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The group $O(3)_\Lambda(T_2\times\bar{T}_2)$ and the hydrogen atom

J W B Hughes and J Yadegar

Department of Applied Mathematics, Queen Mary College, Mile End Road, London E1 4NS, UK

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Abstract. Properties of the seven parameter group $O(3)_\Lambda(T_2\times\bar{T}_2)$ are investigated using shift operator techniques. A complete classification and analysis of unitary irreducible representations is given and it is shown that a single arbitrary irreducible representation contains all those irreducible representations of the group O(4) which are realized by the hydrogen atom. Further, it is shown that the seven parameter group $O(3)_\Lambda(T_2\times\bar{T}_2)$ is equally as good a choice for the dynamical group of the hydrogen atom as the more usual fifteen parameter group O(4, 2).

1. Introduction

Shift operator techniques have been used to analyse irreducible unitary representations (IUR) of groups containing O(3) as a subgroup with respect to IUR of O(3) for the case of SU(3) (Hughes 1973a, b), O(4), O(3, 1) and E(3) (Hughes 1973b) and SL(3, R) (Hughes 1974). In all these cases the additional generators form an irreducible tensor representation $\{T(j,\mu), \mu=-j,\ldots,j\}$ of O(3) corresponding to integral j, and the analysis was performed using operators which shift the l values of states upon which they act by integral amounts ($l(l+1)$ is the eigenvalue of the O(3) Casimir L^2).

In this paper we consider a group in which the generators additional to those of O(3) form a reducible tensor representation of O(3), $\{T(\frac{1}{2},\pm\frac{1}{2}), \bar{T}(\frac{1}{2},\pm\frac{1}{2})\}$, so that the l shift operators constructed out of them change l by half-integral amounts. The group is denoted by $O(3)_\Lambda(T_2\times\bar{T}_2)$, where T_2, $\bar{T}_2$ denote mutually Hermitian two-dimensional translation groups, and is the simplest such group with $T(j,\mu)$ for which j is not integral; the apparently simpler group $O(3)_\Lambda T_2$ has no non-trivial unitary representations and is therefore not considered. The next simplest such group is SU(3) in an SU(2) basis, which has an extra generator of type T(0, 0); surprisingly, the techniques of this paper do yield new information even about that very well studied group, and this will be the subject of a later paper (Hughes and Yadegar 1976).

$O(3)_\Lambda(T_2\times\bar{T}_2)$ is interesting for several reasons. Firstly it is the smallest non-compact group with an O(3) subgroup for which l degeneracy occurs. Moreover, unlike the case of, for instance, SL(3, R) it is possible not only to give a complete classification of its IUR, but also to give explicit formulae for the matrix elements of its generators valid for arbitrary states of an arbitrary IUR.

The second reason why $O(3)_\Lambda(T_2\times\bar{T}_2)$ is interesting is that its enveloping algebra contains, in addition to an invariant, X, three O(3) scalar operators, Y_0 and $Y_\pm$, which, when normalized by a term depending on the eigenvalue x of X, themselves generate an O(3) group whose Casimir equals L^2. Hence for any fixed IUR, $O(3)_\Lambda(T_2\times\bar{T}_2)$ contains an O(4) subgroup and, moreover, this IUR contains, precisely once, each IUR of O(4) of type $l_1 = l_2 = l$. These are just the IUR of O(4) realized by the hydrogen atom (see for instance Hughes (1967) and references therein). $O(3)_\Lambda(T_2 \times \bar{T}_2)$ is therefore an alternative to O(4, 1) as the spectral group of the hydrogen atom.

One may, however, go even further and show that $O(3)_\Lambda(T_2 \times \bar{T}_2)$ is the dynamical group of the hydrogen atom, in the sense of Barut and Kleinert (1966) (see also Kleinert (1968) and Wybourne (1974) for a review of this work). These authors show that operators connecting states of different values of the principal quantum number, n, may be constructed which, together with the generators of the symmetry group O(4), close under commutation to give an IUR of the fifteen parameter group O(4, 2), and obtain expressions for the matrix elements of the dipole operator in terms of those of the O(4, 2) generators (thus justifying the name 'dynamical group').

If we identify our l with $\frac{1}{2}(n-1)$ we find that the n-shifting operators are precisely our l-shifting operators (our O(3) subgroup is not therefore, the group of space rotations generated by the angular momentum operators). Eight of these, together with Y_0, $Y_\pm$, L^2 and the generators l_0, $l_\pm$ of O(3) satisfy, for a fixed IUR of $O(3)_\Lambda(T_2 \times \bar{T}_2)$, the commutation relations of O(4, 2). Hence the IUR of O(4, 2) used by Barut and Kleinert may be replaced by a fixed, but arbitrary, IUR of the far more economical group $O(3)_\Lambda(T_2 \times \bar{T}_2)$. All the matrix elements of the O(4, 2) operators are in fact contained in those of the four operators $T(\frac{1}{2}, \pm\frac{1}{2})$ and their Hermitian conjugates $\bar{T}(\frac{1}{2}, \mp\frac{1}{2})$. The fact that this can be done is not altogether surprising, since the IUR of O(4, 2) used is highly degenerate.

In § 2 the properties of $O(3)_\Lambda(T_2 \times \bar{T}_2)$ will be discussed and the shift operators and their Hermiticity properties derived. The latter will be used in § 3 to give a classification and analysis of the group's IUR. The application of the group to the hydrogen atom is given in § 4.

