Spin-Orbit Matrix Elements in the Atomic f Shell from Automorphisms of SO(8)

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A scrutiny of the matrix elements within the f shell of the spin-other-orbit interaction $H_{\rm soo}$ has revealed many unexpected proportionalities that go beyond an application of the Wigner-Eckart theorem to Racah's groups G_2 and SO(7). An explanation is sought by using the automorphisms of SO(8) by means of which the states of the atomic f shell are generated by two alternative SO(7) bases of the type $(\frac{1}{2}\frac{1}{2}\frac{1}{2})^4$, each augmented by two parity labels. Transformations between the bases can be made by reversing the relative phases of the two angular-momentum states 3 and 0 that comprise any one of the four SO(7) spinors. The method is exemplified by the single-electron spin-orbit interaction $H_{\rm so}$, for which a component can be found that is invariant under the phase reversal. The extension from $H_{\rm so}$ to $H_{\rm soo}$ is described for the component z_6 of $H_{\rm soo}$, and several examples drawn from the comparatively inaccessible configurations near the middle of the f shell are presented.

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The atomic f shell is a source of continuing surprises. Selection rules and proportionalities of blocks of matrix elements often go beyond what would be expected from an application of the Wigner-Eckart theorem to the groups SO(7) and G_2 introduced by Racah [1]. A calculation by Hansen [2] of the matrix elements of the spin-other-orbit interaction $H_{\rm soo}$ for the entire f shell has exposed a large number of unexpected proportionalities, particularly for the components of $H_{\rm soo}$ belonging to the irreducible representation (IR) (30) of G_2. The group labels, which have been known for some time [3], are convenient to work with because contributions to $H_{\rm soo}$ from other sources, such as electrostatically correlated spin-orbit effects (ELSO) [4], can be readily included in spectroscopic analyses. Current work on rare-earth and actinide spectra parametrize $H_{\rm soo}$ with constrained Marvin integrals M^k and ELSO coefficients P^k [5].

Previous experience with the three-electron scalar operators t_i, which can be used to represent the Coulomb interaction between f^N and $f^{N\pm1}l^{\mp1}$, has suggested that the automorphisms of SO(8) may play a key role in understanding the proportionalities. The automorphisms imply the existence of three distinct SO(7) subgroups of SO(8), only one of which is the SO(7) group used by Racah. We refer to the others as SO(7)$'$ and SO(7)$''$. The IRs W' of SO(7)$'$ extend over a different range from the IRs W of SO(7), and a transformation between these two schemes has allowed some of the proportionalities of the t_i matrices to be understood in terms of applications of the Wigner-Eckart theorem to SO(7)$'$ [6]. In contrast, the IRs W'' of SO(7)$''$ extend over the same range as the W, and a recent review has stated that no useful applications have been found for SO(7)$''$ [7]. It is the function of this Letter to show that mere phase changes in going from SO(7) to SO(7)$''$ can determine relations between matrix elements of the spin-orbit type within different configurations f^N and hence supply an explanation for some of the mysterious proportionalities.

The generators of SO(8) can be obtained from those of SO(7) by adjoining sextuple products of creation and annihilation operators for f electrons. However, as recognized by Labarthe [8], it is simpler to introduce four fictitious particles q_θ ($\theta = \lambda, \mu, \nu, \xi$), each belonging to the 8-dimensional IR $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ of SO(7). In other papers, we have called the q_θ quarks because of certain similarities to their namesakes in high-energy physics [7]. The mapping from electrons to the q_θ proceeds in two steps. First, the f electrons are separated into N_A with spin up and N_B with spin down [9], and quasiparticles of the Bogoliubov type [10] are defined by

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

for $-3 \le m \le 3$. Each tensor $\boldsymbol{\theta}^\dagger$ (with components $\theta_m^\dagger$) belongs to the 7-dimensional IR (100) of SO(7). The second step is to make the nonlinear replacements

$$\boldsymbol{\theta}^\dagger = A_\theta(\boldsymbol{q}_\theta^\dagger \boldsymbol{q}_\theta)^{(100)}. \tag{2}$$

