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Complementary groups in the quark model of the atom

B R Judd and G M S Lister

Henry A Rowland Department of Physics and Astronomy, The Johns Hopkins University,
Baltimore, MD 21218, USA

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Abstract. The quark model of the atom is studied with particular regard to its complementary groups. For an atomic l shell, we find that the group complementary to the basic quark group $U(2^l)$ is isomorphic to the double group of the tesseract, W_4^*. Character tables for W_4^* and its subgroup SW_4^* are provided. When $l=3$, the extra symmetry afforded by the automorphisms of SO(8) shows up by providing two further complementary groups. The group $SO_Q(3)''\times SO_S(3)''$ is complementary to $SO(7)''$ and the group W_4', also isomorphic to the group of the tesseract, is complementary to $SU(7)'$. The quark states of the f shell are calculated by diagonalizing a suitably chosen W_4^* scalar operator, and the generalization to the g shell is discussed.

1. Introduction

The concept of atomic quarks introduced recently [1–3] has proved to be a valuable tool in understanding the subtleties of the atomic f shell. The idea is that states of an atomic l shell may be constructed by coupling together just four objects (quarks), each quark belonging to the 2^l-dimensional spinor irreducible representation (irrep) of $SO(2l+1)$. Two parity labels are needed to complete the construction. Having introduced the quark it is natural to consider transformations among its 2^l components, leading us to study the group $U(2^l)$ and its subgroups. Depending on the nature of the quark angular momentum we can introduce the groups $SO(2^l)$ (for integral quark angular momentum), $Sp(2^l)$ (half-integral quark angular momentum) and $SO(2l+2)$. The group schemes for integral (half-integral) quark angular momentum are

$$\begin{aligned} &U(2^l)\supset SO(2^l)(Sp(2^l))\supset SO(2l+1)\\ &U(2^l)\supset SO(2l+2)\supset SO(2l+1). \end{aligned}\tag{1}$$

When we put $l=3$ in equations (1) we have that $2^l=2l+2=8$ and the two schemes are identical. In the first scheme the 8-dimensional irrep [1] of U(8) is associated with the 8-dimensional irrep (1000) of SO(8), while in the second it is associated with the 8-dimensional spinor irrep $(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2})$. Clearly, these two irreps must be equivalent, and indeed we have here an example of the automorphisms exhibited by SO(8). These automorphisms may be visualized as permutations of the three arms of the Dynkin diagram for SO(8) that leave it invariant [4].

In our analysis of the f shell we have used the automorphisms of SO(8) in a slightly different manner from that indicated above. We prefer to reserve the irrep (1000) of SO(8) for a single quark, and to indicate the automorphisms in the form of three alternatives for X in the reduction $SO(8)\supset X\supset G_2$, where G_2 is Cartan's exceptional

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group. The group X can be the SO(7) introduced by Racah [5] or one of the two SO(7)s first introduced by Labarthe [6] in connection with atomic quasiparticles. We indicate the latter by SO(7)′ and SO(7)″. The generators for the three SO(7) groups have been described elsewhere in detail, both in terms of quasiparticles [3] and in terms of quarks [7]. A single quark has the angular momentum structure $s+f$ and can be thought of as deriving from $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ of SO(7), $(100)'+(000)'$ of SO(7)′, or $(\frac{1}{2}\frac{1}{2}\frac{1}{2})''$ of SO(7)″.

An aspect of the atomic-quark model not yet studied concerns the nature of its complementary groups. The idea of the complementary group was introduced by Moshinsky and Quesne [8] and, in those cases where such a group exists, gives us an alternative, yet equivalent, way of characterizing the states of a system. Atomic physicists have used the complementarity of $\mathrm{SO}(2l+1)$ to $\mathrm{SO}_Q(3)\times\mathrm{SO}_S(3)$, where the latter is the product of rotation groups in the quasispin and spin spaces, to yield relations between the matrix elements of operators with well-defined spin and quasispin ranks. The idea has been explored in a broader context in nuclear physics [9]. Le Blanc and Rowe [10] have indicated how the principle of complementarity is related to a technique of Biedenharn *et al* [11] introduced to resolve the outer multiplicity problem for SU(3). Several authors have used the idea of a dual basis to calculate recoupling coefficients for a group by invoking the properties of its complementary group [12–14].

In this paper we discuss the idea of the complementary group as it applies to the quark model of the atom. Because of the rich structure in the atomic f shell associated with the automorphisms of SO(8), new possibilities arise for further complementary group structure. We find several new cases, two of which are based on the group of the tesseract (the 4-dimensional cube) and one of which is of use in simplifying construction of the quark states.

2. Generators

The atomic quasiparticles θ are introduced through the defining relation

$$\theta^{\dagger}_{m}=(\tfrac{1}{2})^{1/2}[a^{\dagger}_{m_s m_l}+(-1)^{b+l-m_l}a_{m_s-m_l}] \tag{2}$$

where $a^{\dagger}(a)$ are creation (annihilation) operators for the electrons with m_s and m_l values indicated by subscripts [15]. The pairs $(m_s,b)=(\frac{1}{2},0)$, $(\frac{1}{2},-1)$, $(-\frac{1}{2},0)$ and $(-\frac{1}{2},-1)$ serve to define the four possibilities λ, μ, ν and ξ for θ. We note that the tensors $\boldsymbol{\theta}$ obey the relations $\boldsymbol{\lambda}^{\dagger}=\boldsymbol{\lambda}$, $\boldsymbol{\mu}^{\dagger}=-\boldsymbol{\mu}$, $\boldsymbol{\nu}^{\dagger}=\boldsymbol{\nu}$ and $\boldsymbol{\xi}^{\dagger}=-\boldsymbol{\xi}$.

The coupled tensors $(\boldsymbol{\theta}^{\dagger}\boldsymbol{\theta})^{(k)}$, for k odd, form the generators of the group $\mathrm{SO}_\theta(2l+1)$. Summing over θ, we obtain the generators of Racah's $\mathrm{SO}(2l+1)$ [5] which is the group familiar to us from classical atomic spectroscopy. However, many more groups can be obtained by forming products of more than two $\boldsymbol{\theta}$s. For f electrons we consider $\boldsymbol{\theta}^n$ for $n=0$, 2, 4 and 6 and assign SO(7) irreps to the products to obtain

$$(\boldsymbol{\theta}^0)^{(000)},(\boldsymbol{\theta}^2)^{(110)},(\boldsymbol{\theta}^4)^{(111)},(\boldsymbol{\theta}^6)^{(100)}. \tag{3}$$

The whole collection comprises 64 operators and forms the generators of $\mathrm{U}_\theta(8)$. Taken together, the operators $(\boldsymbol{\theta}^2)^{(110)}$ and $(\boldsymbol{\theta}^6)^{(100)}$ form the generators for $\mathrm{SO}_\theta(8)$ and $(\boldsymbol{\theta}^2)^{(110)}$ are the $\mathrm{SO}_\theta(7)$ generators. When summing over θ to obtain groups relevant to the entire f shell, we must remember to include the θ dependent phase $\varepsilon^{n/2}$, where $\varepsilon=1$, -1, 1, and -1 for $\theta=\lambda$, μ, ν, and ξ respectively. The need for this phase arises because we chose to write $\boldsymbol{\theta}^n$ rather than $(\boldsymbol{\theta}^{\dagger})^{n/2}\boldsymbol{\theta}^{n/2}$ for the terms in the sequence (3).

2.1. *Spin and quasispin structure*

The operators $(\boldsymbol{\theta}^2)^{(110)}$ can connect f-electron states that are diagonal in electron number as well as states differing by two electrons. The situation for $(\boldsymbol{\theta}^4)^{(111)}$ and $(\boldsymbol{\theta}^6)^{(100)}$ is similar in that these operators have parts that change particle number N by 0, ±2, ±4 and 0, ±2, ±4, ±6 respectively. However, when summed over θ with the appropriate phase factor, those parts changing N by ±2 and ±6 disappear. In the language of quasispin, we say that the group generators can change the z-component of Q by $\Delta M_Q = 0, \pm 2$. A precisely similar situation arises with regard to the z-component of S, that is $\Delta M_S = 0, \pm 2$. It turns out that ΔM_Q and ΔM_S are not entirely independent of each other and the pairs $(\Delta M_Q, \Delta M_S) = (0, \pm 2)$ and $(\pm 2, 0)$ are not allowed. Labarthe has discussed this aspect of multiple products of quasiparticles [6].