2. The group $O(3)_\Lambda(T_2 \times \bar{T}_2)$

The basis for the Lie algebra of $O(3)_\Lambda(T_2 \times \bar{T}_2)$ is most conveniently chosen to consist of the O(3) generators l_0, $l_\pm$ together with two pairs of operators both of which transform under commutation with the l_0, $l_\pm$ as irreducible two-dimensional tensor representations of O(3). We denote these by $T(\frac{1}{2}, \pm\frac{1}{2}) \equiv q_{\pm\frac{1}{2}}$ and $\bar{T}(\frac{1}{2}, \pm\frac{1}{2}) \equiv \bar{q}_{\pm\frac{1}{2}}$ for short. Their non-vanishing commutation relations are

$$\begin{aligned} &[l_0, l_\pm] = \pm l_\pm, \qquad &&[l_+, l_-] = 2l_0 \\ &[l_0, \overset{(-)}{q}_{\pm\frac{1}{2}}] = \pm\tfrac{1}{2}\overset{(-)}{q}_{\pm\frac{1}{2}}, \qquad &&[l_\pm, \overset{(-)}{q}_{\mp\frac{1}{2}}] = \overset{(-)}{q}_{\pm\frac{1}{2}}. \end{aligned} \tag{1}$$

The $q_{\pm\frac{1}{2}}$ and $\bar{q}_{\pm\frac{1}{2}}$ mutually commute, as they have to in order that the Jacobi identity be satisfied for triples of operators such as $\{q_{\frac{1}{2}}, \bar{q}_{\frac{1}{2}}, \bar{q}_{-\frac{1}{2}}\}$.

The Hermiticity properties of the operators are given by

$$l_0^\dagger = l_0, \qquad l_\pm^\dagger = l_\mp, \qquad q_{\pm\frac{1}{2}}^\dagger = \pm\bar{q}_{\mp\frac{1}{2}}. \tag{2}$$

We note here that the group $O(3)_\Lambda T_2$ generated by l_0, $l_\pm$ and $q_{\pm\frac{1}{2}}$ has no non-trivial unitary representations since one cannot self-consistently have $q_{\pm\frac{1}{2}}^\dagger \propto q_{\mp\frac{1}{2}}$. The same applies to any group of the form $O(3)_\Lambda T_{2n}$ with n integral (see Edmonds 1957).

The group has one Casimir given by

$$X = q_{\frac{1}{2}}\bar{q}_{-\frac{1}{2}} - q_{-\frac{1}{2}}\bar{q}_{\frac{1}{2}} \tag{3}$$

and three O(3)-scalar operators:

$$Y_+ = -(2q_{\frac12}q_{-\frac12}l_0 + q_{-\frac12}q_{-\frac12}l_+ - q_{\frac12}q_{\frac12}l_-) \tag{4}$$

$$Y_- = (2\bar q_{\frac12}\bar q_{-\frac12}l_0 + \bar q_{-\frac12}\bar q_{-\frac12}l_+ - \bar q_{\frac12}\bar q_{\frac12}l_-) \tag{5}$$

$$Y_0 = (q_{\frac12}\bar q_{-\frac12}l_0 + q_{-\frac12}\bar q_{\frac12}l_0 + q_{-\frac12}\bar q_{-\frac12}l_+ - q_{\frac12}\bar q_{\frac12}l_-). \tag{6}$$

From (2) one may easily check that X is a positive definite Hermitian operator, and

$$Y_0^\dagger = Y_0, \qquad Y_\pm^\dagger = Y_\mp. \tag{7}$$

In addition, the Y satisfy the commutation relations

$$[Y_0, Y_\pm] = \pm XY_\pm, \qquad [Y_+, Y_-] = 2XY_0 \tag{8}$$

and

$$Y_+Y_- + Y_0^2 - XY_0 = X^2L^2. \tag{9}$$

The IUR of $O(3)_\Lambda(T_2\times \bar T_2)$ are labelled by the eigenvalues x of X, and the states of the IUR will be denoted by $|x; l, k, m\rangle$ where $l(l+1)$ and m are the eigenvalues of L^2 and l_0, and k is an additional parameter needed to distinguish states of the same l and m values in cases of l degeneracy. (k will in fact be chosen to be the eigenvalue of Y_0/x.) Provided we are concerned with a fixed IUR corresponding to $x \neq 0$, we may normalize the Y by dividing them by x. These normalized Y then clearly satisfy the commutation relations of the generators of a new O(3) whose Casimir equals L^2, the Casimir of the original O(3).

The matrix elements of the $\overset{(-)}{q}_{\pm\frac12}$ are given in terms of their reduced matrix elements and the Wigner 3–j symbols by (see Edmonds 1957)

$$\langle x; l', k', m'|\overset{(-)}{q}_\mu|x; l, k, m\rangle = (-1)^{l'-m'}\begin{pmatrix} l' & \frac12 & l \\ -m' & \mu & m\end{pmatrix}\langle x; l', k'\|\overset{(-)}{q}\|x; l, k\rangle \tag{10}$$

where $\mu = \pm\frac12$.

From l_0, $l_\pm$ and $q_{\pm\frac12}$ one can, in a manner completely analogous to that used by Hughes (1973a) construct shift operators which change the l values of states upon which they act by $\pm\frac12$. Since one must then also change m by a half integral amount, we have the choice as to whether we change m by $+\frac12$ or $-\frac12$. In fact, although we shall not need both as far as the analysis of the IUR is concerned, both will be needed in the application to the hydrogen atom. Denoting by R the operator whose eigenvalue is l, these operators, together with their analogues constructed using the $\bar q_{\pm\frac12}$, are

$$\overset{(-)}{O}{}^{\pm\frac12,\frac12} = \overset{(-)}{q}_{\frac12}(l_0 \pm R + \tfrac12(1\pm1)) + \overset{(-)}{q}_{-\frac12}l_+ \tag{11}$$

$$\overset{(-)}{O}{}^{\pm\frac12,-\frac12} = -\overset{(-)}{q}_{-\frac12}(l_0 \mp R - \tfrac12(1\pm1)) + \overset{(-)}{q}_{\frac12}l_-. \tag{12}$$

Provided these operators act upon basis states to the right, l_0 and R may be replaced by their eigenvalues. Their l and m shifting properties follow from the commutation relations

$$\begin{aligned} &[L^2, \overset{(-)}{O}{}^{\frac12,\pm\frac12}] = \overset{(-)}{O}{}^{\frac12,\pm\frac12}(R+\tfrac34), \qquad [L^2, \overset{(-)}{O}{}^{-\frac12,\pm\frac12}] = -\overset{(-)}{O}{}^{-\frac12,\pm\frac12}(R+\tfrac14),\\ &[l_0, \overset{(-)}{O}{}^{\pm\frac12,\frac12}] = \tfrac12\overset{(-)}{O}{}^{\pm\frac12,\frac12}, \qquad [l_0, \overset{(-)}{O}{}^{\pm\frac12,-\frac12}] = -\tfrac12\overset{(-)}{O}{}^{\pm\frac12,-\frac12}.\end{aligned} \tag{13}$$

Note here that whenever there is any doubt about the l and m values of the states upon which these shift operators act we shall prefix them with these l and m values. We shall always do this if in their expressions we are replacing R and l_0 by l and m.