The coefficients A_θ, which are of no special concern to us in this Letter, are phase-adjusted Dirac matrices that preserve the anticommutation of the $\boldsymbol{\theta}^\dagger$. Their rows and columns correspond to the four vacua $|0\rangle_{pp'}$, where p and p' are the parities of N_A and N_B [11]. The products $(\boldsymbol{q}_\theta^\dagger \boldsymbol{q}_\theta)^W$ for which $W = (110)$ form the 21 generators of Racah's SO(7) when summed over θ. All we have to do to get the generators of SO(8) is to add the seven operators for which $W = (100)$. The states of the f shell are now represented by

$$\boldsymbol{q}_\lambda^\dagger \boldsymbol{q}_\mu^\dagger \boldsymbol{q}_\nu^\dagger \boldsymbol{q}_\xi^\dagger |0\rangle_{pp'}. \tag{3}$$

The four vacua, taken with the eight components of each $\boldsymbol{q}_\theta^\dagger$, give the 2^{14} states of the configurations f^N ($0 \le N \le 14$).

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The distinction between SO(7) and SO(7)$''$ appears when the reduction SO(7) $\rightarrow$ SO(3) is made. The IR $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ decomposes into the angular momenta 3 and 0, so $q_\theta \rightarrow f_\theta + s_\theta$. The present paper focuses on the consequences of reversing the relative phases of the states f_θ and s_θ. In view of the arbitrary nature of many phases, it may seem surprising that anything useful can accrue from this operation. Nevertheless, the switch has a dramatic effect when expressed in terms of the usual electron model. The generators of Racah's group SO(7) can be written in the new formalism as

$$\sum_\theta (\boldsymbol{f}_\theta^\dagger \boldsymbol{f}_\theta)^{(1)}, \qquad \sum_\theta (\boldsymbol{f}_\theta^\dagger \boldsymbol{f}_\theta)^{(5)}, \tag{4}$$

$$-\tfrac{1}{2}\sum_\theta (\boldsymbol{f}_\theta^\dagger \boldsymbol{f}_\theta)^{(3)} + \sqrt{\tfrac{3}{8}}\sum_\theta [(\boldsymbol{s}_\theta^\dagger \boldsymbol{f}_\theta)^{(3)} - (\boldsymbol{f}_\theta^\dagger \boldsymbol{s}_\theta)^{(3)}]. \tag{5}$$

To get the generators of SO(7)$''$, we have only to make the replacements

$$\boldsymbol{s}_\theta^\dagger \rightarrow -\boldsymbol{s}_\theta^\dagger \quad \text{and} \quad \boldsymbol{s}_\theta \rightarrow -\boldsymbol{s}_\theta\,. \tag{6}$$

In the electron model, the generators of SO(7)$''$ involve sextuple products of annihilation and creation operators and can connect states in distinct f-electron configurations. The tensors (4) are the generators of the exceptional Lie group G_2 used by Racah and are untouched by the phase reversals, so the connected states belong to identical IRs of G_2. The group SO(7)$'$ possesses the generators $\sum_\theta (\boldsymbol{f}_\theta^\dagger \boldsymbol{f}_\theta)^{(k)}$, with $k = 1$, 3, and 5. It is not relevant to the present work and will not be considered further.

If we do not sum over θ in (4) and (5), we get the generators of the SO(7) group for a single q_θ, which we write as $\mathrm{SO}_\theta(7)$. By summing over θ as is done in (4) and (5), we effect the reduction

$$\mathrm{SO}_\lambda(7) \times \mathrm{SO}_\mu(7) \times \mathrm{SO}_\nu(7) \times \mathrm{SO}_\xi(7) \rightarrow \mathrm{SO}(7)\,. \tag{7}$$

Because of the independence of the q_θ, it is not necessary to make phase reversals for all four θ's simultaneously. The replacement $\theta \equiv \xi$ alone leads to $\mathrm{SO}_\xi(7) \rightarrow \mathrm{SO}_\xi(7)''$ but leaves the three other groups in the direct product above unchanged. We shall focus on this single replacement, although it is clear that eight different combinations of replacements are possible, each one of which leads to a distinct form for the generators (5) and thus to a different SO(7) group on the right-hand side of (7).

Under the phase reversal, q_θ becomes q_θ'' and belongs to $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ of $\mathrm{SO}_\theta(7)''$. In both cases, the f shell is generated by $(\frac{1}{2}\frac{1}{2}\frac{1}{2})^4$. Thus, in addition to the usual set of basis states for the f shell, there is another one of exactly the same type, but which can be distinguished from the first by carrying double primes on N, S, and the IRs W of SO(7). No double primes are needed for the IRs U of G_2 or L of $\mathrm{SO}_L(3)$, which are preserved under the phase reversal.