The duality between spin and quasispin is no accident since, under closer examination, the generators of U(8) are found to be invariant under spin-quasispin interchange. The possible values for the spin (κ) and quasispin (K) ranks for the operators in equation (3) can be found by referring to Flowers' tables of charge-spin supermultiplets [16]. For example, for $(\boldsymbol{\theta}^4)^{(111)}$ we see that $(K\kappa) = (00)$, (11) and (22). However, when summed over θ we find that all of the possible $(K\kappa)$ pairs no longer appear. Just which of the possible values are present must be determined by direct calculation and it turns out that the U(8) generators have the following mixtures of $(K\kappa)$ values:

$$\begin{aligned}
&\textstyle\sum'(\boldsymbol{\theta}^0)^{(000)}\text{: } (00)\\
&\textstyle\sum'(\boldsymbol{\theta}^2)^{(110)}\text{: } (00)\\
&\textstyle\sum'(\boldsymbol{\theta}^4)^{(111)}\text{: } (00), (22)\\
&\textstyle\sum'(\boldsymbol{\theta}^6)^{(100)}\text{: } (00), (22), (33)
\end{aligned} \tag{4}$$

where the primes on the summations indicate that the appropriate phase factors $\varepsilon^{n/2}$ have been included.

3. $\mathbf{W_4}$ and its double group $\mathbf{W_4^*}$

The generators of U(8) are not only invariant under spin–quasispin interchange; the operations of particle-hole conjugation and spin (or quasispin) reversal also leave them invariant. In order to discuss further symmetries we introduce some notation. We adopt the symbol $\{abcd\}$ to represent the following permutation of the basic quasiparticles; $\lambda \to a$, $\mu \to b$, $\nu \to c$ and $\xi \to d$, where a, b, c or d may be another quasiparticle or a phase times a quasiparticle. It is straightforward to show that the operations of spin-quasispin interchange, particle-hole conjugation and spin-up and spin-down interchange are given by the following permutations: $\{\lambda\ \mu\ \nu\ {-\xi}\}$, $\{\nu\ {-\xi}\ {-\lambda}\ \mu\}$ and $\{\nu\ \xi\ \lambda\ \mu\}$.

We can see from equations (4) that permutations of the quasiparticles are good candidates for operations that leave invariant the U(8) generators, and the generators of its subgroups. We must be careful, however, to ensure that permutations of the quasiparticles yield permutations for their adjoints that preserve the basic anticommutation relations, and we are forced to consider permutations such as $\{-\lambda\ \mathrm{i}\nu\ \mathrm{i}\xi\ \mu\}$, where $\mathrm{i} = \sqrt{-1}$. Under this permutation, the relations

$$[\theta_m^\dagger, \theta_{m'}]_+ = (-1)^{l-m+b}[\theta_{-m}, \theta_{m'}]_+ = \delta(m, m')$$

remain unchanged, since the factors i^2 entering when the substitutions $\mu \rightarrow i\nu$ and $\nu \rightarrow i\xi$ are made exactly compensate the factors $(-1)^b$ that differ for the pairs (μ, ν) and (ν, ξ). At the same time, the $SO(7)$ generator

$$(\boldsymbol{\lambda\lambda})^{(k)} - (\boldsymbol{\mu\mu})^{(k)} + (\boldsymbol{\nu\nu})^{(k)} - (\boldsymbol{\xi\xi})^{(k)} \qquad \text{(for } k \text{ odd)} \tag{5}$$

becomes

$$(\boldsymbol{\lambda\lambda})^{(k)} - (\mathrm{i})^2(\boldsymbol{\nu\nu})^{(k)} + (\mathrm{i})^2(\boldsymbol{\xi\xi})^{(k)} - (\boldsymbol{\mu\mu})^{(k)}$$

and is thus left invariant. That this permutation leaves the remaining U(8) generators invariant follows directly from equations (4). From this simple example it is not difficult to see that any permutation $\{\varepsilon_1\lambda\ \varepsilon_2 i\nu\ \varepsilon_3 i\xi\ \varepsilon_4\mu\}$, where ε_i can be ± 1, will reproduce the required result. For a fixed choice of ε s, there are 24 permutations which close under multiplication (by multiplication, we mean the usual rule for a product of permutations) to give the group S_4, the permutation group on four objects. Allowing each ε to be ± 1 independently, we find that the $2^4 \times 24 = 384$ operations again close under multiplication and form a group isomorphic to the symmetry group of the tesseract [17]. We use the symbol W_4 to denote this group although it has many different names throughout the literature [18–21].

The 4-dimensional (irreducible) representation of W_4 that we have just described is not the most convenient for use with our U(8) group because there is no simple connection with the spin and quasispin. We can generate a 6-dimensional (irreducible) representation by considering the action of our basic permutations on the components of the spin and quasispin vectors:

$$\begin{aligned} S_x &= \tfrac{1}{2}(2l+1)^{1/2}[(\boldsymbol{\lambda\xi})^{(0)} - (\boldsymbol{\mu\nu})^{(0)}] \\ S_y &= \tfrac{1}{2}(2l+1)^{1/2}[\mathrm{i}(\boldsymbol{\mu\xi})^{(0)} - \mathrm{i}(\boldsymbol{\lambda\nu})^{(0)}] \\ S_z &= \tfrac{1}{2}(2l+1)^{1/2}[(\boldsymbol{\lambda\mu})^{(0)} - (\boldsymbol{\nu\xi})^{(0)}] \end{aligned} \tag{6}$$

and

$$\begin{aligned} Q_x &= \tfrac{1}{2}(2l+1)^{1/2}[-(\boldsymbol{\lambda\xi})^{(0)} - (\boldsymbol{\mu\nu})^{(0)}] \\ Q_y &= \tfrac{1}{2}(2l+1)^{1/2}[-\mathrm{i}(\boldsymbol{\mu\xi})^{(0)} - \mathrm{i}(\boldsymbol{\lambda\nu})^{(0)}] \\ Q_z &= \tfrac{1}{2}(2l+1)^{1/2}[(\boldsymbol{\lambda\mu})^{(0)} + (\boldsymbol{\nu\xi})^{(0)}]. \end{aligned} \tag{7}$$

Permutations of the θs induce permutations among the components of $\boldsymbol{S}$ and $\boldsymbol{Q}$, and we denote the permutation $S_x \rightarrow a$, $S_y \rightarrow b$, $S_z \rightarrow c$, $Q_x \rightarrow d$, $Q_y \rightarrow e$ and $Q_z \rightarrow f$ by the symbol $\{abcdef\}$. In table 1 we list representative permutations for the 4- and 6-dimensional irreps considered above; one for each class of W_4. Also listed in table 1 are the number of elements in each class. Our classes are ordered in the the same way as those listed by Littlewood [19].

The characters for this group have been worked out by several authors [18–21]. A glance at Littlewood's character table [19] indicates that this group is itself a double group; a result that we might have anticipated since the basic quasiparticles belong to the irrep $D_{1/2} \times D_{1/2}$ of $SO_Q(3) \times SO_S(3)$. The single-valued representations have bases with integral spin and quasispin. When we consider the effect of W_4 transformations on basis states with integral spin and half integral quasispin, we find that we need to go to its double group W_4^* in order to correctly classify these states. To proceed further we construct a 4-dimensional representation in the basis given by the direct sum of states with $S=0$, $Q=\tfrac{1}{2}$ and $S=\tfrac{1}{2}$, $Q=0$. The matrices of this representation are determined by noting that the permutations listed in table 1 for the 6-dimensional

Table 1. Listing of the classes of the groups W_4 and W_4'. The number of elements in a class is listed under the heading D; columns 3 and 4 contain representative group elements for each class for the permutations of the quasiparticles (column 3) and for the components of S and Q (column 4). Column 5 contains a representative group element for each of the classes of the group W_4'. The classes are listed in the same order as those of Littlewood [19].

