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On R(4) Symmetries in Atomic Structure

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By defining a new rotation group in four dimensions we show that previous phase discrepancies can be accounted for. Furthermore we demonstrate that the new R(4) group is the one to be used in the study of atomic correlation.

1. Introduction

It is well known, Fock [1] and Bargmann [2], that the full symmetry group of the non-relativistic hydrogen atom is the rotation group in four dimensions R(4) provided only bound states are considered.

Between 1962 and 1975 several workers have investigated the possibility of using the group R(4) as an approximate symmetry group for atoms with more than one electron, Moshinsky [3], Wulfman [4], [5], Alper and Sinanoglu [6], Alper [7], Butler and Wybourne [8], [9], Rau [10], Alper [11], Sinanoglu and Herrick [12], [13], [14]. These authors came to differing conclusions on the validity of using R(4) for many-electron atoms. These conflicting views have not yet been satisfactorily explained. In this paper we critically examine the above authors' work in an attempt to finally understand the nature of R(4) symmetry in many-electron atoms.

We find that a new R(4) group can be introduced and we define its generators. We employ the use of generalized Racah tensors since operators representing physical properties can be taken to be irreducible tensor operators. We find that this new R(4) group can be used to explain the discrepancies in the various phase conventions discussed by Alper [11].

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2. Generators for the Group R(4)

The four dimensional rotation group R(4) is a six parameter semi-simple Lie group. We thus have six generators for the Lie algebra D_2 of $R(4)$ which we denote by $\hat{l}_1, \hat{l}_2, \hat{l}_3, \hat{R}_1, \hat{R}_2, \hat{R}_3$. The generators satisfy the commutation relations (CR's)

$$[\hat{l}_i, \hat{R}_j] = \sum_k \varepsilon_{ijk} i \hat{R}_k$$

$$\hat{\boldsymbol{l}} \times \hat{\boldsymbol{l}} = i\hat{\boldsymbol{l}} \qquad \hat{\boldsymbol{R}} \times \hat{\boldsymbol{R}} = i\boldsymbol{l} \tag{1}$$

where ε_{ijk} is the usual Levi–Civita tensor.

From these CR's it can be shown, Chisholm [15], that

$$D_2 = B_1 + B_1 \tag{2}$$

where B_1 is the Lie algebra for the three dimensional rotation group $R(3)$. As a consequence of Eq. (2) we have the result that $R(4) = R(3) \times R(3)$ and so the well known properties of $R(3)$ can be used to obtain the properties of $R(4)$.

The irreducible representations (IR) of $R(3)$ can be labelled by a symbol (j) where $j = 0, 1, 2, 3 \ldots$ (or $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$ in the case of the double group $R^*(3)$). The dimension of the IR (j) is $(2j+1)$. Since $R(4) = R(3) \times R(3)$ we find that the IR's of $R(4)$ can be labelled by a symbol $(j_1 j_2)$ and that the dimension of $(j_1 j_2)$ is $(2j_1+1)(2j_2+1)$. It is often convenient to label the IR's of $R(4)$ by $[p, q]$ where $p = j_1 + j_2$ and $q = j_1 - j_2$.

Because $R(4)$ is a rank two Lie group there exists two invariant operators which may be taken to be $\hat{R}^2 + \hat{l}^2$ and $\hat{\boldsymbol{R}} \cdot \hat{\boldsymbol{l}}$. The eigenvalues of $\hat{R}^2 + \hat{l}^2$ are given by $p(p+2) + q^2$ while those of $\hat{\boldsymbol{R}} \cdot \hat{\boldsymbol{l}}$ are given by $q(p+1)$.