From (2) one may, again in a manner completely analogous to that employed by Hughes (1973a), derive the Hermiticity properties of the shift operators. These are conveniently expressed by the equation

$$\langle x; l+\tfrac{1}{2}, k', m\pm\tfrac{1}{2}|O^{\frac{1}{2},\pm\frac{1}{2}}_{l,m}|x; l, k, m\rangle = \mp\frac{(2l+1)}{2(l+1)}\langle x; l+\tfrac{1}{2}, k', m\pm\tfrac{1}{2}|(\bar{O}^{-\frac{1}{2},\mp\frac{1}{2}}_{l+\frac{1}{2},m\pm\frac{1}{2}})^{\dagger}|x; l, k, m\rangle \tag{14}$$

and

$$\langle x; l-\tfrac{1}{2}, k', m\pm\tfrac{1}{2}|O^{-\frac{1}{2},\pm\frac{1}{2}}_{l,m}|x; l, k, m\rangle$$
$$= \mp\frac{(2l+1)}{2l}\langle x; l-\tfrac{1}{2}, k', m\pm\tfrac{1}{2}|(\bar{O}^{\frac{1}{2},\mp\frac{1}{2}}_{l-\frac{1}{2},m\pm\frac{1}{2}})^{\dagger}|x; l, k, m\rangle. \tag{15}$$

For the purpose of considering the IUR of $O(3)_{\Lambda}(T_2\times\bar{T}_2)$ it suffices to consider the normalized shift operators

$$\overset{(-)}{A}{}^{\pm\frac{1}{2}}_{l} = (l+m+\tfrac{1}{2}(1\pm1))^{-\frac{1}{2}}\,\overset{(-)}{O}{}^{\pm\frac{1}{2},\pm\frac{1}{2}}_{l,m}. \tag{16}$$

This effectively means that the internal O(3) structure of the IUR of $O(3)_{\Lambda}(T_2\times\bar{T}_2)$ has been divided out.

Equations (14) and (15) now imply

$$\langle x; l\pm\tfrac{1}{2}, k'|A^{\pm\frac{1}{2}}_{l}|x; l, k\rangle = \frac{\mp(2l+1)}{2(l+\frac{1}{2}\pm\frac{1}{2})}\langle x; l\pm\tfrac{1}{2}, k'|(\bar{A}^{\mp\frac{1}{2}}_{l\pm\frac{1}{2}})^{\dagger}|x; l, k\rangle \tag{17}$$

where the m dependence of the states has been suppressed.

One may now use (14) and (17) to obtain various useful relations between the matrix elements of those products of two O or two A which commute with L^2 and l_0. For brevity we write these down only for the A, the ones for the O being easily derivable from them. They are:

$$\begin{aligned}\langle x; l, k|A^{\pm\frac{1}{2}}_{l\mp\frac{1}{2}}\bar{A}^{\mp\frac{1}{2}}_{l}|x; l, k\rangle &= \mp\frac{2(l+\frac{1}{2}\mp\frac{1}{2})}{(2l+1)}\sum_{k'}|\langle x; l\mp\tfrac{1}{2}, k'|\bar{A}^{\mp\frac{1}{2}}_{l}|x; l, k\rangle|^2\\ &= \mp\frac{(2l+1)}{2(l+\frac{1}{2}\mp\frac{1}{2})}\sum_{k'}|\langle x; l, k|A^{\pm\frac{1}{2}}_{l\mp\frac{1}{2}}|x; l\mp\tfrac{1}{2}, k'\rangle|^2\end{aligned} \tag{18}$$

$$\begin{aligned}\langle x; l, k|\bar{A}^{\pm\frac{1}{2}}_{l\mp\frac{1}{2}}A^{\mp\frac{1}{2}}_{l}|x; l, k\rangle &= \pm\frac{2(l+\frac{1}{2}\mp\frac{1}{2})}{(2l+1)}\sum_{k'}|\langle x; l\mp\tfrac{1}{2}, k'|A^{\mp\frac{1}{2}}_{l}|x; l, k\rangle|^2\\ &= \pm\frac{(2l+1)}{2(l+\frac{1}{2}\mp\frac{1}{2})}\sum_{k'}|x; l, k|\bar{A}^{\pm\frac{1}{2}}_{l\mp\frac{1}{2}}|x; l\mp\tfrac{1}{2}, k'\rangle|^2.\end{aligned} \tag{19}$$

From these equations we see that $A^{-\frac{1}{2}}\bar{A}^{\frac{1}{2}}$ and $\bar{A}^{\frac{1}{2}}A^{-\frac{1}{2}}$ are positive definite Hermitian operators, whereas $A^{\frac{1}{2}}\bar{A}^{-\frac{1}{2}}$ and $\bar{A}^{-\frac{1}{2}}A^{\frac{1}{2}}$ are negative definite and Hermitian.

Finally, from the definitions of the shift operators and the Y_0, $Y_{\pm}$, one may readily verify the following equations:

$$A^{\frac{1}{2}}_{l-\frac{1}{2}}A^{-\frac{1}{2}}_{l} = A^{-\frac{1}{2}}_{l+\frac{1}{2}}A^{\frac{1}{2}}_{l} = Y_{+} \tag{20}$$

$$\bar{A}^{\frac{1}{2}}_{l-\frac{1}{2}}\bar{A}^{-\frac{1}{2}}_{l} = \bar{A}^{-\frac{1}{2}}_{l+\frac{1}{2}}\bar{A}^{\frac{1}{2}}_{l} = -Y_{-} \tag{21}$$

$$A^{\pm\frac12}_{l\mp\frac12}\bar A^{\mp\frac12}_{l}=\mp((l+\tfrac12(1\mp1))X\pm Y_0) \tag{22}$$

$$\bar A^{\pm\frac12}_{l\mp\frac12}A^{\mp\frac12}_{l}=\pm((l+\tfrac12(1\mp1))X\mp Y_0). \tag{23}$$

We now have all the mathematical apparatus necessary to consider the problem of classifying the IUR of $O(3)_\wedge(T_2\times\bar T_2)$, which we do in the following section.