Class	D	$\{a\,b\,c\,d\}$	$\{a'\,b'\,c'\,d'\,e'\,f'\}$	$\{\bar{a}\,\bar{b}\,\bar{c}\,\bar{d}\}$
1	1	$\{\lambda\,\mu\,\nu\,\xi\}$	$\{S_x\,S_y\,S_z\,Q_x\,Q_y\,Q_z\}$	$\{\lambda\,\mu\,\nu\,\xi\}$
2	4	$\{\lambda\,\mu\,\nu\,-\xi\}$	$\{Q_x\,Q_y\,Q_z\,S_x\,S_y\,S_z\}$	$\{\lambda\,\mu\,\nu\,\xi''\}$
3	12	$\{\lambda\,-\xi\,\nu\,\mu\}$	$\{S_z\,S_y\,-S_x\,-Q_z\,Q_y\,Q_x\}$	$\{\lambda\,-\xi\,\nu\,-\mu''\}$
4	12	$\{\lambda\,\xi\,\nu\,\mu\}$	$\{Q_z\,Q_y\,-Q_x\,-S_z\,S_y\,S_x\}$	$\{\lambda\,-\xi''\,\nu\,-\mu''\}$
5	6	$\{\lambda\,\mu\,-\nu\,-\xi\}$	$\{-S_x\,-S_y\,S_z\,-Q_x\,-Q_y\,Q_z\}$	$\{\lambda\,\mu\,\nu''\,\xi''\}$
6	32	$\{\lambda\,\mathrm{i}\nu\,\mathrm{i}\xi\,\mu\}$	$\{Q_z\,-Q_x\,-Q_y\,-S_z\,S_x\,-S_y\}$	$\{\lambda\,\mathrm{i}\nu\,\mathrm{i}\xi\,-\mu''\}$
7	24	$\{\lambda\,-\mu\,\mathrm{i}\xi\,\mathrm{i}\nu\}$	$\{-Q_y\,-Q_x\,-Q_z\,S_y\,S_x\,-S_z\}$	$\{\lambda\,\mu''\,\mathrm{i}\xi\,-\mathrm{i}\nu''\}$
8	24	$\{\lambda\,-\mu\,\mathrm{i}\xi\,-\mathrm{i}\nu\}$	$\{S_y\,S_x\,-S_z\,-Q_y\,-Q_x\,-Q_z\}$	$\{\lambda\,\mu''\,\mathrm{i}\xi\,-\mathrm{i}\nu\}$
9	4	$\{-\lambda\,-\mu\,-\nu\,\xi\}$	$\{Q_x\,Q_y\,Q_z\,S_x\,S_y\,S_z\}$	$\{\lambda''\,\mu''\,\nu''\,\xi\}$
10	32	$\{\lambda\,-\mathrm{i}\nu\,\mathrm{i}\xi\,\mu\}$	$\{S_z\,S_x\,S_y\,-Q_z\,-Q_x\,Q_y\}$	$\{\lambda\,\mathrm{i}\nu''\,\mathrm{i}\xi\,-\mu''\}$
11	48	$\{-\mathrm{i}\mu\,\mathrm{i}\nu\,\mathrm{i}\xi\,\mathrm{i}\lambda\}$	$\{-S_z\,-S_y\,-S_x\,Q_z\,Q_y\,-Q_x\}$	$\{\mathrm{i}\mu''\,\mathrm{i}\nu\,\mathrm{i}\xi\,\mathrm{i}\lambda\}$
12	48	$\{\mathrm{i}\mu\,\mathrm{i}\nu\,\mathrm{i}\xi\,\mathrm{i}\lambda\}$	$\{Q_z\,-Q_y\,Q_x\,-S_z\,S_y\,S_x\}$	$\{\mathrm{i}\mu\,\mathrm{i}\nu\,\mathrm{i}\xi\,\mathrm{i}\lambda\}$
13	12	$\{-\nu\,-\xi\,\lambda\,\mu\}$	$\{-S_x\,S_y\,-S_z\,Q_x\,Q_y\,Q_z\}$	$\{-\nu\,-\xi\,-\lambda''\,-\mu''\}$
14	24	$\{-\nu\,\xi\,\lambda\,\mu\}$	$\{-Q_x\,Q_y\,-Q_z\,S_x\,S_y\,S_z\}$	$\{-\nu\,-\xi''\,-\lambda''\,-\mu''\}$
15	12	$\{-\lambda\,-\xi\,-\nu\,\mu\}$	$\{-S_z\,S_y\,S_x\,Q_z\,Q_y\,-Q_x\}$	$\{\lambda''\,-\xi\,\nu''\,-\mu''\}$
16	32	$\{-\lambda\,\mathrm{i}\nu\,\mathrm{i}\xi\,\mu\}$	$\{-S_z\,-S_x\,S_y\,Q_z\,Q_x\,Q_y\}$	$\{\lambda''\,\mathrm{i}\nu\,\mathrm{i}\xi\,-\mu''\}$
17	32	$\{-\lambda\,-\mathrm{i}\nu\,\mathrm{i}\xi\,\mu\}$	$\{-Q_z\,Q_x\,-Q_y\,S_z\,-S_x\,-S_y\}$	$\{\lambda''\,\mathrm{i}\nu''\,\mathrm{i}\xi\,-\mu''\}$
18	12	$\{-\lambda\,\xi\,-\nu\,\mu\}$	$\{-Q_z\,Q_y\,Q_x\,S_z\,S_y\,-S_x\}$	$\{\lambda''\,-\xi''\,\nu''\,-\mu''\}$
19	12	$\{\nu\,\xi\,\lambda\,\mu\}$	$\{S_x\,-S_y\,-S_z\,-Q_x\,-Q_y\,Q_z\}$	$\{-\nu''\,-\xi''\,-\lambda''\,-\mu''\}$
20	1	$\{-\lambda\,-\mu\,-\nu\,-\xi\}$	$\{S_x\,S_y\,S_z\,Q_x\,Q_y\,Q_z\}$	$\{\lambda''\,\mu''\,\nu''\,\xi''\}$

irrep, based on S and Q, are easily converted into rotations. For example, the representative permutation from class 11, $\{-S_z\,-S_y\,-S_x\,Q_z\,Q_y\,-Q_x\}$, corresponds to a product of three rotations: the first by $-\pi/2$ about the y-axis in quasispin space, the second by π about the z-axis in spin space and the third a rotation by $\pi/2$ about the y-axis in spin space. Some operators in the 6-dimensional irrep, for example, those from classes 1 and 20, are identical and we must determine the form of the corresponding rotations by appealing to the known transformations of the 4-dimensional bases with $S=\frac{1}{2}$ and $Q=\frac{1}{2}$. Once we have the rotation operators, their matrix elements are evaluated using angular momentum theory. It is a straightforward matter to find the new class structure when we augment the representation matrices by $-I$, the matrix of the operation corresponding to rotation by 2π in both spin and quasispin space. It turns out that five new classes appear, deriving from classes 1, 3, 10, 11 and 13. We denote these as classes 1*, 3*, 10*, 11* and 13*. Thus W_4^* has five new representations ($\Gamma_{21}-\Gamma_{25}$) whose characters we have worked out and tabulated in table 2. In table 2 we give only those characters for the new irreps of W_4^*. The complete character table for W_4^* can be obtained by augmenting Littlewood's table [19] with the entries of table 2 and noting that for the single-valued irreps, the characters for the new classes C^* satisfy the relation $\chi(C^*)=\chi(C)$, where C is the class in W_4 from which C^* is derived.

3.1. A subgroup of W_4

The group W_4 is too general for our purposes, since it contains an element interchanging the spin and quasispin. We usually wish to work within a single irrep of $SO_Q(3)\times SO_S(3)$

Table 2. The characters for the new irreps of W_4^*. Columns are labelled by the class and below the class label, the number of elements in that class. The full character table may be obtained by adding this table to Littlewood's character table [19] and using the relation $\chi(C^*)=\chi(C)$ (see section 3) for the single-valued irreps.

	1	1*	2	3	3*	4	5	6	7	8	9	10	10*	11	11*	12	13	13*	14	15	16	17	18	19	20
	1	1	8	12	12	24	12	64	48	48	8	32	32	48	48	96	12	12	48	24	64	64	24	24	2
Γ_{21}	4	−4	0	$2(2)^{1/2}$	$-2(2)^{1/2}$	0	0	0	0	0	0	2	−2	$(2)^{1/2}$	$-(2)^{1/2}$	0	2	−2	0	0	0	0	0	0	0
Γ_{22}	4	−4	0	$-2(2)^{1/2}$	$2(2)^{1/2}$	0	0	0	0	0	0	2	−2	$-(2)^{1/2}$	$(2)^{1/2}$	0	2	−2	0	0	0	0	0	0	0
Γ_{23}	8	−8	0	0	0	0	0	0	0	0	0	−2	2	0	0	0	4	−4	0	0	0	0	0	0	0
Γ_{24}	12	−12	0	$2(2)^{1/2}$	$-2(2)^{1/2}$	0	0	0	0	0	0	0	0	$-(2)^{1/2}$	$(2)^{1/2}$	0	−2	2	0	0	0	0	0	0	0
Γ_{25}	12	−12	0	$-2(2)^{1/2}$	$2(2)^{1/2}$	0	0	0	0	0	0	0	0	$(2)^{1/2}$	$-(2)^{1/2}$	0	−2	2	0	0	0	0	0	0	0

Table 5. The characters for the new irreps of SW_4^*. Columns are labelled by the class and below the class label, the number of elements in that class. The full character table may be obtained by adding this table to table 4 and using the relation $\chi(C^*)=\chi(C)$ for the single-valued irreps (see section 3.1).