The basis functions for the IR's of $R(4)$ can be classified by the usual quantum numbers l and m because the branching rule for the reduction $R(4) \to R(3)$ shows that

$$l = p, p-1, \ldots, |q|.$$

It is well known, Chisholm [15], that for the hydrogen atom the three operators $\hat{l}_1$, $\hat{l}_2$, $\hat{l}_3$ are just the components of the orbital angular momentum while $\hat{R}_1, \hat{R}_2, \hat{R}_3$ are the components of the reduced Runge–Lenz vector which for the hydrogen atom is an additional constant of motion. The reduced Runge–Lenz vector is defined (in atomic units) by

$$\hat{\boldsymbol{R}} = \frac{1}{\sqrt{-2E}} \hat{\boldsymbol{M}} \quad \text{where } \hat{\boldsymbol{M}} = \tfrac{1}{2}(\hat{\boldsymbol{p}} \times \hat{\boldsymbol{l}} - \hat{\boldsymbol{l}} \times \hat{\boldsymbol{p}}) - \frac{Z\boldsymbol{r}}{r}.$$

3. Generalized Racah Tensors

Following Judd [16] and Butler and Wybourne [8] we introduce a set of irreducible tensor operators $\hat{v}_q^{(k)}(A,B)$ which satisfy the fundamental CR's

$$[\hat{l}_z, \hat{v}_q^{(k)}(A,B)] = q\hat{v}_q^{(k)}(A,B)$$

$$[\hat{l}_\pm, \hat{v}_q^{(k)}(A,B)] = \sqrt{k(k+1)-q(q\pm 1)}\,\hat{v}_{q\pm 1}^{(k)}(A,B) \tag{3}$$

with respect to the angular momentum operators $\hat{l}_z$ and $\hat{l}_\pm = \hat{l}_x \pm i\hat{l}_y$.

Using the Wigner–Eckart theorem the matrix elements between two single particle eigenfunctions become

$$\langle l', m'|\hat{v}_q^{(k)}(A,B)|l, m\rangle = (-1)^{l'-m'}\begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix}\langle l'\|\hat{v}^{(k)}(A,B)\|l\rangle. \tag{4}$$

In Eq. (4) $(\because)$ is a 3-j symbol and the reduced matrix element is defined by

$$\langle l'\|\hat{v}^{(k)}(A,B)\|l\rangle = \delta_{Al'}\delta_{Bl}[k]^{1/2}. \tag{5}$$

For convenience we use the abbreviation

$$[x, y, \ldots, z] = (2x+1)(2y+1)\ldots(2z+1).$$

For given values of A and B (≥ 0) non-zero operators can be constructed according to

$$|A-B| \leq k \leq A+B, \qquad q = 0, \pm 1, \pm 2, \ldots \pm k$$

for each value of k.

The operators can equally well be defined for half-integral quantum numbers. However in this paper we only study orbital transformations and half-integral numbers will not appear.

The general commutator can now be evaluated to give the result

$$\begin{aligned}[\hat{v}_{q_1}^{(k_1)}(A,B), \hat{v}_{q_2}^{(k_2)}(C,D)] = \sum_{k,q} (-1)^{k-q}[k_1, k_2, k]^{1/2}\begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} \\ \times\left[\delta_{BC}(-1)^{A+D+k_1+k_2}\begin{Bmatrix} k_1 & k_2 & k \\ D & A & B \end{Bmatrix}\hat{v}_q^{(k)}(A,D)\right. \\ \left. -\delta_{AD}(-1)^{B+C+k}\begin{Bmatrix} k_1 & k_2 & k \\ C & B & A \end{Bmatrix} v_q^{(k)}(C,B)\right]\end{aligned} \tag{6}$$

where $\{\because\}$ is a 6-j symbol.