3. The IUR of $O(3)_\wedge(T_2\times\bar T_2)$

The first task is to give a classification of the types of IUR that may occur; this amounts to classifying the possible values of x and $l_{\min}$ consistent with the Hermiticity condition x real and $x\geqslant0$, and the condition that $l_{\min}$ be a non-negative integer or half integer. The second task is to analyse the IUR, i.e. for a given IUR to specify the l values occurring and their degeneracies, to find a suitable labelling for states of the same l value, and to give the matrix elements between them of the generators $\overset{(-)}{q}_{\pm\frac12}$.

Clearly one must first perform the first task. We suppose a given IUR to correspond to the value x of X and to have the minimum l value $\underline{l}$. We suppress the m values of the states and when we refer to l being degenerate we do not count the $(2l+1)$-fold degeneracy due to the interval O(3) structure. For $\underline{l}$ to be the minimum value of l, we clearly must have

$$\overset{(-)}{A}{}^{-\frac12}_{\underline{l}}|x;\underline{l},k\rangle=0 \tag{24}$$

and this clearly implies that

$$A^{\frac12}_{\underline{l}-\frac12}A^{-\frac12}_{\underline{l}}|x;\underline{l},k\rangle=\bar A^{\frac12}_{\underline{l}-\frac12}\bar A^{-\frac12}_{\underline{l}}|x;\underline{l},k\rangle=0 \tag{25}$$

and

$$\bar A^{\frac12}_{\underline{l}-\frac12}A^{-\frac12}_{\underline{l}}|x;\underline{l},k\rangle=A^{\frac12}_{\underline{l}-\frac12}\bar A^{-\frac12}_{\underline{l}}|x;\underline{l},k\rangle=0. \tag{26}$$

Using equations (20)–(23) we see that

$$Y_\pm|x;\underline{l},k\rangle=Y_0|x;\underline{l},k\rangle=\underline{l}X|x;\underline{l},k\rangle=0. \tag{27}$$

Clearly then we must have $\underline{l}x=0$, which may be satisfied either if $x=0$, in which case we may have $\underline{l}=0,\frac12,1,\ldots$, or if $\underline{l}=0$, in which case x may take on any non-negative real value. These are the only types of IUR that may arise and we give first an analysis of the first type.

3.1. *The IUR $x=0$*

Here $\underline{l}$ may be any non-negative integer or half integer. Equation (8) shows that Y_0, $Y_\pm$ mutually commute so that they generate a group isomorphic to the three-dimensional translation group. All IUR of this Abelian group are one-dimensional, so any l value which may occur must be non-degenerate. Equation (9) implies that

$$Y_+Y_-+Y_0^2=0. \tag{28}$$

However, from the Hermiticity relation (7) it is readily verified that both Y_+Y_- and Y_0^2 are positive definite operators, so (28) implies that, for any value of l occurring in the IUR,

$$Y_\pm|l\rangle=Y_0|l\rangle=0.$$

Equations (20)–(23) then show that

$$\overset{(-)}{A}{}_l^{\pm\frac{1}{2}}|l\rangle = 0$$

so that there is no possibility of connecting states of different l values, in other words that the only l value occurring is $l = \underline{l}$. Also, since the matrix elements of the shift operators are proportional to the reduced matrix elements of the $\overset{(-)}{q}_{\pm\frac{1}{2}}$, we see that

$$\overset{(-)}{q}_{\pm\frac{1}{2}}|l, m\rangle = 0,$$

in other words the only generators with non-vanishing matrix elements are l_0 and $l_\pm$. We may therefore conclude that the $x = 0$ IUR of $O(3)_\Lambda(T_2 \times \bar{T}_2)$ are just the IUR of the O(3) subgroup. This is entirely analogous to the case of the Euclidean group $O(3)_\Lambda T_3$ (Hughes 1973c) which also possesses two types of IUR, one of which contains just a single l value and which is such that the matrix elements of the T_3 generators all vanish.

As far as the group $O(3)_\Lambda(T_2 \times \bar{T}_2)$ is concerned, we may therefore regard the $x = 0$ IUR as trivial. The $x \neq 0$ IUR, which we now consider, are by no means trivial.

3.2. *The* IUR $x \neq 0, \underline{l} = 0$

We restrict ourselves to the IUR specified by a fixed value of $x > 0$, and define

$$\hat{Y}_0 = \frac{1}{x} Y_0, \qquad \hat{Y}_\pm = \frac{1}{x} Y_\pm. \tag{29}$$

These normalized operators clearly satisfy the Hermiticity relations (7), and the commutation relations of the generators of an O(3) group. Whenever confusion may arise we label it $O^Y(3)$, to distinguish it from $O^l(3)$. Thus, for such an IUR, $O(3)_\Lambda(T_2 \times \bar{T}_2)$ contains in its enveloping algebra the group $O^l(3) \times O^Y(3)$, which is isomorphic to the group O(4). Not all IUR of O(4) may be realized in this way, since (9) implies

$$\hat{Y}_+\hat{Y}_- + \hat{Y}_0^2 - \hat{Y}_0 = L^2 = l_+l_- + l_0^2 - l_0 \tag{30}$$

so that the Casimirs of the two O(3) groups are equal. The IUR of O(4) realized are therefore precisely those realized by the hydrogen atom (Hughes 1967).

We may therefore choose the label k for the states $|x; l, k\rangle$ to be the eigenvalue of $\hat{Y}_0$. Using the well known properties of IUR of $O^Y(3)$ we see that for a fixed value of l, k takes on the range of values $k = -l, -l+1, \ldots, l-1, l$. Hence l is $(2l+1)$-fold degenerate or, if we include the degeneracy due to the internal $O^l(3)$ structure given by $m = -l, -l+1, \ldots, l-1, l$, l is $(2l+1)^2$-fold degenerate, this being the dimension of the IUR of O(4) specified by l.