	1	1*	3	3*	5	8	10	10*	11	11*	11′	11′*	13	13*	13′	13′*	15	15*	16	16*	19	20	20*
	1	1	12	12	12	48	32	32	24	24	24	24	6	6	6	6	12	12	32	32	24	1	1
Γ_{14}	2	−2	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	1	−1	0	0	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	2	−2	$(2)^{1/2}$	$-(2)^{1/2}$	1	−1	0	2	−2
Γ_{15}	2	−2	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	1	−1	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	2	−2	0	0	$-(2)^{1/2}$	$(2)^{1/2}$	−1	1	0	−2	2
Γ_{16}	2	−2	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	1	−1	0	0	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	2	−2	$-(2)^{1/2}$	$(2)^{1/2}$	1	−1	0	2	−2
Γ_{17}	2	−2	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	1	−1	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	2	−2	0	0	$(2)^{1/2}$	$-(2)^{1/2}$	−1	1	0	−2	2
Γ_{18}	6	−6	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	0	0	0	0	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	−2	2	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	0	6	−6
Γ_{19}	6	−6	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	0	0	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	−2	2	0	0	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	0	−6	6
Γ_{20}	6	−6	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	0	0	0	0	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	−2	2	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	0	6	−6
Γ_{21}	6	−6	$-(2)^{1/2}$	$(2)^{1/2}$	0	0	0	0	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	−2	2	0	0	$(2)^{1/2}$	$-(2)^{1/2}$	0	0	0	−6	6
Γ_{22}	4	−4	0	0	0	0	−1	1	0	0	0	0	0	0	4	−4	0	0	−1	1	0	4	−4
Γ_{23}	4	−4	0	0	0	0	−1	1	0	0	0	0	4	−4	0	0	0	0	1	−1	0	−4	4

and so restrict our attention accordingly. The group we seek is obtained simply by striking out those entries in table 1 for which the Qs appear to the left of the Ss. In other words we remove all elements in classes 2, 4, 6, 7, 9, 12, 14, 17 and 18. The remaining 192 elements again form a group. This group has been studied by Baake *et al* [20, 21] who denote it as SW_4. We have used standard techniques (see for example, [22]) to work out its classes and characters. In table 3 we list a representative element from each class for the 4- and 6-dimensional representations considered earlier. Our notation is designed to indicate from which class of W_4 the classes of SW_4 derive. For example, class 13 of W_4 gives rise to two classes in SW_4, 13 and 13′; the reason being that the elements needed to put the members of classes 13 and 13′ into the same

Table 3. Listing of the classes of the group SW_4. The number of elements in a class is listed under the heading D; columns 3 and 4 contain representative group elements for each class for the permutations of the quasiparticles (column 3) and for the components of $\boldsymbol{S}$ and $\boldsymbol{Q}$ (column 4). Classes are labelled according to their origins in W_4. Classes with primes attached derive from a single class of W_4.

Class	D	$\{a\, b\, c\, d\}$	$\{a'\, b'\, c'\, d'\, e'\, f'\}$
1	1	$\{\lambda\ \mu\ \nu\ \xi\}$	$\{S_x\ S_y\ S_z\ Q_x\ Q_y\ Q_z\}$
3	12	$\{\lambda\ -\xi\ \nu\ \mu\}$	$\{S_z\ S_y\ -S_x\ -Q_z\ Q_y\ Q_x\}$
5	6	$\{\lambda\ \mu\ -\nu\ -\xi\}$	$\{-S_x\ -S_y\ S_z\ -Q_x\ -Q_y\ Q_z\}$
8	24	$\{\lambda\ -\mu\ \mathrm{i}\xi\ -\mathrm{i}\nu\}$	$\{S_y\ S_x\ -S_z\ -Q_y\ -Q_x\ -Q_z\}$
10	32	$\{\lambda\ -\mathrm{i}\nu\ \mathrm{i}\xi\ \mu\}$	$\{S_z\ S_x\ S_y\ -Q_z\ -Q_x\ Q_y\}$
11	24	$\{-\mathrm{i}\mu\ \mathrm{i}\nu\ \mathrm{i}\xi\ \mathrm{i}\lambda\}$	$\{-S_z\ -S_y\ -S_x\ Q_z\ Q_y\ -Q_x\}$
11′	24	$\{\mathrm{i}\mu\ -\mathrm{i}\nu\ \mathrm{i}\xi\ \mathrm{i}\lambda\}$	$\{S_z\ S_y\ -S_x\ -Q_z\ -Q_y\ -Q_x\}$
13	6	$\{-\nu\ -\xi\ \lambda\ \mu\}$	$\{-S_x\ S_y\ -S_z\ Q_x\ Q_y\ Q_z\}$
13′	6	$\{\nu\ -\xi\ -\lambda\ \mu\}$	$\{S_x\ S_y\ S_z\ -Q_x\ Q_y\ -Q_z\}$
15	12	$\{-\lambda\ -\xi\ -\nu\ \mu\}$	$\{-S_z\ S_y\ S_x\ Q_z\ Q_y\ -Q_x\}$
16	32	$\{-\lambda\ \mathrm{i}\nu\ \mathrm{i}\xi\ \mu\}$	$\{-S_z\ -S_x\ S_y\ Q_z\ Q_x\ Q_y\}$
19	12	$\{\nu\ \xi\ \lambda\ \mu\}$	$\{S_x\ -S_y\ -S_z\ -Q_x\ -Q_y\ Q_z\}$
20	1	$\{-\lambda\ -\mu\ -\nu\ -\xi\}$	$\{S_x\ S_y\ S_z\ Q_x\ Q_y\ Q_z\}$

Table 4. The characters for the irreps of SW_4. Columns are labelled by the class and below the class label, the number of elements in that class.

	1	3	5	8	10	11	11′	13	13′	15	16	19	20
	1	12	6	24	32	24	24	6	6	12	32	12	1
Γ_1	1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	−1	1	−1	1	−1	−1	1	1	−1	1	1	1
Γ_3	2	0	2	0	−1	0	0	2	2	0	−1	2	2
Γ_4	3	1	3	1	0	−1	−1	−1	−1	1	0	−1	3
Γ_5	3	−1	3	−1	0	1	1	−1	−1	−1	0	−1	3
Γ_6	3	1	−1	−1	0	−1	1	−1	3	1	0	−1	3
Γ_7	3	1	−1	−1	0	1	−1	3	−1	1	0	−1	3
Γ_8	3	−1	−1	1	0	1	−1	−1	3	−1	0	−1	3
Γ_9	3	−1	−1	1	0	−1	1	3	−1	−1	0	−1	3
Γ_{10}	6	0	−2	0	0	0	0	−2	−2	0	0	2	6
Γ_{11}	4	2	0	0	1	0	0	0	0	−2	−1	0	−4
Γ_{12}	4	−2	0	0	1	0	0	0	0	2	−1	0	−4
Γ_{13}	8	0	0	0	−1	0	0	0	0	0	1	0	−8

conjugacy class are of the type that interchange spin and quasispin and are not present in SW_4. For SW_4, the 6-dimensional representation is not irreducible; it transforms as $\Gamma_6+\Gamma_7$. The 4-dimensional representation remains irreducible and transforms as Γ_{11}. The character table for SW_4 is presented in table 4, where we see again that SW_4 is itself a double group. We shall be interested in bases for irreps of SW_4 with integral spin and half-integral quasispin and so shall need to consider SW_4^*, the double group of SW_4. Following the procedure outlined in section 3 for W_4, we find that 10 new classes appear for SW_4^* and hence 10 new irreps, Γ_{14}–Γ_{23}. In table 5 we give the characters for these new irreps and again appeal to the relation $\chi(C^*)=\chi(C)$ to get the characters of the single-valued irreps for the new classes.

4. U(2^l) and complementarity

Diagonalizing an operator that is a scalar with respect to SW_4^* in an $SO_S(3)\times SO_Q(3)$ basis yields states that transform as bases for irreps of SW_4^*. We know that the U(8) generators are invariant under W_4^* transformations and hence under SW_4^* transformations also; so by diagonalizing the U(8) generators we obtain states transforming as bases for SW_4^* irreps which have, at the same time, good U(8) labels. Under certain circumstances the reverse of this argument may be true, that is, by diagonalizing a suitably chosen SW_4^* scalar we get states that transform as bases for irreps of U(8). This idea is familiar to us from atomic physics, where the diagonalization of $\boldsymbol{Q}^2$ and $\boldsymbol{S}^2$, both of which commute with the generators of SO($2l+1$), yields states with good SO($2l+1$) symmetry. The labels obtained this way, namely, Q and S on the one hand and the SO($2l+1$) irrep labels on the other, are complementary in the sense of Moshinsky and Quesne [8]. That is, specifying S and Q uniquely determines the SO($2l+1$) labels.

A good candidate for an SW_4^* scalar, to play an analogous role to that of $\boldsymbol{Q}^2$ and $\boldsymbol{S}^2$, is

$$2Q_0^{(2)}S_0^{(2)}+(Q_2^{(2)}+Q_{-2}^{(2)})(S_2^{(2)}+S_{-2}^{(2)}) \tag{8}$$

where $\boldsymbol{Q}^{(2)}$ and $\boldsymbol{S}^{(2)}$ are rank-2 tensors, with arbitrary strengths, in the quasispin and spin spaces. The K, κ, M_K and M_κ structure of (8) matches that of the third of equations (4) except for an ineffective part with $(K\kappa)=(00)$. We find that by diagonalizing equation (8) in the bases $(Q, S)=(0,\frac{1}{2}), (0,\frac{3}{2}), (0,\frac{5}{2}), (1,\frac{1}{2}), (1,\frac{3}{2})$ and $(2,\frac{1}{2})$ we obtain just those states for the d shell calculated earlier by diagonalizing the many-electron U(4) generators [3]. It turns out that there is a one-to-one correspondence, for Q integral and S half-integral, between the U(4) irreps and the SW_4^* irreps and so we can say that SW_4^* is the complementary group to U(4). The same correspondence exists for the case of Q half-integral and S integral. If we follow the definition of Moshinsky and Quesne [8] in the strictest sense, our statements concerning complementarity are not quite correct since the correspondence should hold for a single irrep of SW_4^*. However, by limiting our attention to one half of the atomic shell we are assured that our remarks are not in error; and should the need arise we can always rephrase our language in terms of W_4^* for which the correspondence is unique. We find by direct calculation that an analogous relationship holds for the irreps of U(8) and those of SW_4^* for the f shell, and it is seems likely that SW_4^* (or strictly speaking W_4^*) is the complementary group to U(2^l). The correspondence between irreps of U(8) and SW_4^*

for Q half-integral (integral) and S integral (half-integral) is as follows:

$$\begin{aligned}
&[4] \simeq \Gamma_{15}(\Gamma_{14})\\
&[31] \simeq \Gamma_{19}(\Gamma_{18})\\
&[22] \simeq \Gamma_{23}(\Gamma_{22})\\
&[211] \simeq \Gamma_{21}(\Gamma_{20})\\
&[1111] \simeq \Gamma_{17}(\Gamma_{16}).
\end{aligned} \tag{9}$$