If, then, we are studying an operator H of physical interest that is invariant under the phase reversal (for a particular θ or set of θ's), we have

$$\langle \Psi_a'' | H | \Psi_b'' \rangle = \langle \Psi_a | H | \Psi_b \rangle, \tag{8}$$

where Ψ_a'' and Ψ_b'' are constructed by taking the labels describing Ψ_a and Ψ_b and simply attaching double primes to those that need them. Once Ψ_a'' and Ψ_b'' are expressed as sums over the unprimed states, Eq. (8) becomes a matrix equation comprising as many relations between the unprimed matrix elements as there are cells in the matrix. Many of these relations may be superpositions of others and therefore not useful, but we might hope that others may go beyond what is to be expected from applications of the Wigner-Eckart theorem to G_2 or SO(7).

The transformation between the unprimed and doubly primed states can be worked out by first adding the generators of $\mathrm{SO}_\lambda(7)$, $\mathrm{SO}_\mu(7)$, and $\mathrm{SO}_\nu(7)$ to give the subgroup $\mathrm{SO}_\eta(7)$ of their direct product. It is known that the states of either even or odd N of the f shell span the spinor IR $(\frac{1}{2}\cdots\frac{1}{2}\pm\frac{1}{2})$ of SO(28), and that

$$\mathrm{SO}(28) \supset \mathrm{SO}_T(3) \times \mathrm{SO}_\eta(7) \times \mathrm{SO}_\xi(7)\,, \tag{9}$$

where the generators of $\mathrm{SO}_T(3)$ are the components of $\boldsymbol{T} = \boldsymbol{S} + \boldsymbol{Q}$, the sum of the spin and quasispin [12]. The components of $\boldsymbol{T}$ are given by the SO(7) scalars

$$T_x = -(\boldsymbol{\mu}^\dagger \cdot \boldsymbol{\nu}), \quad T_y = -i(\boldsymbol{\nu}^\dagger \cdot \boldsymbol{\lambda}), \quad T_z = (\boldsymbol{\lambda}^\dagger \cdot \boldsymbol{\mu}) \tag{10}$$

and do not involve $\boldsymbol{\xi}^\dagger$ at all. The branching runs

$$\begin{aligned}(\tfrac{1}{2}\cdots\tfrac{1}{2}\pm\tfrac{1}{2}) \rightarrow\ & (\tfrac{1}{2}) \times (\tfrac{3}{2}\tfrac{3}{2}\tfrac{3}{2}) \times (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) + (\tfrac{3}{2}) \\ & \times (\tfrac{3}{2}\tfrac{3}{2}\tfrac{1}{2}) \times (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) + (\tfrac{5}{2}) \times (\tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2}) \\ & \times (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) + (\tfrac{7}{2}) \times (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) \times (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2})\end{aligned}$$

with dimension check

$$\begin{aligned}2^{13} = {} & 2 \times 112 \times 8 + 4 \times 112 \times 8 + 6 \times 48 \times 8 \\ & + 8 \times 8 \times 8\,.\end{aligned}$$

This indicates that the IRs W_T of $\mathrm{SO}_\eta(7)$ are uniquely tied to the quantum numbers T. Consider any state within the f shell in the basis

$$|(QS)TM_T\Psi\rangle = |(QS)TM_T WU\tau LM_L\rangle, \tag{11}$$

where τ distinguishes duplicated L values in a given U. Its expansion in terms of the states in which q_ξ is separated out is given by the isoscalar factor

$$(W_T U_1 + (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2})U_2 \,|\, WU) \tag{12}$$

in the notation of Racah [1]. These isoscalars are known [11]. As an example, the factors for which $U = (21)$, $T = \frac{3}{2}$, and $W_T = (\frac{3}{2}\frac{3}{2}\frac{1}{2})$ are collected in Table I.

The next step is to reverse the phase for s_ξ as in (6) with $\theta = \xi$. This is done for the example in hand by reversing the signs of the coefficients in the column headed (21) + (00) in Table I. At the same time, double primes are added to the IRs W in the first column. The multiplicities $2S + 1$ and $2Q + 1$ are abbreviated to $[S]$ and $[Q]$. We now regard Table I and its converted form as two orthogonal

TABLE I. The isoscalars (12) for $U = (21)$ and $T = \frac{3}{2}$. The prefixed multiplicities $[K]$ stand for $2K + 1$.