We may also use the well known properties of IUR of O(3) to obtain

$$\begin{aligned} \hat{Y}_0|x; l, k\rangle &= k|x; l, k\rangle \\ \hat{Y}_\pm|x; l, k\rangle &= [(l \mp k)(l \pm k + 1)]^{\frac{1}{2}}|x; l, k \pm 1\rangle. \end{aligned} \tag{31}$$

This also fixes the relative phases of states corresponding to the same l but different k values.

Equations (20)–(23) may now be used to obtain the following actions of the double shift operators:

$$A^{\pm\frac12}_{l\mp\frac12}A^{\mp\frac12}_{l}|x;l,k\rangle=x[(l-k)(l+k+1)]^{\frac12}|x;l,k+1\rangle \tag{32}$$

$$\bar A^{\pm\frac12}_{l\mp\frac12}\bar A^{\mp\frac12}_{l}|x;l,k\rangle=-x[(l+k)(l-k+1)]^{\frac12}|x;l,k-1\rangle \tag{33}$$

$$A^{\pm\frac12}_{l\mp\frac12}\bar A^{\mp\frac12}_{l}|x;l,k\rangle=\mp x[l\pm k+\tfrac12\mp\tfrac12]|x;l,k\rangle \tag{34}$$

$$\bar A^{\pm\frac12}_{l\pm\frac12}A^{\mp\frac12}_{l}|x;l,k\rangle=\pm x[l\mp k+\tfrac12\mp\tfrac12]|x;l,k\rangle. \tag{35}$$

The effect of these operators on the k values of the states is due to the following easily verifiable commutation relations:

$$[Y_0,A^{\mp\frac12}_l]=\tfrac12 xA^{\pm\frac12}_l,\qquad [Y_0,\bar A^{\pm\frac12}_l]=-\tfrac12 x\bar A^{\pm\frac12}_l \tag{36}$$

i.e. $A^{\mp\frac12}_l$ raise, and $\bar A^{\mp\frac12}_l$ lower, k by $\frac12$.

If we insert equations (34) and (35) into (18) and (19) we obtain the values of the modulus of the matrix elements of $\overset{(-)}{A}{}^{\pm\frac12}$. The relative phases of states corresponding to values of l differing by $\pm\frac12$ can be fixed using equations (32) and (33). In this way we obtain the following actions:

$$A^{\pm\frac12}_l|x;l,k\rangle=\left(\frac{x(2l+1)(l\pm k+\frac12\pm\frac12)}{2(l+\frac12\pm\frac12)}\right)^{\frac12}|x;l\pm\tfrac12,k+\tfrac12\rangle \tag{37}$$

$$\bar A^{\pm\frac12}_l|x;l,k\rangle=\pm\left(\frac{x(2l+1)(l\mp k+\frac12\pm\frac12)}{2(l+\frac12\pm\frac12)}\right)^{\frac12}|x;l\pm\tfrac12,k-\tfrac12\rangle. \tag{38}$$

Since $|k|\leqslant l$, we see that $\overset{(-)}{A}{}^{+\frac12}$ never annihilates $|x;l,k\rangle$; hence there is no maximum l value and the IUR of $O(3)_\Lambda(T_2\times\bar T_2)$ is infinite dimensional. The states up to $l=\frac32$, together with the actions of the $\overset{(-)}{A}{}^{\pm}$, are depicted in figure 1.

We may now introduce the internal $O^l(3)$ structure of the IUR and reintroduce the m label. From equation (16) we obtain immediately

$$O^{\pm\frac12,\pm\frac12}_{l,m}|x;l,k,m\rangle=\left(\frac{x(2l+1)(l\pm k+\frac12\pm\frac12)(l+m+\frac12\pm\frac12)}{2(l+\frac12\pm\frac12)}\right)^{\frac12}|x;l\pm\tfrac12,k+\tfrac12,m\pm\tfrac12\rangle \tag{39}$$

$$\bar O^{\pm\frac12,\pm\frac12}_{l,m}|x;l,k,m\rangle=\pm\left(\frac{x(2l+1)(l\mp k+\frac12\pm\frac12)(l+m+\frac12\pm\frac12)}{2(l+\frac12\pm\frac12)}\right)^{\frac12}|x;l\pm\tfrac12,k-\tfrac12,m\pm\tfrac12\rangle. \tag{40}$$

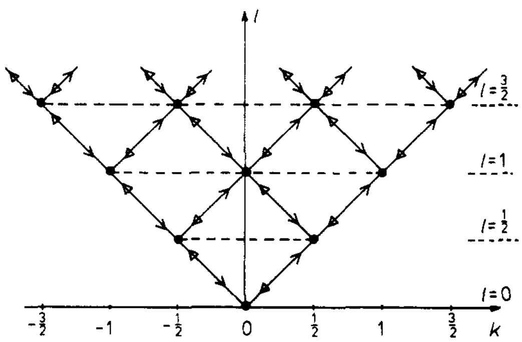

Figure 1. The O(3) content of the IUR $x>0$, $l_{\min}=0$ of $O(3)_\Lambda(T_2\times\bar T_2)$ for the first four l values. The IUR of O(3) are indicated by full circles; open arrows and closed arrows indicate the actions of the operators $A^{\pm\frac12}$ and $\bar A^{\pm\frac12}$, respectively.