Because of the isomorphism between U(4) and SO(6), W_4^* serves as the complementary group to both; however, this is not the case for higher l, and we must attempt to construct SW_4^* scalars that can separate the $U(2^l)$ states on the basis of the groups appearing in the sequences (1). For f electrons we need an operator with $K=3$ and $\kappa=3$ in order to correctly match the spin and quasispin of the fourth of equations (4), and which can change M_Q and M_S by 0 or ±2, subject to the restrictions discussed in section 2.1. We can see from table 6 that only one SW_4^* scalar can be constructed from tensors for which $K=\kappa=3$, and the following operator has all the required properties:

$$(Q_2^{(3)}-Q_{-2}^{(3)})(S_2^{(3)}-S_{-2}^{(3)}). \tag{10}$$

Table 6. Branching rules for the reduction $SO_Q(3)\times SO_S(3)\rightarrow SW_4^*$.

Q	S	Γ_i
0	0	Γ_1
0	$\frac{1}{2}$	Γ_{14}
$\frac{1}{2}$	0	Γ_{15}
0	1	Γ_6
1	0	Γ_7
0	$\frac{3}{2}$	Γ_{22}
$\frac{3}{2}$	0	Γ_{23}
0	2	$\Gamma_3+\Gamma_8$
2	0	$\Gamma_3+\Gamma_9$
$\frac{1}{2}$	2	$\Gamma_{21}+\Gamma_{23}$
2	$\frac{1}{2}$	$\Gamma_{20}+\Gamma_{22}$
0	3	$\Gamma_2+\Gamma_6+\Gamma_8$
3	0	$\Gamma_2+\Gamma_7+\Gamma_9$
0	4	$\Gamma_1+\Gamma_3+\Gamma_7+\Gamma_9$
4	0	$\Gamma_1+\Gamma_3+\Gamma_6+\Gamma_8$
$\frac{1}{2}$	1	Γ_{19}
1	$\frac{1}{2}$	Γ_{18}
1	1	$\Gamma_4+\Gamma_{10}$
1	$\frac{3}{2}$	$\Gamma_{18}+\Gamma_{20}$
$\frac{3}{2}$	1	$\Gamma_{19}+\Gamma_{21}$
$\frac{3}{2}$	$\frac{3}{2}$	$\Gamma_{11}+\Gamma_{12}+\Gamma_{13}$
$\frac{3}{2}$	2	$\Gamma_{15}+\Gamma_{17}+\Gamma_{19}+\Gamma_{21}+\Gamma_{23}$
2	$\frac{3}{2}$	$\Gamma_{14}+\Gamma_{16}+\Gamma_{18}+\Gamma_{20}+\Gamma_{22}$
2	2	$\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4+\Gamma_6+\Gamma_7+\Gamma_8+\Gamma_9+\Gamma_{10}$
2	$\frac{5}{2}$	$\Gamma_{15}+\Gamma_{17}+2\Gamma_{19}+\Gamma_{21}+2\Gamma_{23}$
$\frac{5}{2}$	2	$\Gamma_{14}+\Gamma_{16}+2\Gamma_{18}+\Gamma_{20}+2\Gamma_{22}$
3	3	$\Gamma_1+2\Gamma_4+2\Gamma_5+\Gamma_6+\Gamma_7+\Gamma_8+\Gamma_9+4\Gamma_{10}$
4	4	$2\Gamma_1+\Gamma_2+3\Gamma_3+2\Gamma_4+2\Gamma_5+3\Gamma_6+3\Gamma_7+3\Gamma_8+3\Gamma_9+4\Gamma_{10}$

In table 7 we give the U(8) and SO(8) classification of the states of the f shell obtained using equations (8) and (10). Only one quarter of the states are listed; those with parity labels gg, gu and ug can be obtained using the following equations:

$$
\begin{aligned}
&M_S^{\mathrm{gu}}=-M_S^{\mathrm{ug}} \qquad && M_Q^{\mathrm{gu}}=-M_Q^{\mathrm{ug}} \qquad && M_S^{\mathrm{uu}}=M_Q^{\mathrm{ug}} \\
&M_Q^{\mathrm{uu}}=M_S^{\mathrm{ug}} \qquad && M_S^{\mathrm{gg}}=-M_S^{\mathrm{uu}} \qquad && M_Q^{\mathrm{gg}}=-M_Q^{\mathrm{uu}}.
\end{aligned}
\tag{11}
$$

Table 7. States of the f shell with parities uu. The labels a, b, c attached to the irreducible representations of SO(8) distinguish states on the basis of the U(8) representations specified in the adjacent column for the spin-up and spin-down spaces. The quasispins Q and spins S are indicated by prefaced multiplicities $2Q+1$ and $2S+1$ to W.

