\dagger &= (\tfrac{1}{2})^{1/2}[a_{-1/2,m}^\dagger + (-1)^{l-m} a_{-1/2,-m}]\,,\\ \xi_m^\dagger &= (\tfrac{1}{2})^{1/2}[a_{-1/2,m}^\dagger - (-1)^{l-m} a_{-1/2,-m}]\,.\end{aligned} \tag{1}$$

The four coupled tensors $(\boldsymbol{\theta}^\dagger\boldsymbol{\theta})^{(k)}$ (with odd k) form the generators for $SO_\theta(2l+1)$; their sum yields the generators for the group $SO(2l+1)$ that reduces to the SO(7) of Racah [7] when $l=3$. To embrace all the states of the f shell, four quasiparticle vacua are required, corresponding to either an even or an odd number of electrons in the spin-up and spin-down spaces. The generators of each group $SO_\theta(7)$, when acting on any of the four vacua, produce the eight-dimensional spinor irreducible representation (irrep) $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ of $SO_\theta(7)$, whose angular-momentum structure is $0+3$. The 16384 states of the entire f shell are generated by the quadruple Kronecker product $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})^4$ and two parity labels [10]. As a simple example of how this works, we consider just the spin-up space for an even number of electrons. The Kronecker square $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})^2$ yields (000), (100), (110), and (111), corresponding exactly to Racah's labels for the terms of maximum multiplicity in f^0, f^6, f^2, and f^4, respectively. The L values are just those appearing in $(s+f)^2$, namely, $2S+P+D+3F+G+H+I$.

We propose to consider each spinor $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ as an entity in its own right and to refer to it as a quark, q_θ. Its angular-momentum structure is $s+f$. Like their counterparts in particle physics, the four quarks cannot be separately observed; but this need not diminish their usefulness. We can, for example, consider the mapping from the states of the quark configuration q^4 to the fifteen electronic configurations f^N $(0 \le N \le 14)$. There are four ways of doing this, depending on our choice of parity labels. We can also consider transformations among the eight components of each quark; this leads to the groups $SO_\theta(8)$ and $U_\theta(8)$. If a single quark is taken to span the irreps [1] of $U_\theta(8)$ and (1000) of $SO_\theta(8)$, the generators of $SU_\theta(8)$ can be written as the collection of coupled products $(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(W)}$, where $W=(2000)$ and (1100); the latter constitutes the generators of $\mathrm{SO}_\theta(8)$. By summing over θ, we obtain the generators of SU(8) and SO(8). The connection between these generators and those referring to the f electrons was considered in a slightly different language some years ago by Labarthe [11]. In schematic form, we have

$$(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(1100)(110)} \leftrightarrow (\boldsymbol{\theta}^\dagger \boldsymbol{\theta})^{(110)},$$
$$(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(1100)(100)} \leftrightarrow (\boldsymbol{\theta}^\dagger \boldsymbol{\theta}^\dagger \boldsymbol{\theta}^\dagger \boldsymbol{\theta}\boldsymbol{\theta}\boldsymbol{\theta})^{(100)}, \quad (2)$$
$$(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(2000)(111)} \leftrightarrow (\boldsymbol{\theta}^\dagger \boldsymbol{\theta}^\dagger \boldsymbol{\theta}\boldsymbol{\theta})^{(111)},$$

where the superscripted SO(7) irreps refer to the subgroup $\mathrm{SO}_\theta(7)$ of $\mathrm{SO}_\theta(8)$.

It is here that a new symmetry appears. The group SO(8) exhibits automorphisms, a fact familiar to us today from its importance in several areas of physics [12]. From a mathematical point of view, the automorphisms are associated with the rotational symmetry of the Dynkin diagram for SO(8), which consists of three equal arms springing from a central node. The implications of the associated triality have been discussed by Cartan [13] and Littlewood [14], among others. In addition to the irrep (1000) of SO(8), there are two spinor irreps, $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2})$ and $(\frac{1}{2}\,\frac{1}{2}\,\frac{1}{2}\,-\frac{1}{2})$, that are also of dimension 8 and that we could have chosen to label our quarks. We prefer to cope with this ambiguity by retaining (1000) as our quark label and introducing two alternative SO(7) groups, SO(7)′ and SO(7)″, whose generators of ranks 1 and 5 in SO(3) are unchanged, but whose generators of rank 3, corresponding to the irrep (10) of G_2, are given by

$$-\tfrac{1}{2}(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(1100)(110)(10)} \pm (\tfrac{3}{4})^{1/2}(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(1100)(100)(10)}, \quad (3)$$

corresponding to the irreps (110)′ of SO(7)′ (lower sign) and (110)″ of SO(7)″ (upper sign). With our choice of phases, it is the generators of SO(7)′ rather than SO(7)″ that only involve the f component of the quark (and not the s). The existence of SO(7)′ and SO(7)″ was noticed by Labarthe [11], though he did not relate these groups to the automorphisms of SO(8).

The independence of the four quarks means that all five Young tableaux involving four cells (namely, [1111], [211], [22], [31], and [4]) occur in the U(8) descriptions of the states of q^4. The irreps of SO(8) produced in the decompositions of these tableaux are themselves decomposed into irreps of SO(7) and SO(7)′ in Table I. We see, for example, that spectroscopic terms labeled by (222) in Racah's scheme can occur only in (4000) of SO(8), while those labeled by (211) are mixtures of (2110) and (3100).

The assignment of SO(8) labels to physical operators is rather more intricate. To illustrate our methods, we work towards an explanation for the two unexpected zeros

$$\langle f^7(222)(30)\,^2L|t_i|f^7(221)(31)\,^2L\rangle = 0 \quad (i=2,4), \quad (4)$$

TABLE I. Selected branching rules for SO(8) → SO(7) and SO(8) → SO(7)′.