Using equations (14) and (15), the above two equations can be used to obtain the actions of the $\overset{(-)}{q}_{\pm\frac{1}{2}}$. These are easily found to be

$$q_{\pm\frac{1}{2}}|x;l,k,m\rangle=\left(\frac{x(l+k+1)(l\pm m+1)}{2(2l+1)(l+1)}\right)^{\frac{1}{2}}|x;l+\tfrac{1}{2},k+\tfrac{1}{2},m\pm\tfrac{1}{2}\rangle$$
$$\pm\left(\frac{x(l-k)(l\mp m)}{2l(2l+1)}\right)^{\frac{1}{2}}|x;l-\tfrac{1}{2},k+\tfrac{1}{2},m\pm\tfrac{1}{2}\rangle \tag{41}$$

and

$$\bar{q}_{\pm\frac{1}{2}}|x;l,k,m\rangle=\left(\frac{x(l-k+1)(l\pm m+1)}{2(2l+1)(l+1)}\right)^{\frac{1}{2}}|x;l+\tfrac{1}{2},k-\tfrac{1}{2},m\pm\tfrac{1}{2}\rangle$$
$$\mp\left(\frac{x(l+k)(l\mp m)}{2l(2l+1)}\right)^{\frac{1}{2}}|x;l-\tfrac{1}{2},k-\tfrac{1}{2},m\pm\tfrac{1}{2}\rangle. \tag{42}$$

Putting these back into the parts of equations (14) and (15) relating to $\overset{(-)}{O}{}_{l}^{\pm\frac{1}{2},\mp\frac{1}{2}}$, yields

$$O_{l,m}^{\pm\frac{1}{2},\mp\frac{1}{2}}|x;l,k,m\rangle=\pm\left(\frac{x(2l+1)(l\pm k+\frac{1}{2}\pm\frac{1}{2})(l-m+\frac{1}{2}\pm\frac{1}{2})}{2(l+\frac{1}{2}\pm\frac{1}{2})}\right)^{\frac{1}{2}}|x;l\pm\tfrac{1}{2},k+\tfrac{1}{2},m\mp\tfrac{1}{2}\rangle \tag{43}$$

$$\bar{O}_{l,m}^{\pm\frac{1}{2},\mp\frac{1}{2}}|x;l,k,m\rangle=\left(\frac{x(2l+1)(l\mp k+\frac{1}{2}\pm\frac{1}{2})(l-m+\frac{1}{2}\pm\frac{1}{2})}{2(l+\frac{1}{2}\pm\frac{1}{2})}\right)^{\frac{1}{2}}|x;l\pm\tfrac{1}{2},k-\tfrac{1}{2},m\mp\tfrac{1}{2}\rangle. \tag{44}$$

Finally, using equation (10), the reduced matrix elements of $\overset{(-)}{q}$ can be obtained. The only non-vanishing ones are

$$\langle x;l\pm\tfrac{1}{2},k+\tfrac{1}{2}||q||x;l,k\rangle=\mp[x(l\pm k+\tfrac{1}{2}\pm\tfrac{1}{2})]^{\frac{1}{2}} \tag{45}$$

and

$$\langle x;l\pm\tfrac{1}{2},k-\tfrac{1}{2}||\bar{q}||x;l,k\rangle=-[x(l\mp k+\tfrac{1}{2}\pm\tfrac{1}{2})]^{\frac{1}{2}}. \tag{46}$$

This completes the analysis of the $x\neq 0$ IUR of $O(3)_\Lambda(T_2\times\bar{T}_2)$. The whole structure of the IUR is contained in equations (41) and (42), or alternatively in (45) and (46). The full weight diagram, together with the actions of the O shift operators, is depicted for l values up to $l=1$ in figure 2. One sees that every IUR of O(4) of hydrogenic type occurs precisely once, where we identify $l=\frac{1}{2}(n-1)$, n being the principal quantum number. $O(3)_\Lambda(T_2\times\bar{T}_2)$ may therefore be regarded as the spectral group of the hydrogen atom, in place of the usual O(4, 1). The given IUR of $O(3)_\Lambda(T_2\times\bar{T}_2)$ is clearly identical to the IUR of O(4, 1) used for this purpose. Also, there is a continuously infinite set of such IUR, all with this structure, corresponding to all positive real values of x. We shall see in the following section that $O(3)_\Lambda(T_2\times\bar{T}_2)$ is in fact the dynamical group of the hydrogen atom.

4. $O(3)_\Lambda(T_2\times\bar{T}_2)$ and the hydrogen atom

The O(4) symmetry of the hydrogen atom is a consequence (see Pauli 1926, Hughes 1967) of the fact that the quantum-mechanical angular momentum operator, $\boldsymbol{J}$, and the normalized Runge–Lenz vector $\hat{\boldsymbol{M}}$ commute with the Hamiltonian operator. If one defines

$$\hat{\boldsymbol{Y}}=\tfrac{1}{2}(\boldsymbol{J}+\hat{\boldsymbol{M}}),\qquad \boldsymbol{I}=\tfrac{1}{2}(\boldsymbol{J}-\hat{\boldsymbol{M}}) \tag{47}$$

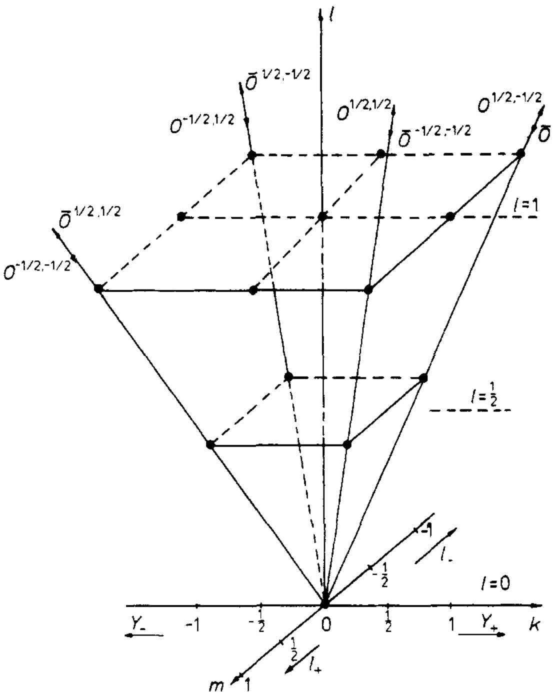

Figure 2. The states of the IUR $x>0$, $l_{\min}=0$ of $O(3)_\Lambda(T_2\times\bar{T}_2)$ for the first three l values, showing the directions of action of the various shift operators. The states $|x; l, k, m\rangle$ are indicated by full circles.