U(8)	SO(8)	$\mathrm{U_A}(8)\times\mathrm{U_B}(8)$	$\vert M_Q, M_S, {}^{2Q+1\,2S+1}W\rangle$
[4]	(4000)	[2]×[2]	$\vert-\frac12, 0, {}^{21}(222)\rangle$
	(2000)	[2]×[2]	$(\frac12)^{1/2}\vert-\frac12, 0, {}^{45}(111)\rangle+\frac12\vert\frac32, 2, {}^{45}(111)\rangle+\frac12\vert\frac32, -2, {}^{45}(111)\rangle$
	(0000)	[2]×[2]	$(\frac{7}{12})^{1/2}\vert-\frac12, 0, {}^{81}(000)\rangle+(\frac{5}{12})^{1/2}\vert\frac72, 0, {}^{81}(000)\rangle$
[31]	$(3100)_a$	[2]×[2]	$\vert-\frac12, 0, {}^{23}(221)\rangle, \vert-\frac12, 0, {}^{43}(211)\rangle$
	$(3100)_b$	[11]×[2]	$\vert\frac12, 1, {}^{23}(221)\rangle, (\frac34)^{1/2}\vert-\frac32, -1, {}^{43}(211)\rangle+\frac12\vert\frac12, 1, {}^{43}(211)\rangle$
	$(3100)_c$	[2]×[11]	$\vert\frac12, -1, {}^{23}(221)\rangle, (\frac34)^{1/2}\vert-\frac32, 1, {}^{43}(211)\rangle+\frac12\vert\frac12, -1, {}^{43}(211)\rangle$
	$(2000)_a$	[2]×[2]	$(\frac12)^{1/2}\vert\frac32, 2, {}^{45}(111)\rangle-(\frac12)^{1/2}\vert\frac32, -2, {}^{45}(111)\rangle$
	$(2000)_b$	[11]×[2]	$\frac12\vert-\frac32, -1, {}^{45}(111)\rangle+(\frac34)^{1/2}\vert\frac12, 1, {}^{45}(111)\rangle$
	$(2000)_c$	[2]×[11]	$\frac12\vert-\frac32, 1, {}^{45}(111)\rangle+(\frac34)^{1/2}\vert\frac12, -1, {}^{45}(111)\rangle$
	$(1100)_a$	[2]×[2]	$\vert-\frac12, 0, {}^{63}(110)\rangle, \vert-\frac12, 0, {}^{27}(100)\rangle$
	$(1100)_b$	[11]×[2]	$(\frac18)^{1/2}\vert-\frac32, -1, {}^{63}(110)\rangle+\frac12\vert\frac12, 1, {}^{63}(110)\rangle+(\frac58)^{1/2}\vert\frac52, -1, {}^{63}(110)\rangle,$ $(\frac38)^{1/2}\vert\frac12, 1, {}^{27}(100)\rangle+(\frac58)^{1/2}\vert\frac12, -3, {}^{27}(100)\rangle$
	$(1100)_c$	[2]×[11]	$(\frac18)^{1/2}\vert-\frac32, 1, {}^{63}(110)\rangle+\frac12\vert\frac12, -1, {}^{63}(110)\rangle+(\frac58)^{1/2}\vert\frac52, 1, {}^{63}(110)\rangle,$ $(\frac38)^{1/2}\vert\frac12, -1, {}^{27}(100)\rangle+(\frac58)^{1/2}\vert\frac12, 3, {}^{27}(100)\rangle$
[22]	$(2200)_a$	[11]×[11]	$\vert\frac32, 0, {}^{41}(220)\rangle, (\frac12)^{1/2}\vert-\frac12, 2, {}^{25}(210)\rangle+(\frac12)^{1/2}\vert-\frac12, -2, {}^{25}(210)\rangle,$ $(\frac16)^{1/2}\vert\frac32, 0, {}^{61}(200)\rangle+(\frac56)^{1/2}\vert-\frac52, 0, {}^{61}(200)\rangle$
	$(2200)_b$	[2]×[2]	$\vert-\frac12, 0, {}^{41}(220)\rangle, \vert-\frac12, 0, {}^{25}(210)\rangle, \vert-\frac12, 0, {}^{61}(200)\rangle$
	$(2000)_a$	[11]×[11]	$(\frac12)^{1/2}\vert\frac32, 0, {}^{45}(111)\rangle+\frac12\vert-\frac12, 2, {}^{45}(111)\rangle+\frac12\vert-\frac12, -2, {}^{45}(111)\rangle$
	$(2000)_b$	[2]×[2]	$(\frac12)^{1/2}\vert-\frac12, 0, {}^{45}(111)\rangle-\frac12\vert\frac32, 2, {}^{45}(111)\rangle-\frac12\vert\frac32, -2, {}^{45}(111)\rangle$
	$(0000)_a$	[11]×[11]	$(\frac34)^{1/2}\vert\frac32, 0, {}^{81}(000)\rangle+\frac12\vert-\frac52, 0, {}^{81}(000)\rangle$
	$(0000)_b$	[2]×[2]	$(\frac{5}{12})^{1/2}\vert-\frac12, 0, {}^{81}(000)\rangle-(\frac{7}{12})^{1/2}\vert\frac72, 0, {}^{81}(000)\rangle$
[211]	$(2110)_a$	[11]×[11]	$\vert\frac32, 0, {}^{43}(211)\rangle, (\frac12)^{1/2}\vert-\frac12, 2, {}^{25}(210)\rangle-(\frac12)^{1/2}\vert-\frac12, -2, {}^{25}(210)\rangle,$ $(\frac12)^{1/2}\vert-\frac12, 2, {}^{45}(111)\rangle-(\frac12)^{1/2}\vert-\frac12, -2, {}^{45}(111)\rangle,$ $(\frac56)^{1/2}\vert\frac32, 0, {}^{63}(110)\rangle-(\frac16)^{1/2}\vert-\frac52, 0, {}^{63}(110)\rangle$
	$(2110)_b$	[11]×[2]	$\vert\frac12, 1, {}^{25}(210)\rangle, \frac12\vert-\frac32, -1, {}^{43}(211)\rangle-(\frac34)^{1/2}\vert\frac12, 1, {}^{43}(211)\rangle,$ $(\frac34)^{1/2}\vert-\frac32, -1, {}^{45}(111)\rangle-\frac12\vert\frac12, 1, {}^{45}(111)\rangle,$ $(\frac56)^{1/2}\vert-\frac32, -1, {}^{63}(110)\rangle-(\frac16)^{1/2}\vert\frac52, -1, {}^{63}(110)\rangle$
	$(2110)_c$	[2]×[11]	$\vert\frac12, -1, {}^{25}(210)\rangle, \frac12\vert-\frac32, 1, {}^{43}(211)\rangle-(\frac34)^{1/2}\vert\frac12, -1, {}^{43}(211)\rangle,$ $(\frac34)^{1/2}\vert-\frac32, 1, {}^{45}(111)\rangle-\frac12\vert\frac12, -1, {}^{45}(111)\rangle,$ $(\frac56)^{1/2}\vert-\frac32, 1, {}^{63}(110)\rangle-(\frac16)^{1/2}\vert\frac52, 1, {}^{63}(110)\rangle$
	$(1100)_a$	[11]×[11]	$(\frac16)^{1/2}\vert\frac32, 0, {}^{63}(110)\rangle+(\frac56)^{1/2}\vert-\frac52, 0, {}^{63}(110)\rangle,$ $(\frac12)^{1/2}\vert-\frac12, 2, {}^{27}(100)\rangle+(\frac12)^{1/2}\vert-\frac12, -2, {}^{27}(100)\rangle$
	$(1100)_b$	[11]×[2]	$(\frac{1}{24})^{1/2}\vert-\frac32, -1, {}^{63}(110)\rangle-(\frac34)^{1/2}\vert\frac12, 1, {}^{63}(110)\rangle+(\frac{5}{24})^{1/2}\vert\frac52, -1, {}^{63}(110)\rangle,$ $(\frac58)^{1/2}\vert\frac12, 1, {}^{27}(100)\rangle-(\frac38)^{1/2}\vert\frac12, -3, {}^{27}(100)\rangle$
	$(1100)_c$	[2]×[11]	$(\frac{1}{24})^{1/2}\vert-\frac32, 1, {}^{63}(110)\rangle-(\frac34)^{1/2}\vert\frac12, -1, {}^{63}(110)\rangle+(\frac{5}{24})^{1/2}\vert\frac52, 1, {}^{63}(110)\rangle,$ $(\frac58)^{1/2}\vert\frac12, -1, {}^{27}(100)\rangle-(\frac38)^{1/2}\vert\frac12, 3, {}^{27}(100)\rangle$
[1111]	(111−1)	[11]×[11]	$(\frac12)^{1/2}\vert\frac32, 0, {}^{45}(111)\rangle-\frac12\vert-\frac12, 2, {}^{45}(111)\rangle-\frac12\vert-\frac12, -2, {}^{45}(111)\rangle$
	(1111)	[11]×[11]	$(\frac56)^{1/2}\vert\frac32, 0, {}^{61}(200)\rangle-(\frac16)^{1/2}\vert-\frac52, 0, {}^{61}(200)\rangle,$ $(\frac12)^{1/2}\vert-\frac12, 2, {}^{27}(100)\rangle-(\frac12)^{1/2}\vert-\frac12, -2, {}^{27}(100)\rangle,$ $\frac12\vert\frac32, 0, {}^{81}(000)\rangle-(\frac34)^{1/2}\vert-\frac52, 0, {}^{81}(000)\rangle$

5. Generalizations

The generalization of these ideas to higher l values is straightforward. The generators of $U(2^l)$ are invariant under W_4^* and SW_4^* transformations and so these groups again provide the base upon which we construct our quark states. The analysis becomes more complicated due to the increasing number of $(K\kappa)$ values associated with the $U(2^l)$ generators. For g electrons, for example, we have the situation that the generators of U(16) have in addition to parts with $(K\kappa)=(00)$, (22) and (33), contributions with $(K\kappa)=(44)$, for which M_K and M_κ can assume the values 0, ±2, or ±4. The components M_K and M_κ do not take on these values independently: the actual values assumed are discussed below. The distribution of the $(K\kappa)$ among the various generators of U(16) can be found by extending the analysis of Flowers [16]. The generators of the subgroups of U(16), found by setting $l=4$ in equations (1), along with their various mixtures of $(K\kappa)$ values are as follows:

$$\begin{aligned}
&\mathrm{SO}(9)\colon \textstyle\sum'(\boldsymbol{\theta}^2)^{(1100)} && (00) \\
&\mathrm{SO}(10)\colon\ \textstyle\sum'(\boldsymbol{\theta}^2)^{(1100)}, \sum'(\boldsymbol{\theta}^8)^{(1000)} && (00), (22), (33), (44) \\
&\mathrm{SO}(16)\colon\ \textstyle\sum'(\boldsymbol{\theta}^2)^{(1100)}, \Sigma'(\boldsymbol{\theta}^6)^{(1110)} && (00), (22), (33)
\end{aligned} \tag{12}$$

where the superscripted numbers give the transformation properties with respect to SO(9) and the primes attached to the summations have the same significance as in equations (4). U(16) has one additional generator, namely $\Sigma'(\boldsymbol{\theta}^4)^{(1111)}$, for which $(K\kappa)=(00)$ and (22). We find by looking at table 6 that (44) of $\mathrm{SO}_Q(3)\times\mathrm{SO}_S(3)$ contains Γ_1 of SW_4^* twice, and hence we can construct two SW_4^* invariants from tensors with spin and quasispin ranks of 4. Knowing that the U(16) generators cannot have parts that change M_K and M_κ by ±1 or ±3, we can use the octahedral eigenfunctions given by Lea *et al* [23] to help us construct the two following invariants:

$$((\tfrac{5}{24})^{1/2}Q_4^{(4)}+(\tfrac{14}{24})^{1/2}Q_0^{(4)}+(\tfrac{5}{24})^{1/2}Q_{-4}^{(4)})((\tfrac{5}{24})^{1/2}S_4^{(4)}+(\tfrac{14}{24})^{1/2}S_0^{(4)}+(\tfrac{5}{24})^{1/2}S_{-4}^{(4)}) \tag{13}$$

and

$$\begin{aligned}
&((\tfrac{7}{24})^{1/2}Q_4^{(4)}-(\tfrac{10}{24})^{1/2}Q_0^{(4)}+(\tfrac{7}{24})^{1/2}Q_{-4}^{(4)})((\tfrac{7}{24})^{1/2}S_4^{(4)}-(\tfrac{10}{24})^{1/2}S_0^{(4)}+(\tfrac{7}{24})^{1/2}S_{-4}^{(4)}) \\
&\qquad +(Q_2^{(4)}+Q_{-2}^{(4)})(S_2^{(4)}+S_{-2}^{(4)}).
\end{aligned} \tag{14}$$