For a many-electron system we can construct generalized Racah tensors by

$$\hat{V}_q^{(k)}(A,B) = \sum_i \hat{v}_q^{(k)}(A,B)_i.$$

4. Generalized Racah Tensors for the $R(4)$ Group

The simplest case of generalized Racah tensors occurs when $B = A$. In this case we have the three rank one operators $\hat{v}_q^{(1)}(A, A)$, $q = 0, \pm 1$ which are related to the spherical components of orbital angular momentum by, Judd [16]

$$\hat{l}_q^{(1)} = \sum_{A=0}^{n-1} \sqrt{\frac{A(A+1)(2A+1)}{3}}\, \hat{v}_q^{(1)}(A, A) \tag{7}$$

where n is the principal quantum number. It follows that the three operators $\hat{v}_q^{(1)}(A, A)$ are generators for the group $R(3)$.

When $|B-A| = 1$ we can construct the following six tensor operators $\hat{v}_q^{(1)}(A, A+1)$, $\hat{v}_q^{(1)}(A+1, A)$; $q = 0, \pm 1$. Three of these operators can be related to the spherical components of the reduced Runge–Lenz vector as follows

$$\hat{R}_q^{(1)} = \sum_{A=0}^{n-2} \sqrt{\frac{(A+1)(n^2-(A+1)^2)}{3}}\, [\hat{v}_q^{(1)}(A+1, A) - \hat{v}_q^{(1)}(A, A+1)]. \tag{8}$$

The set of six operators $\hat{l}_q^{(1)}$, $\hat{R}_q^{(1)}$ can be taken as the generators of an $R(4)$ group, Butler and Wybourne [8]. In what follows we shall refer to this $R(4)$ group as the R group.

In addition to the operators given by Eq. (8) we can also define three other tensor operators by

$$\hat{Q}_q^{(1)} = \sum_{A=0}^{n-2} \sqrt{\frac{(A+1)(n^2-(A+1)^2)}{3}}\, i[\hat{v}_q^{(1)}(A+1, A) + \hat{v}_q^{(1)}(A, A+1)] \tag{9}$$

and the Cartesian components of these operators can be shown to be Hermitian.

Using Eq. (6) we have evaluated the CR's in Cartesian components and we find that

$$[\hat{l}_i, \hat{Q}_j] = \sum_k \varepsilon_{ijk} i \hat{Q}_k \tag{10a}$$

$$\hat{\boldsymbol{Q}} \times \hat{\boldsymbol{Q}} = i\hat{\boldsymbol{l}}. \tag{10b}$$

By comparing Eqs. (1) and (10a), (10b) we see that the commutators of Eqs. (10a) and (10b) correspond to a Lie algebra which is isomorphic to that for $R(4)$. Since in the particular case of $R(4)$ this result contradicts Butler and Wybourne's [8] general assertion we present in an appendix a detailed derivation of Eqs. (10a) and (10b). We agree that the generators used by Alper and Sinanoglu [6] do not give an $R(4)$ group. However the generators that we have defined do give an $R(4)$ group. Because our generators have not been considered before we have a new $R(4)$ group which is not related to the work in [6], [7]. In what follows we shall refer to this new $R(4)$ group as the Q group. As we shall see, it is this new mathematical $R(4)$ group which gives approximate diagonalisation of the Coulomb interaction.

5. $\boldsymbol{R}(4)$ Groups and Phase Conventions

In previous work with $R(4)$ two different phase conventions have been used for the basis functions. One is the usual Condon and Shortley phase while the other is that introduced by Biedenharn [17].

Now the reduced matrix element of $\hat{\boldsymbol{R}}^{(1)}$ is given by

$$\langle n, l+1\|\hat{R}^{(1)}\|n, l\rangle = -\sqrt{(l+1)(n^2-(l+1)^2)}$$

and for this result to be true the Condon and Shortley phase convention must be used. For the $\hat{\boldsymbol{Q}}^{(1)}$ operators we find the relation

$$\langle n, l+1\|\hat{Q}^{(1)}\|n, l\rangle = -i\langle n, l+1\|\hat{R}^{(1)}\|n, l\rangle$$

The matrix representations of $\hat{R}_q^{(1)}$ and $\hat{Q}_q^{(1)}$ are thus related by a basis transformation corresponding to $|n, l, m\rangle_Q = (-i)^l|n, l, m\rangle_R$ where the subscripts on the kets indicate to which $R(4)$ group the kets belong. It follows that the matrix representations in the two $R(4)$ groups are equivalent. By simply using $|n, l, m\rangle_Q$ instead of $|n, l, m\rangle_R$ we now find that $|n, l, m\rangle_Q$ satisfy the Biedenharn phase convention.