SO(8)	SO(7)	SO(7)′
(0000)	(000)	(000)′
(1100)	(100)(110)	(100)′(110)′
(1111)	(000)(100)(200)	(111)′
(111−1)	(111)	(111)′
(2000)	(111)	(000)′(100)′(200)′
(2110)	(110)(111)(210) (211)	(110)′(111)′(210)′ (211)′
(2200)	(200)(210)(220)	(200)′(210)′(220)′
(3100)	(211)(221)	(100)′(110)′(200)′ (210)′(300)′(310)′
(4000)	(222)	(000)′(100)′(200)′ (300)′(400)′

which have been found [9] when sifting the computer output of Carnall [6]. Both t_2 and t_4 are three-electron operators, scalar with respect to SO(3); they belong to the SO(7) and G_2 irrep pairs (220)(22) and (222)(40), respectively [15]. Our first step is to show that the effective SO(8) labels are (2200) and (4000). We take t_4 for a detailed study.

The quark operator

$$[(\mathbf{q}_\lambda^\dagger \mathbf{q}_\lambda)(\mathbf{q}_\mu^\dagger \mathbf{q}_\mu)]^{(4000)} + [(\mathbf{q}_\nu^\dagger \mathbf{q}_\nu)(\mathbf{q}_\xi^\dagger \mathbf{q}_\xi)]^{(4000)} \quad (5)$$

must necessarily involve the intermediate couplings $(\mathbf{q}_\theta^\dagger \mathbf{q}_\theta)^{(2000)}$, which, being proportional to some of the generators of $\mathrm{U}_\theta(8)$, correspond to the quasiparticle product $(\boldsymbol{\theta}^\dagger \boldsymbol{\theta}^\dagger \boldsymbol{\theta}\boldsymbol{\theta})^{(111)}$ by the last of Eqs. (2). The triple products $(\boldsymbol{\theta}^\dagger \boldsymbol{\theta}^\dagger \boldsymbol{\theta}^\dagger)^{(111)}$ and $(\boldsymbol{\theta}\boldsymbol{\theta}\boldsymbol{\theta})^{(111)}$ also belong to (2000) of SO(8) because the quasiparticle shell closes at seven members; and, for a resultant (222), the operator

$$[(\boldsymbol{\lambda}^\dagger \boldsymbol{\lambda}^\dagger \boldsymbol{\lambda}^\dagger)^{(111)}(\boldsymbol{\mu}\boldsymbol{\mu}\boldsymbol{\mu})^{(111)}]^{(222)} + [(\boldsymbol{\nu}^\dagger \boldsymbol{\nu}^\dagger \boldsymbol{\nu}^\dagger)^{(111)}(\boldsymbol{\xi}\boldsymbol{\xi}\boldsymbol{\xi})^{(111)}]^{(222)} \quad (6)$$

matches (5) and necessarily belongs to (4000) of SO(8). If we ignore contributions that change electron number, the first part of (6) acts in the spin-up space, and connects the $M_S=\frac{3}{2}$ states of f^3; the second part acts in the spin-down space and connects the $M_S=-\frac{3}{2}$ states of f^3. As such, (6) is a linear superposition of two tensors whose spin ranks are 2 and 0, say $\mathbf{T}^{(2)}+T^{(0)}$. The part $T^{(0)}$ must be proportional to some superposition of the components t_4' and t_4'', whose quasispin ranks are 3 and 1; from Table XVI of Ref. [15] the required combination is found to be simply $t_4'-t_4''$. However, the seniorities of the states in the matrix element (4) are 5 and 7, implying quasispin ranks of 1 and 0. Thus t_4' cannot contribute, and so $T^{(0)}$ is effectively proportional to t_4 itself. Furthermore, $\mathbf{T}^{(2)}$ cannot contribute to the matrix element either, because the spins of the bra and ket are both $\frac{1}{2}$. The upshot is that the contributing part of t_4 is proportional to (6); that is, it has the effective SO(8) label

(4000). Similar arguments can be developed to show that the corresponding label for t_2 is (2200).

We are now ready to account for Eq. (4). From that equation and Table I, the SO(8) and G_2 labels of bra, operator, and ket are (4000)(30) for the bra, (2200)(22) or (4000)(40) for the operator, and (3100)(31) for the ket. Since G_2 is a common subgroup of SO(7) and SO(7)′, we can use the branching rules, as tabulated, for example, by Wybourne [16], to determine the acceptable irreps of SO(7)′ to sandwich between the irreps of SO(8) and G_2 given above. The result is (300)′ for the bra, (220)′ or (400)′ for the operator, and (310)′ for the ket. However, a straightforward calculation reveals that neither (220)′ nor (400)′ occurs in the reduction of the Kronecker product (300)′×(310)′. Thus the vanishing of the matrix elements can be regarded as a direct application of the Wigner-Eckart theorem to the group SO(7)′, that is, to the group whose transformations involve only the f components of our quarks.

Several examples of matrix-element proportionality have been established by methods such as these. We have also embarked on a more ambitious plan in which atomic shell theory is recast in terms of quarks. All the cfp up to q^4 have been calculated, and we have also determined the various mixtures of Racah's states that correspond to pure SO(8) states (a problem we evaded in the analysis above by taking states of peculiar simplicity). The d shell, for which the analogs of SU(8) and SO(8), namely, SU(4) and SO(6), coincide in virtue of the isomorphism SU(4)≡SO(6), is simple and less interesting to treat.

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