It is to be noticed that the values of the pairs (M_K, M_κ) are restricted. For example, the values (4, 2) and (2, 0) never appear; the allowed values of M_K and M_κ just match those of the U(16) generators. We have found that by diagonalizing some combination of the operators of equations (8), (10), (13) and (14), it is possible to obtain the states of the g shell in both schemes of equation (1). We find, for example, in the $U(16)\supset SO(16)\supset SO(9)$ scheme the following gg parity states as linear combinations of the kets $|M_Q\, M_S\, {}^{2Q+1,2S+1}(w_1w_2w_3w_4)\rangle$:

$$\begin{aligned}
&|[4](00\,..\,0)(0000)\rangle \\
&\qquad =(\tfrac{7}{12})^{1/2}|-\tfrac{1}{2}\,0\ {}^{10,1}(0000)\rangle+(\tfrac{1}{24})^{1/2}|\tfrac{7}{2}\,0\ {}^{10,1}(0000)\rangle+(\tfrac{3}{8})^{1/2}|-\tfrac{9}{2}\,0\ {}^{10,1}(0000)\rangle \\
&|[22](00\,..\,0)(0000)\rangle \\
&\qquad =-(\tfrac{7}{20})^{1/2}|-\tfrac{1}{2}\,0\ {}^{10,1}(0000)\rangle-(\tfrac{1}{40})^{1/2}|\tfrac{7}{2}\,0\ {}^{10,1}(0000)\rangle+(\tfrac{5}{8})^{1/2}|-\tfrac{9}{2}\,0\ {}^{10,1}(0000)\rangle \\
&|[22](220\,..\,0)(0000)\rangle \\
&\qquad =-(\tfrac{1}{15})^{1/2}|-\tfrac{1}{2}\,0\ {}^{10,1}(0000)\rangle+(\tfrac{14}{15})^{1/2}|\tfrac{7}{2}\,0\ {}^{10,1}(0000)\rangle
\end{aligned} \tag{15}$$

while in the U(16) ⊃ SO(10) ⊃ SO(9) scheme, we have:

$$
\begin{aligned}
&|[4](20000)(0000)\rangle \\
&\qquad = (\tfrac{7}{12})^{1/2}|-\tfrac{1}{2}\,0\ ^{10,1}(0000)\rangle + (\tfrac{1}{24})^{1/2}|\tfrac{7}{2}\,0\ ^{10,1}(0000)\rangle + (\tfrac{3}{8})^{1/2}|-\tfrac{9}{2}\,0\ ^{10,1}(0000)\rangle \\
&|[22](20000)(0000)\rangle \\
&\qquad = -(\tfrac{5}{12})^{1/2}|-\tfrac{1}{2}\,0\ ^{10,1}(0000)\rangle + (\tfrac{7}{120})^{1/2}|\tfrac{7}{2}\,0\ ^{10,1}(0000)\rangle + (\tfrac{21}{40})^{1/2}|-\tfrac{9}{2}\,0\ ^{10,1}(0000)\rangle \\
&|[22](00000)(0000)\rangle \\
&\qquad = -(\tfrac{9}{10})^{1/2}|\tfrac{7}{2}\,0\ ^{10,1}(0000)\rangle + (\tfrac{1}{10})^{1/2}|-\tfrac{9}{2}\,0\ ^{10,1}(0000)\rangle.
\end{aligned}
\tag{16}
$$

There appears to be no difficulty in extending this approach to cope with higher l values.

6. Complementary group to SO(7)″

With respect to the group SO(7)″, a single quark transforms as $(\frac{1}{2}\frac{1}{2}\frac{1}{2})''$ and the states of the f shell can be constructed by considering the product $((\frac{1}{2}\frac{1}{2}\frac{1}{2})'')^4$. The SO(7)″ irreps appearing in this scheme are identical to those that arise for the analysis based on SO(7), so we anticipate a complementary group $\mathrm{SO}_Q(3)''\times\mathrm{SO}_S(3)''$ in analogy with the familiar spin and quasispin groups of classical SO(7) theory. An examination of the generators of SO(7) and SO(7)″, as expressed in terms of the annihilation and creation operators of the quarks $s+f$ [7], reveals that one can pass from one group to the other simply by reversing the phase of the s quark relative to the f quark. However, to convert the $\boldsymbol{S}$ and $\boldsymbol{Q}$ of equations (6) and (7) to $\boldsymbol{S}''$ and $\boldsymbol{Q}''$ we need the corresponding substitutions for quasiparticles. These are not so easy to obtain. Our starting point is the observation that the seven components of a tensor $\boldsymbol{\theta}$ belong to the irreps (1100), (100) and (10) of $\mathrm{SO}_\theta(8)$, $\mathrm{SO}_\theta(7)$ and $\mathrm{G}_{2\theta}$. The transformed $\boldsymbol{\theta}$, namely $\boldsymbol{\theta}''$, must belong to (1100), (100)″ and (10) of $\mathrm{SO}_\theta(8)$, $\mathrm{SO}_\theta(7)''$ and $\mathrm{G}_{2\theta}$. Thus (100) is replaced by (100)″, but the other descriptions are unchanged. The only other irrep of SO(7) that derives from (1100) of SO(8) and contains (10) of G_2 is (110), and the corresponding operator can only be provided by the quintuple tensor product $(\boldsymbol{\theta}^5)^{(110)}$. We can conclude that the required substitutions are of the form

$$\boldsymbol{\theta}\rightarrow\boldsymbol{\theta}''=A\boldsymbol{\theta}+B(\boldsymbol{\theta}^5)^{(110)(10)3}.$$

The two coefficients A and B can be found by requiring that the components of $\boldsymbol{\theta}''$ satisfy the same anticommutation relations as those of $\boldsymbol{\theta}$. In terms of the components θ_q of the tensors $\boldsymbol{\theta}$, we ultimately arrive at the substitutions:

$$
\begin{aligned}
\theta_3 &\rightarrow \theta_3''=\tfrac{1}{2}\theta_3+\tfrac{1}{2}(\theta_3c_1c_2+(8)^{1/2}\theta_2\theta_1\theta_0c_3) \\
\theta_2 &\rightarrow \theta_2''=\tfrac{1}{2}\theta_2+\tfrac{1}{2}(\theta_2c_3c_1+(8)^{1/2}\theta_3\theta_0\theta_{-1}c_2) \\
\theta_1 &\rightarrow \theta_1''=\tfrac{1}{2}\theta_1-\tfrac{1}{2}(\theta_1c_3c_2+(8)^{1/2}\theta_3\theta_0\theta_{-2}c_1) \\
\theta_0 &\rightarrow \theta_0''=\tfrac{1}{2}\theta_0+\tfrac{1}{2}\theta_0(c_1c_2+c_1c_3-c_2c_3)
\end{aligned}
\tag{17}
$$

where

$$c_i=[\theta_i,\theta_{-i}].$$

Direct calculation shows that the substitutions (17) transform the generators of SO(7) into those of SO(7)″, and vice versa, while leaving invariant the generators of SO(7)′.

7. Complementary group to SU(7)′

As an alternative to equation (1), we consider the group scheme

$$\mathrm{U}(8) \supset \mathrm{Y} \supset \mathrm{X} \supset \mathrm{G}_2 \tag{18}$$

where Y can be SU(7), SU(7)′ or SU(7)″ according to whether X is SO(7), SO(7)′ or SO(7)″. We find that the complementary group to SU(7)′ is a group isomorphic to W_4, which we denote W_4'. To see this, consider the transformation $\{-\nu\ -\eta''\ -\lambda''\ -\nu''\}$, where now we have added double primes to some of the quasiparticles appearing in the permutation to indicate that the substitutions (17) have been made for those quasiparticles. Applying this operation to the SU(7)′ generators $\Sigma'(\boldsymbol{\theta}^4)^{(200)'}$ shows that they do indeed remain invariant. Other SU(7)′ generators are more difficult to handle when written in terms of quasiparticles, and a simpler way to proceed is to write them as $\Sigma_\theta(\boldsymbol{f}_\theta^\dagger \boldsymbol{f}_\theta)^{(k)}$, for $k=1, 2, \ldots, 6$, noting that under the transformation $\theta \to \theta''$, we have $\boldsymbol{f}_\theta^\dagger \to \boldsymbol{f}_\theta^\dagger$ and $\boldsymbol{s}_\theta^\dagger \to -\boldsymbol{s}_\theta^\dagger$, from which the required invariance follows.