As we shall see this has a profound significance when calculations are done using the different bases functions.

In connection with the work of Alper [11] the R group corresponds to his mathematical group. By introducing the Q group we have obtained a new mathematical group.

6. Doubly Excited States of Helium

In previous work with $R(4)$ symmetry the most studied application has been on doubly excited states of helium particularly the ^1S states arising from the configurations $2s^2$ and $2p^2$. With the usual $R(3)$ configurational basis these configurations are very strongly mixed with respect to the Coulomb interaction. If $R(4)$ symmetry basis functions are used for these states instead of the configurational basis functions the question arises as to whether the Coulomb interaction is approximately diagonalized. Alper and Sinanoglu [6] claim that their $R(4)$ basis functions do approximately diagonalize the Coulomb interaction but Rau [10] and Butler and Wybourne [9] have refuted this by stating that their generators do not give an $R(4)$ group.

Using hydrogenic functions the results of calculations on the diagonalization of the Coulomb interaction using the various bases sets are given in Table 1.

From Table 1 we can infer the following conclusions. In the configurational basis the $2s^2$ and $2p^2$ configurations are strongly mixed. In the R group basis used by Rau [10] and by Butler and Wybourne [9] there is no improvement on the mixing. However when the Q group basis is used the Coulomb interaction is very nearly diagonalized. It would thus appear that in this case at least the Q group is an

Table 1. Coulomb interaction eigenvectors for the doubly excited ^1S states of He

Eigenvalue (a.u.)	Configurational basis[a] $2s^2$	$2p^2$	R group basis[a] [0, 0]	[2, 0]	Q group basis[a] [0, 0]	[2, 0]
0.2459	0.7738	0.2262	0.7255	0.2745	0.0008	0.9992
0.4885	0.2262	0.7738	0.2745	0.7255	0.9992	0.0008

[a] Squares of eigenvector components.

approximate symmetry group. Unfortunately we have not yet been able to attach any physical interpretation to the Q group.

7. Conclusions

By introducing the Q group as a new $R(4)$ group we have resolved the phase anomaly pointed out by Rau [10].

Calculations on doubly excited states of helium indicate that the Q group might be an approximate symmetry group. Since however we cannot give a physical interpretation to the Q group we must conclude that the good approximate diagonalization of the Coulomb interaction in helium seems to be a fortuitous result.

Appendix

In this appendix we present a detailed derivation of Eqs. (10a) and (10b). For convenience we define a quantity $F(x)$ by

$$F(x)=\left[\frac{(x+1)(n^2-(x+1)^2)}{3}\right]^{1/2}. \tag{A1}$$

Using the definition of the $\hat{Q}$ operators given by Eq. (9) we can express the commutator relations between the spherical components as

$$[\hat{Q}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = -\sum_{A=0}^{n-2}\sum_{B=0}^{n-2} F(A)F(B)[\hat{v}^{(1)}_{q_1}(A, A+1) + \hat{v}^{(1)}_{q_1}(A+1, A), \hat{v}^{(1)}_{q_2}(B, B+1)+\hat{v}^{(1)}_{q_2}(B+1, B)]. \tag{A2}$$