$^{([Q][S])[T]}WU$	$(21) + (00)$	$(11) + (10)$	$(20) + (10)$	$(21) + (10)$
$^{(25)4}(210)\,(21)$	$\frac{\sqrt{5}}{4\sqrt{2}}$	$-\frac{\sqrt{3}}{4\sqrt{2}}$	$\frac{\sqrt{3}}{4\sqrt{14}}$	$-\frac{\sqrt{165}}{4\sqrt{14}}$
$^{(43)4}(211)\,(21)$	$\frac{\sqrt{5}}{4}$	$-\frac{1}{4\sqrt{3}}$	$\frac{13}{4\sqrt{21}}$	$\frac{\sqrt{55}}{4\sqrt{21}}$
$^{(41)4}(220)\,(21)$	$\frac{\sqrt{3}}{4}$	$-\frac{\sqrt{5}}{4}$	$-\frac{3\sqrt{5}}{4\sqrt{7}}$	$\frac{\sqrt{11}}{4\sqrt{7}}$
$^{(23)4}(221)\,(21)$	$-\frac{\sqrt{11}}{4\sqrt{2}}$	$-\frac{\sqrt{55}}{4\sqrt{6}}$	$\frac{\sqrt{55}}{4\sqrt{42}}$	$\frac{1}{4\sqrt{42}}$

matrices B and B'' connected by the transformation

$$B'' = (B'' \cdot B^t) \cdot B = M \cdot B\,, \tag{13}$$

where t indicates a transposition. It turns out that

$$M = \begin{bmatrix} \frac{11}{16} & -\frac{5\sqrt{2}}{16} & -\frac{\sqrt{30}}{16} & \frac{\sqrt{55}}{16} \\ -\frac{5\sqrt{2}}{16} & \frac{3}{8} & -\frac{\sqrt{15}}{8} & \frac{\sqrt{110}}{16} \\ -\frac{\sqrt{30}}{16} & -\frac{\sqrt{15}}{8} & \frac{5}{8} & \frac{\sqrt{66}}{16} \\ \frac{\sqrt{55}}{16} & \frac{\sqrt{110}}{16} & \frac{\sqrt{66}}{16} & \frac{5}{16} \end{bmatrix}. \tag{14}$$

Notice that $M^2 = M \cdot M^t = 1$ as expected. This gives the required transformation matrix for the states in the first column of Table I.

We now turn to the problem of expressing our physical operators in terms of operators satisfying (8). The vector $\boldsymbol{T}$ is again useful. The operator $\boldsymbol{\xi}^\dagger$, given in the last of Eqs. (1), is a scalar with respect to $\boldsymbol{T}$; suppressing the IR (100), we write $\boldsymbol{\xi}^\dagger = \boldsymbol{a}^{(0)}$. By coupling the spin and quasispin ranks of $\frac{1}{2}$ to 1, the other $\boldsymbol{\theta}^\dagger$'s appear as the three components of $\boldsymbol{a}^{(1)}$. All combinations of the vector $\boldsymbol{a}^{(1)}$ are devoid of $\boldsymbol{\xi}^\dagger$ and thus invariant with respect to phase changes for s_ξ. For single-electron operators like $H_{\rm so}$, we need to know the W and T assignments that occur in the various products $\boldsymbol{a}^{(t)}\boldsymbol{a}^{(t')}$. They can easily be found from the fermionic nature of the $\boldsymbol{a}^{(t)}$, and are set out (with T specified by the prefixed multiplicity $[T] = 2T + 1$) in Table II. Although the operators in this table do not conserve electron number, all those that overlap the characterizations (S, Q, W) of $H_{\rm so}$, namely, $\mathbf{(}1, 1, (110)\mathbf{)}$, are potential contributors. There is only one operator $H^{(QS)T}$ of the type $H^{(11)2}$, and, being formed from $\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)}$, is an invariant under s_ξ phase reversals. There are, however, two of the type $H^{(11)0}$, and we might anticipate having to form an appropriate linear combination of $\boldsymbol{a}^{(0)}\boldsymbol{a}^{(0)}$ with $(\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)})^{(0)}$ to satisfy $S = Q = 1$. However, $\boldsymbol{a}^{(0)}\boldsymbol{a}^{(0)} \sim \boldsymbol{\xi}^\dagger\boldsymbol{\xi}$, and the condition that the overall orbital rank be 1, as it is for $H_{\rm so}$, excludes any s_ξ term, just as it does in the first of Eqs. (4). We can conclude that we have two invariants we can use for $H_{\rm so}$, namely, $H^{(11)0}$ and $H^{(11)2}$.