The new permutations considered above form the group W_4', obtained by adding to the group of permutations among the quasiparticles, the substitution $\theta \to \theta''$. Making this substitution twice sends $\theta \to (\theta'')'' \to \theta$, so the operation of adding a double prime is formally similar to the sign change ε_i that we considered in section 3. This property leads to the isomorphism between W_4 and W_4'. In table 1 we list representative group elements for each of the classes of W_4', which are the images of the elements of W_4, listed in column 3, under the isomorphism.

We are now in a position to classify the SU(7)′ states according to W_4'. There are two ways to proceed; either by constructing states in the quasiparticle picture or by using our knowledge of the quarks. The first approach soon becomes very cumbersome, whereas in the second, states can be separated naturally according to the number of occurrences of a particular m_l component among the quark creation operators. For example, the quark states $f_{\lambda 3}^\dagger f_{\mu 2}^\dagger f_{\nu 2}^\dagger f_{\xi 2}^\dagger|0\rangle$, $f_{\lambda 2}^\dagger f_{\mu 3}^\dagger f_{\nu 2}^\dagger f_{\xi 2}^\dagger|0\rangle$, $f_{\lambda 2}^\dagger f_{\mu 2}^\dagger f_{\nu 3}^\dagger f_{\xi 2}^\dagger|0\rangle$ and $f_{\lambda 2}^\dagger f_{\mu 2}^\dagger f_{\nu 2}^\dagger f_{\xi 3}^\dagger|0\rangle$, which we denote collectively as {3222}, transform as $\Gamma_1+\Gamma_9$ of W_4'. The states {3111}, {3000}, $\{3-1-1-1\}\ldots$ behave similarly; in other words, those states obtained by acting on the quark vacuum with four f-quark creation operators, three of which have identical m_l values, transform as $\Gamma_1+\Gamma_9$. A similar state of affairs exists for the other possible distributions of m_l values among four quarks. In table 8 we list, for the configurations $f^{4-n}s^n$ with $0 \leqslant n \leqslant 4$, the transformation properties of the various types of states that can occur, along with the number of states of each type. The classification proceeds by starting from the state {3333}, which has $m_l=12$ and belongs to [4]′ of SU(7)′, and stepping down in units of m_l until reaching $m_l=0$. At each stage those irreps of W_4' already assigned to SU(7)′ states are subtracted out, allowing us to determine the complementary-group labels for the remaining SU(7)′ states. The results are as follows:

$$\begin{aligned}
&[4]' \simeq \Gamma_1, [31]' \simeq \Gamma_9, [22]' \simeq \Gamma_5, [211]' \simeq \Gamma_{11}\\
&[3]' \simeq \Gamma_{13}, [21]' \simeq \Gamma_{19}, [111]' \simeq \Gamma_{15}\\
&[2]' \simeq \Gamma_7, [11]' \simeq \Gamma_{18}\\
&[1]' \simeq \Gamma_{13}\\
&[0]' \simeq \Gamma_1.
\end{aligned} \tag{19}$$

Table 8. Transformation properties with respect to W_4' of the various quark states in the configurations $f^{4-n}s^n$ $(0 \leqslant n \leqslant 4)$. The symbols in braces are the m_l values $(-3 \leqslant m_l \leqslant 3)$, to be distributed among the four quarks. The number of states of a particular type is listed under the heading D. An explicit zero in the braces refers to the m_l value of an s quark.

Configuration	D	$\{m_1m_2m_3m_4\}$	Γ_i
f^4	24	$\{m_1m_2m_3m_4\}$	$\Gamma_1+\Gamma_3+2\Gamma_5+3\Gamma_9+3\Gamma_{11}$
	12	$\{m_1m_2m_3m_3\}$	$\Gamma_1+\Gamma_5+2\Gamma_9+\Gamma_{11}$
	6	$\{m_1m_1m_2m_2\}$	$\Gamma_1+\Gamma_5+\Gamma_9$
	4	$\{m_1m_2m_2m_2\}$	$\Gamma_1+\Gamma_9$
	1	$\{m_1m_1m_1m_1\}$	Γ_1
f^3s	24	$\{m_1m_2m_30\}$	$\Gamma_{13}+\Gamma_{15}+2\Gamma_{19}$
	12	$\{m_1m_2m_20\}$	$\Gamma_{13}+\Gamma_{19}$
	4	$\{m_1m_1m_10\}$	Γ_{13}
f^2s^2	12	$\{m_1m_200\}$	$\Gamma_7+\Gamma_{18}$
	6	$\{m_1m_100\}$	Γ_7
fs^3	4	$\{m_1000\}$	Γ_{13}
s^4	1	$\{0000\}$	Γ_1

8. Application

Much of the discussion in this paper has been of a formal nature. An example of the usefulness of the complementary group idea in the atomic quark model should serve to bring us into contact with our previous analysis. In [1] we considered the three-electron operator t_4, used in configuration-interaction studies, and gave an explanation for the vanishing of the matrix element $\langle \mathrm{f}^7(222)(30)|t_4|\mathrm{f}^7(221)(31)\rangle$ in terms of the group SO(7)′. It turned out that the operator t_4 could be expressed as a two-quark operator of the form

$$((\boldsymbol{q}_\lambda^\dagger \boldsymbol{q}_\lambda)^{(2000)}(\boldsymbol{q}_\mu^\dagger \boldsymbol{q}_\mu)^{(2000)})^{(4000)(222)} + ((\boldsymbol{q}_\nu^\dagger \boldsymbol{q}_\nu)^{(2000)}(\boldsymbol{q}_\xi^\dagger \boldsymbol{q}_\xi)^{(2000)})^{(4000)(222)} \tag{20}$$

where the SO(8) and SO(7) labels are specified as superscripts. If, now, we turn to our complementary group W_4' and consider the transformations of the six operators

$$((\boldsymbol{q}_\theta^\dagger \boldsymbol{q}_\theta)^{(2000)}(\boldsymbol{q}_{\theta'}^\dagger \boldsymbol{q}_{\theta'})^{(2000)})^{(4000)} \qquad [(\theta\theta') \equiv (\lambda\mu), (\lambda\nu), (\lambda\xi), (\mu\nu), (\mu\xi), (\nu\xi)] \tag{21}$$

it is straightforward to show that they belong to the representation $\Gamma_1+\Gamma_5+\Gamma_9$ and these, therefore, are the irreps available for labelling t_4. The states appearing in the bra and ket of the above matrix element belong to Γ_{13} and Γ_9, respectively, so the matrix element has the form $\langle \Gamma_{13}|\Gamma_1+\Gamma_5+\Gamma_9|\Gamma_9\rangle$, when written in terms of the complementary group representations. A matrix element with these W_4' labels must vanish, since the Kronecker product $\Gamma_{13}\times\Gamma_9$ does not contain any of the irreps labelling the operator. Thus the complementary group W_4' has provided an alternative to our earlier approach.

We anticipate other applications as we proceed to study 3-quark and 4-quark operators. Just as the dependence of the matrix elements of operators on spin or quasispin has been usefully represented in the past by the 3-j symbols of the groups $\mathrm{SO}_S(3)$ and $\mathrm{SO}_Q(3)$, so we expect relations between our quark operators to involve Clebsch-Gordan coefficients for our new complementary groups. The absence of useful tabulations of such coefficients means that any proportionalities we might establish between sets of matrix elements will lack numerical coefficients; but this would be a minor price to pay for the gain in structural information.

9. Complementary group to G_2

Unexpected relations between matrix elements frequently occur in the f shell: indeed, they are the motivating force for the analysis presented above. Because all the states are characterized by irreps of G_2, it is natural to ask whether a complementary group Z to G_2 exists, and, if so, whether the surprising simplifications that have accumulated over the years could be explained at a single stroke in terms of the irreps of Z. As pointed out some years ago [24], this possibility would not yield anything of value if Z was simply the direct product

$$U(4)\times U(8)\times U(12)\times\ldots\times U(60) \tag{22}$$

where the dimensions of the unitary groups are merely the number of occurrences of the irreps (40), (31), (30), ..., (00).

We are now in a position to construct a complementary group to G_2 because we have at our disposal the four operators S, Q, S'' and Q'' which commute with the generators of G_2. If we take the various commutators of these four vectors, the commutators of these commutators, and so on, the fermionic character of the component creation and annihilation operators that form the resultant operators guarantees closure. Since S'' and Q'' involve quintuple products of annihilation and creation operators, the procedure is technically difficult, and there seems no reason to suppose that an interesting early closure will be obtained. We have studied in detail what happens if attention is limited just to the spin-up space, and indeed a trivial direct product of unitary groups is produced. This a rather disappointing conclusion, but not, perhaps, too surprising. After all, there is no simple Lie group with irreps with the required dimensions 4, 8, 12, ..., 60. There remains, however, the possibility that a finite group might exist to play the role of Z. It would have to be a subgroup of the product (22) and itself contain both W_4^* and W_4' as subgroups. The smallest group to contain both W_4^* and W_4' comprises 12288 elements. Although the structure of this group can be identified as the double group of a wreath product (of D_2 with S_4) we prefer to set it aside as a topic for future study.

Acknowledgments

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