Carrying out the summation over B we obtain

$$[\hat{Q}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = -\sum_{A=0}^{n-2} F(A)[F(A+1)\{[\hat{v}^{(1)}_{q_1}(A, A+1), \hat{v}^{(1)}_{q_2}(A+1, A+2)] + [\hat{v}^{(1)}_{q_1}(A+1, A), \hat{v}^{(1)}_{q_2}(A+2, A+1)]\} + F(A)\{[\hat{v}^{(1)}_{q_1}(A, A+1), \hat{v}^{(1)}_{q_2}(A+1, A)] + [\hat{v}^{(1)}_{q_1}(A+1, A), \hat{v}^{(1)}_{q_2}(A, A+1)]\}$$

$$+F(A-1)\{[\hat{v}_{q_1}^{(1)}(A,A+1),\hat{v}_{q_2}^{(1)}(A-1,A)]$$
$$+[\hat{v}_{q_1}^{(1)}(A+1,A),\hat{v}_{q_2}^{(1)}(A,A-1)]\}]. \tag{A3}$$

Eq. (A3) can now be reduced using the general commutator relation Eq. (6) to give

$$\begin{aligned}
[\hat{Q}_{q_1}^{(1)},\hat{Q}_{q_2}^{(1)}] = -\sum_{A=0}^{n-2} F(A)\sum_{k,q}(-1)^{k-q}3[k]^{1/2}\begin{pmatrix}1 & 1 & k\\ q_1 & q_2 & -q\end{pmatrix}\\
\times\Bigg[F(A+1)\begin{Bmatrix}1 & 1 & k\\ A+2 & A & A+1\end{Bmatrix}\\
\times[\hat{v}_q^{(k)}(A,A+2)-(-1)^k\hat{v}_q^{(k)}(A+2,A)]\\
+F(A)(1-(-1)^k)\\
\times\left[\begin{Bmatrix}1 & 1 & k\\ A & A & A+1\end{Bmatrix}\hat{v}_q^{(k)}(A,A)+\begin{Bmatrix}1 & 1 & k\\ A+1 & A+1 & A\end{Bmatrix}\hat{v}_q^{(k)}(A+1,A+1)\right]\\
+F(A-1)\begin{Bmatrix}1 & 1 & k\\ A-1 & A+1 & A\end{Bmatrix}\\
\times[\hat{v}_q^{(k)}(A+1,A-1)-(-1)^k\hat{v}_q^{(k)}(A-1,A+1)]\Bigg].
\end{aligned} \tag{A4}$$

Using the properties of the 6-j symbols we find that non-zero contributions will occur for only $k=1$ and 2 in the separate terms of Eq. (A4). Thus Eq. (A4) reduces to

$$\begin{aligned}
[\hat{Q}_{q_1}^{(1)},\hat{Q}_{q_2}^{(1)}] = -\sum_{A=0}^{n-2} F(A)\Bigg\{\sum_q 3\sqrt{5}(-1)^q\begin{pmatrix}1 & 1 & 2\\ q_1 & q_2 & -q\end{pmatrix}\\
\times\Bigg[F(A+1)\begin{Bmatrix}1 & 1 & 2\\ A+2 & A & A+1\end{Bmatrix}\\
\times[\hat{v}_q^{(2)}(A,A+2)-\hat{v}_q^{(2)}(A+2,A)]+F(A-1)\\
\times\begin{Bmatrix}1 & 1 & 2\\ A-1 & A+1 & A\end{Bmatrix}\\
\times[\hat{v}_q^{(2)}(A+1,A-1)-\hat{v}_q^{(2)}(A-1,A+1)]\Bigg]\\
+\sum_q 6\sqrt{3}(-1)^q\begin{pmatrix}1 & 1 & 1\\ q_1 & q_2 & -q\end{pmatrix}F(A)\Bigg[\begin{Bmatrix}1 & 1 & 1\\ A & A & A+1\end{Bmatrix}\hat{v}_q^{(1)}(A,A)\\
+\begin{Bmatrix}1 & 1 & 1\\ A+1 & A+1 & A\end{Bmatrix}\hat{v}_q^{(1)}(A+1,A+1)\Bigg]\Bigg\}.
\end{aligned} \tag{A5}$$