one may easily see that the components of $\hat{\boldsymbol{Y}}$ and $\boldsymbol{l}$ satisfy the same Hermiticity properties and commutation relations as do the l and $\hat{Y}$ operators of this paper, i.e. those of the group $O(4)=O^l(3)\times O^Y(3)$. Moreover, since $\boldsymbol{J}.\hat{\boldsymbol{M}}=\hat{\boldsymbol{M}}.\boldsymbol{J}=0$, one may easily deduce that the Casimirs of the two O(3) subgroups are equal and have the eigenvalues $l(l+1)$, where $l=0, \frac{1}{2}, 1, \ldots$, so the IUR of O(4) pertaining to the hydrogen atom are just the ones that occur for the $x>0$ IUR of $O(3)_\Lambda(T_2\times\bar{T}_2)$. Also, $2l+1=n$ is just the principal quantum number. Our states, for which l_0 and $\hat{Y}_0$ are diagonal, correspond to the Stark states of the hydrogen atom, $|n_1, n_2, M\rangle$, obtained by separating out the Schrödinger equation in parabolic cylinder coordinates (M is the eigenvalue of the angular momentum operator J_0). Hence we make the identification

$$|x; l, k, m\rangle \equiv |n_1, n_2, M\rangle \tag{48}$$

where we suppress the x label from the hydrogenic states, and (l, k, m) are related to (n_1, n_2, M) by

$$l=\tfrac{1}{2}(n_1+n_2+M), \qquad k=\tfrac{1}{2}(M+n_2-n_1), \qquad m=\tfrac{1}{2}(M-n_2+n_1) \tag{49}$$

whose inverse is

$$M=m+k, \qquad n_1=l-\tfrac{1}{2}k+\tfrac{1}{2}m-\tfrac{1}{2}|m+k|, \qquad n_2=l+\tfrac{1}{2}k-\tfrac{1}{2}m-\tfrac{1}{2}|m+k|. \tag{50}$$

Using equations (39), (40), (43) and (44) we may rewrite the actions of the O operators on $|n_1, n_2, M\rangle$, noting that raising l by $\pm\frac{1}{2}$ is equivalent to raising n by ± 1. Unfortunately the presence of the $|M|$ in the above two equations means that for four of these operators (the ones that change M), the cases $M>0$ and $M<0$ must be treated separately, which does make them a little tedious to write out. The actions are as follows for all values of M:

$$O^{\frac{1}{2},-\frac{1}{2}}|n_1, n_2, M\rangle = \left(\frac{xn(n_2+1)(n_2+|M|+1)}{(n+1)}\right)^{\frac{1}{2}}|n_1, n_2+1, M\rangle \tag{51}$$

$$O^{-\frac{1}{2},-\frac{1}{2}}|n_1, n_2, M\rangle = \left(\frac{xn\, n_1(n_1+|M|)}{(n-1)}\right)^{\frac{1}{2}}|n_1-1, n_2, M\rangle \tag{52}$$

$$\bar{O}^{\frac{1}{2},\frac{1}{2}}|n_1, n_2, M\rangle = \left(\frac{xn(n_1+1)(n_1+|M|+1)}{(n+1)}\right)^{\frac{1}{2}}|n_1+1, n_2, M\rangle \tag{53}$$

$$\bar{O}^{-\frac{1}{2},\frac{1}{2}}|n_1, n_2, M\rangle = \left(\frac{xn\, n_2(n_2+|M|)}{(n-1)}\right)^{\frac{1}{2}}|n_1, n_2-1, M\rangle \tag{54}$$

and

$$O^{\frac{1}{2},\frac{1}{2}}|n_1, n_2, M\rangle = \begin{cases} \left(\dfrac{xn(n_1+M+1)(n_2+M+1)}{(n+1)}\right)^{\frac{1}{2}}|n_1, n_2, M+1\rangle & \text{for } M\geqslant 0 \\ \left(\dfrac{xn(n_1+1)(n_2+1)}{(n+1)}\right)^{\frac{1}{2}}|n_1+1, n_2+1, M+1\rangle & \text{for } M<0 \end{cases} \tag{55}$$

$$O^{-\frac{1}{2},\frac{1}{2}}|n_1, n_2, M\rangle = \begin{cases} -\left(\dfrac{xnn_1n_2}{(n-1)}\right)^{\frac{1}{2}}|n_1-1, n_2-1, M+1\rangle & \text{for } M\geqslant 0 \\ -\left(\dfrac{xn(n_1-M)(n_2-M)}{(n-1)}\right)^{\frac{1}{2}}|n_1, n_2, M+1\rangle & \text{for } M<0 \end{cases} \tag{56}$$

$$\bar{O}^{-\frac{1}{2},-\frac{1}{2}}|n_1, n_2, M\rangle = \begin{cases} -\left(\dfrac{xn(n_1+M)(n_2+M)}{(n-1)}\right)^{\frac{1}{2}}|n_1, n_2, M-1\rangle & \text{for } M>0 \\ -\left(\dfrac{xnn_1n_2}{(n-1)}\right)^{\frac{1}{2}}|n_1-1, n_2-1, M-1\rangle & \text{for } M\leqslant 0 \end{cases} \tag{57}$$

$$\bar{O}^{\frac{1}{2},-\frac{1}{2}}|n_1, n_2, M\rangle = \begin{cases} \left(\dfrac{xn(n_1+1)(n_2+1)}{(n+1)}\right)^{\frac{1}{2}}|n_1+1, n_2+1, M-1\rangle & \text{for } M>0 \\ \left(\dfrac{xn(n_1-M+1)(n_2-M+1)}{(n+1)}\right)^{\frac{1}{2}}|n_1, n_2, M-1\rangle & \text{for } M\leqslant 0. \end{cases} \tag{58}$$