The operators of the type $H^{(QS)T}$ do not, in general, conserve electron number. However, this is immaterial. We may calculate them in the basis (11) by means of the equation

$$\mathbf{(}(Q'S')T'\Psi'\|H^{(QS)T}\|(\overline{Q}\,\overline{S})\overline{T}\,\overline{\Psi}\mathbf{)} = \{[T'][T][\overline{T}]\}^{1/2}(Q'S'\Psi'\|H^{(QS)}\|\overline{Q}\,\overline{S}\,\overline{\Psi})\begin{Bmatrix} Q' & Q & \overline{Q} \\ S' & S & \overline{S} \\ T' & T & \overline{T} \end{Bmatrix}, \tag{15}$$

where the matrix element (a_i, say) preceding the 9-j symbol is reduced with respect to both $\boldsymbol{Q}$ and $\boldsymbol{S}$. We write the unknown values of a_i for the four states $^{[Q][S]}W$ of Table I as the matrix

$$A = \begin{bmatrix} a_1 & a_4 & 0 & a_5 \\ a_4 & a_2 & a_6 & a_7 \\ 0 & -a_6 & 0 & a_8 \\ -a_5 & -a_7 & a_8 & a_3 \end{bmatrix}. \tag{16}$$

The zeros above are due to the spin selection rules. The entries of A are now multiplied by the 9-j symbol and $\{[T'][T][\overline{T}]\}^{1/2}$ to give a new matrix $E^{(T)}$. We insist that $E^{(T)} = M \cdot E^{(T)} \cdot M^t$ for our two possibilities $T = 0, 2$. Solving the two matrix equations simultaneously, we get

$$\begin{aligned} a_1 &= -\tfrac{3}{2}a_6, \qquad a_5 = \tfrac{\sqrt{3}}{2\sqrt{11}}(\sqrt{2}\,a_2 - a_6)\,, \\ a_3 &= \tfrac{\sqrt{5}}{22}(2\sqrt{2}\,a_2 + 9a_6)\,, \\ a_7 &= \tfrac{-1}{2\sqrt{110}}(7a_2 - 9\sqrt{2}\,a_6)\,, \\ a_4 &= \tfrac{\sqrt{3}}{2\sqrt{2}}(a_2 + \sqrt{2}\,a_6), \qquad a_8 = \tfrac{-1}{2\sqrt{55}}(9a_2 + \sqrt{2}\,a_6)\,. \end{aligned} \tag{17}$$

These equations are valid for any component of the IR (110) appropriate to $H_{\rm so}$. In particular, they hold for the component for which $UL \equiv (11)1$. Since the IR (11) of G_2 occurs twice in the Kronecker product $(21)^2$ [13], a simple proportionality between matrix elements is not expected; indeed, Eqs. (17) express six of the a_i in terms of the two others, a_2 and a_6. However, the first equation gives a direct proportionality. When converted to a relation involving the classic double tensor $V^{(11)}$ of Racah [14], where the superscripts now refer to spin and orbital ranks,

TABLE II. Classification of one-body operators in two different group schemes.

Operator	$\mathrm{SO}(21) \times \mathrm{SO}_\xi(7)$	$^{[T]}W$
$\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)}$	$(110^8) \times (000)$	$^1(110)\,^3(000)\,^3(200)\,^5(110)$
$\boldsymbol{a}^{(0)}\boldsymbol{a}^{(0)}$	$(0^{10}) \times (110)$	$^1(110)$
$\boldsymbol{a}^{(1)}\boldsymbol{a}^{(0)}$	$(10^9) \times (100)$	$^3(000)\,^3(110)\,^3(200)$

it becomes

$$(f^6(210)\,(21)^5L\|V^{(11)}\|f^6(210)\,(21)^5L') = -\sqrt{\tfrac{5}{2}}\,(f^4(211)\,(21)^3L\|V^{(11)}\|f^4(220)\,(21)^1L') \tag{18}$$

for all L and L'. In getting this result, which goes beyond what the Wigner-Eckart theorem would predict when applied to G_2, we chose M_Q values appropriate for each f^N according to the relation $N = 2M_Q + 7$ [15]. It should be noted that Eq. (18) differs (by a sign) from what the tables of Nielson and Koster [16] would give. Phase differences of this kind come from the different choices inherent in the formalism (3) and the electron model.