By a trivial rearrangement of the summation range over A we find that the terms involving tensor operators of rank two cancel each other out. For the remaining two rank one operator terms we obtain, by rearranging the summation over A in the second term,

$$[\hat{Q}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = \sum_q 2\sqrt{3}(-1)^q \begin{pmatrix} 1 & 1 & 1 \\ q_1 & q_2 & -q \end{pmatrix}$$

$$\times \sum_{A=1}^{n-1} \Big[(A+1)(n^2-(A+1)^2) \begin{Bmatrix} 1 & 1 & 1 \\ A & A & A+1 \end{Bmatrix}$$

$$+ A(n^2-A^2) \begin{Bmatrix} 1 & 1 & 1 \\ A & A & A-1 \end{Bmatrix} \Big] \hat{v}^{(1)}_q(A,A) \quad \text{(A6)}$$

By explicitly evaluating the 6-j symbols Eq. (A6) becomes

$$[\hat{Q}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = \sum_q (-1)^{1-q}\sqrt{6} \begin{pmatrix} 1 & 1 & 1 \\ q_1 & q_2 & -q \end{pmatrix} \sum_{A=1}^{n-1} \frac{[A(A+1)(2A+1)]^{1/2}}{\sqrt{3}} \hat{v}^{(1)}_q(A,A) \quad \text{(A7)}$$

Using Eq. (7) we see that Eq. (A7) can be written as

$$[\hat{Q}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = \sum_q (-1)^{1-q}\sqrt{6} \begin{pmatrix} 1 & 1 & 1 \\ q_1 & q_2 & -q \end{pmatrix} \hat{l}^{(1)}_q. \quad \text{(A8)}$$

Now Eq. (10b) is immediately obtained by transferring from spherical components to Cartesian components, using the well known result that

$$\hat{l}^{(1)}_1 = -\frac{1}{\sqrt{2}}(\hat{l}_x + i\hat{l}_y), \qquad \hat{l}^{(1)}_0 = \hat{l}_z, \qquad \hat{l}^{(1)}_1 = \frac{1}{\sqrt{2}}(\hat{l}_x - i\hat{l}_y).$$

Consider next the commutators

$$[\hat{l}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = i \sum_{A=0}^{n-2} F(A) \sum_{B=0}^{n-1} \left[\frac{B(B+1)(2B+1)}{3}\right]^{1/2}$$

$$\times [\hat{v}^{(1)}_{q_1}(B,B), \hat{v}^{(1)}_{q_2}(A,A+1) + \hat{v}^{(1)}_{q_2}(A+1,A)]$$

$$= i \sum_{A=0}^{n-2} F(A) \Big[\left[\frac{A(A+1)(2A+1)}{3}\right]^{1/2} \{[\hat{v}^{(1)}_{q_1}(A,A), \hat{v}^{(1)}_{q_2}(A,A+1)]$$

$$+ [\hat{v}^{(1)}_{q_1}(A,A), \hat{v}^{(1)}_{q_2}(A+1,A)\}$$

$$+ \left[\frac{(A+1)(A+2)(2A+3)}{3}\right]^{1/2} \{[\hat{v}^{(1)}_{q_1}(A+1,A+1), \hat{v}^{(1)}_{q_2}(A,A+1)]$$

$$+ [\hat{v}^{(1)}_{q_1}(A+1,A+1), \hat{v}^{(1)}_{q_2}(A+1,A)]\} \Big]. \quad \text{(A9)}$$

Again using Eq. (6) this reduces to

$$[\hat{l}^{(1)}_{q_1}, \hat{Q}^{(1)}_{q_2}] = i \sum_{A=0}^{n-2} F(A) \sum_{k,q} (-1)^{k-q} 3[k]^{1/2} \begin{pmatrix} 1 & 1 & k \\ q_1 & q_2 & -q \end{pmatrix}$$

$$\times \Big[-\left[\frac{A(A+1)(2A+1)}{3}\right]^{1/2} \times \begin{Bmatrix} 1 & 1 & k \\ A+1 & A & A \end{Bmatrix}$$

$$\times[\hat{v}_q^{(k)}(A, A+1)-(-1)^k\hat{v}_q^{(k)}(A+1, A)]$$
$$+\left[\frac{(A+1)(A+2)(2A+3)}{3}\right]^{1/2}\times\begin{Bmatrix}1 & 1 & k\\ A & A+1 & A+1\end{Bmatrix}$$
$$\times[(-1)^k\hat{v}_q^k(A, A+1)-\hat{v}_q^{(k)}(A+1, A)]\Big]. \tag{A10}$$

We now proceed as in the evaluation of the commutators $[\hat{Q}_{q_1}^{(1)}, \hat{Q}_{q_2}^{(1)}]$ and find that in the present case the only non-zero terms arise from tensors of rank one. By evaluating the 6-j symbols we find that Eq. (A10) becomes

$$[\hat{l}_{q_1}^{(1)}, \hat{Q}_{q_2}^{(1)}]=i\sum_{A=0}^{n-2}F(A)\sqrt{6}\sum_q(-1)^{1-q}\begin{pmatrix}1 & 1 & 1\\ q_1 & q_2 & -q\end{pmatrix}$$
$$\times[\hat{v}_q^{(1)}(A, A+1)+\hat{v}_q^{(1)}(A+1, A)]$$
$$=\sum_q(-1)^{1-q}\sqrt{6}\begin{pmatrix}1 & 1 & 1\\ q_1 & q_2 & -q\end{pmatrix}\hat{Q}_q^{(1)} \tag{A11}$$

where we have used the definition of $\hat{Q}_q^{(1)}$ given in Eq. (9). Eq. (A11) is clearly just that given by (10a) when we transfer to Cartesian components.

It must be stressed that the derivation in this appendix is for an $R(4)$ group only and thus cannot be compared to the result of Butler and Wybourne [8] who were concerned with generators for rotation groups of general even dimension. The fact that our generators for the new $R(4)$ group are closed under commutation probably stems from the fact that $R(4)$ is the only semi-simple rotation group in even dimensions. All the higher even dimension rotation groups are simple groups.

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References

1. Fock, V.: Z. Physik **98**, 145 (1935)
2. Bargmann, V.: Z. Physik **99**, 576 (1936)
3. Moshinsky, M.: Phys. Rev. **126**, 1880 (1962)
4. Wulfman, C. E.: Phys. Letters **26A**, 397 (1968)
5. Wulfman, C. E., in: Group theory and its applications, Vol. II., E. M. Loebl Ed. New York: Academic Press 1971
6. Alper, J. S., Sinanoglu, O.: Phys. Rev. **177**, 77 (1969)
7. Alper, J. S: Phys. Rev. **177**, 86 (1969)
8. Butler, P. H., Wybourne, B. G.: J. Math. Phys. **11**, 2512 (1970)
9. Butler, P. H., Wybourne, B. G.: J. Math. Phys. **11**, 2519 (1970)
10. Rau, A. R. P.: Phys. Rev. **A2**, 1600 (1970)
11. Alper, J. S.: Phys. Rev. **A2**, 1603 (1970)
12. Sinanoglu, O., Herrick, D. R.: J. Chem. Phys. **62**, 886 (1975)
13. Herrick, D. R., Sinanoglu, O.: Phys. Rev. A, **11**, 97 (1975)
14. Sinanoglu, O., Herrick, D. R.: Chem. Phys. Letters **31**, 373 (1975)

15. Chisholm, C. D. H., in: Group theoretical techniques in quantum chemistry. London: Academic Press 1976
16. Judd, B. R., in: Operator techniques in atomic spectroscopy. New York: McGraw-Hill 1963
17. Bidenharn, L. C.: J. Math. Phys. **2**, 433 (1961)

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