The above analysis is easily extended to deal with two-electron operators. As an example, we choose the component z_6 of $H_{\rm soo}$ with group labels $(Q, S, L, W, U) = (2, 1, 1, (211), (30))$ [3]. An obvious s_ξ invariant is the form $(\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)})^{(T)}$. Being symmetric with respect to an S-Q interchange, it can produce combinations of the operators $H^{(QS)T}$ such as $H^{(21)3} + H^{(12)3}$ and $H^{(21)2} - H^{(12)2}$. Arguments similar to those that showed $H^{(11)0}$ is an invariant for $H_{\rm so}$ indicate that $(\boldsymbol{a}^{(1)}\boldsymbol{a}^{(1)}\boldsymbol{a}^{(0)}\boldsymbol{a}^{(0)})^{(2)}$ (the only other possible contributor to $H^{(21)2} - H^{(12)2}$) is also an s_ξ phase invariant for $WU = (211)\,(30)$. Equation (15) can now be used for $H^{(21)T} \pm H^{(12)T}$ with $T = 3$ and 2. The matrix element on the right becomes

$$A = \begin{bmatrix} 0 & a_4 & 0 & 0 \\ a_4 & a_2 & a_7 & a_8 \\ 0 & -a_7 & 0 & a_9 \\ 0 & -a_8 & a_9 & 0 \end{bmatrix} \pm \begin{bmatrix} \overline{a}_1 & \overline{a}_4 & \overline{a}_5 & \overline{a}_6 \\ \overline{a}_4 & \overline{a}_2 & 0 & \overline{a}_8 \\ -\overline{a}_5 & 0 & 0 & 0 \\ -\overline{a}_6 & -\overline{a}_8 & 0 & \overline{a}_3 \end{bmatrix} \tag{19}$$

instead of (16), where the bars refer to the matrix elements of the unwanted operator $H^{(12)T}$. Fortunately, these matrix elements can be converted to those of $H^{(21)T}$ by means of the spin-quasispin interchange. This entails a parity change in the electron number N [12]. Invariance under (14) results in relations similar to those in (17); two of them are $\overline{a}_1 = \sqrt{77}\,\overline{a}_6$ and $\overline{a}_5 = -\sqrt{\frac{2}{5}}\,a_4$. They lead to analogs of (18):

$$(f^3(210)\,(21)^2L\|z_6\|f^3(210)\,(21)^2L') = -\sqrt{44}\,(f^5(210)\,(21)^2L\|z_6\|f^5(221)\,(21)^2L'), \tag{20}$$

$$(f^7(210)\,(21)^2L\|z_6\|f^7(220)\,(21)^4L') = -\tfrac{2}{\sqrt{5}}(f^6(210)\,(21)^5L\|z_6\|f^6(211)\,(21)^3L'). \tag{21}$$

We can also start with states belonging to different IRs of G_2. As examples, we cite the simple proportionalities

$$(f^5(210)\,(21)^2L\|z_6\|f^5(221)\,(31)^2L') = \tfrac{3}{\sqrt{2}}(f^6(220)\,(21)^1L\|z_6\|f^6(221)\,(31)^3L'), \tag{22}$$

$$(f^7(210)\,(21)^2L\|z_6\|f^7(222)\,(40)^2L') = -\sqrt{6}\,(f^6(211)\,(21)^3L\|z_6\|f^6(222)\,(40)^1L'), \tag{23}$$

$$(f^4(211)\,(30)^3L\|z_6\|f^4(220)\,(22)^1L') = -\sqrt{2}\,(f^6(221)\,(30)^3L\|z_6\|f^6(220)\,(22)^1L'). \tag{24}$$

Equations (20)–(24) go beyond the Wigner-Eckart theorem for G_2 since, in all cases, the product of the G_2 IRs in the bra and ket contain (30) of z_6 at least twice. Preliminary work with other components of $H_{\rm soo}$ yield results of a similar kind. They are consequences of the s_ξ phase reversals and demonstrate very effectively the relevance and power of the automorphisms of SO(8).

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