We now define the operators $N^{\pm}_{1,2}$, $A^{\pm}_{\pm}$, $A^{\mp}_{\pm}$ by

$$\begin{aligned} N_1^+ &= -\left(\frac{n+1}{xn}\right)^{\frac{1}{2}}\bar{O}^{\frac{1}{2},\frac{1}{2}}, & N_2^+ &= \left(\frac{n+1}{xn}\right)^{\frac{1}{2}}O^{\frac{1}{2},-\frac{1}{2}} \\ N_1^- &= -\left(\frac{n-1}{xn}\right)^{\frac{1}{2}}O^{-\frac{1}{2},-\frac{1}{2}}, & N_2^- &= \left(\frac{n-1}{xn}\right)^{\frac{1}{2}}\bar{O}^{-\frac{1}{2},\frac{1}{2}} \\ A_+^+ &= 2\left(\frac{n+1}{xn}\right)^{\frac{1}{2}}O^{\frac{1}{2},\frac{1}{2}}, & A_+^- &= 2\left(\frac{n-1}{xn}\right)^{\frac{1}{2}}O^{-\frac{1}{2},\frac{1}{2}} \\ A_-^- &= 2\left(\frac{n-1}{xn}\right)^{\frac{1}{2}}\bar{O}^{-\frac{1}{2},-\frac{1}{2}}, & A_-^+ &= -2\left(\frac{n+1}{xn}\right)^{\frac{1}{2}}\bar{O}^{\frac{1}{2},-\frac{1}{2}} \\ N &= 2R+1. \end{aligned} \tag{59}$$

Using equations (51)–(58) one may readily verify that the operators given by equations (59) have precisely the same actions on the $|n_1, n_2, M\rangle$ as do those of the same name introduced by Barut and Kleinert (1966). These authors showed that the above operators, together with the O(4) generators, generate the group O(4, 2), where N is the generator of the O(2) subgroup occurring in the chain $O(4,2)\supset O(4)\times O(2)\supset O(2)$. In fact the expressions of Barut and Kleinert for these operators contain M, not $|M|$; for instance they write $n=n_1+n_2+M+1$, which is valid only for $M\geqslant 0$, rather than $n=n_1+n_2+|M|+1$. Their expressions for the actions of the $N^{\pm}_{1,2}$, $A^{\pm}_{\pm}$ and $A^{\mp}_{\pm}$ on $|n_1, n_2, M\rangle$ are therefore valid only for $M\geqslant 0$, whereas ours are valid for all values of M. It is easy to check that the commutation relations for our operators are the same for negative M as for positive M and may therefore be regarded as the generalizations to all values of M of the operators of Barut and Kleinert. Note that the expressions for the operators of equation (59) contain an n-dependent normalization; this is entirely analogous to the fact that our shift operators contain factors containing l in their expressions in terms of the generators of $O(3)_\Lambda(T_2\times\bar T_2)$.

Barut and Kleinert show that the matrix elements of the dipole operator can be given in terms of those of the O(4, 2) operators, and therefore call O(4, 2) the 'dynamical group' of the hydrogen atom. We see from the above that we may call $O(3)_\Lambda(T_2\times\bar T_2)$ the dynamical group of the hydrogen atom. Everything that can be done using the fifteen parameter group O(4, 2) can be achieved using our seven parameter group. In fact both the symmetry and dynamical properties of the hydrogen atom are contained in the actions of the generators of $O(3)_\Lambda(T_2\times\bar T_2)$, which we give below:

$$l_0|n_1, n_2, M\rangle=\tfrac{1}{2}(M-n_2+n_1)|n_1, n_2, M\rangle \tag{60}$$

$$l_+|n_1, n_2, M\rangle=\begin{cases}[n_2(n_1+M+1)]^{\frac{1}{2}}|n_1, n_2-1, M+1\rangle & \text{for } M\geqslant 0\\ [(n_1+1)(n_2-M)]^{\frac{1}{2}}|n_1+1, n_2, M+1\rangle & \text{for } M<0\end{cases} \tag{61}$$

$$l_-|n_1, n_2, M\rangle=\begin{cases}[(n_2+1)(n_1+M)]^{\frac{1}{2}}|n_1, n_2+1, M-1\rangle & \text{for } M>0\\ [n_1(n_2-M+1)]^{\frac{1}{2}}|n_1-1, n_2, M-1\rangle & \text{for } M\leqslant 0\end{cases} \tag{62}$$

$$\begin{aligned}q_{-\frac{1}{2}}|n_1, n_2, M\rangle&=\left(\frac{x(n_2+1)(n_2+|M|+1)}{n(n+1)}\right)^{\frac{1}{2}}|n_1, n_2+1, M\rangle\\&\quad-\left(\frac{xn_1(n_1+|M|)}{n(n-1)}\right)^{\frac{1}{2}}|n_1-1, n_2, M\rangle\end{aligned} \tag{63}$$

$$\begin{aligned}\bar q_{\frac{1}{2}}|n_1, n_2, M\rangle&=\left(\frac{x(n_1+1)(n_1+|M|+1)}{n(n+1)}\right)^{\frac{1}{2}}|n_1+1, n_2, M\rangle\\&\quad-\left(\frac{xn_2(n_2+|M|)}{n(n-1)}\right)^{\frac{1}{2}}|n_1, n_2-1, M\rangle\end{aligned} \tag{64}$$

$$\begin{aligned}q_{\frac{1}{2}}|n_1, n_2, M\rangle&=\left(\frac{x(n_1+M+1)(n_2+M+1)}{n(n+1)}\right)^{\frac{1}{2}}|n_1, n_2, M+1\rangle\\&\quad+\left(\frac{xn_1n_2}{n(n-1)}\right)^{\frac{1}{2}}|n_1-1, n_2-1, M+1\rangle \qquad \text{for } M\geqslant 0\\ q_{\frac{1}{2}}|n_1, n_2, M\rangle&=\left(\frac{x(n_1+1)(n_2+1)}{n(n+1)}\right)^{\frac{1}{2}}|n_1+1, n_2+1, M+1\rangle\end{aligned} \tag{65}$$

$$
\begin{aligned}
&\qquad +\left(\frac{x(n_1-M)(n_2-M)}{n(n-1)}\right)^{\frac{1}{2}}|n_1, n_2, M+1\rangle && \text{for } M<0 \\
\bar{q}_{-\frac{1}{2}}|n_1, n_2, M\rangle &= \left(\frac{x(n_1+M)(n_2+M)}{n(n-1)}\right)^{\frac{1}{2}}|n_1, n_2, M-1\rangle \\
&\qquad +\left(\frac{x(n_1+1)(n_2+1)}{n(n+1)}\right)^{\frac{1}{2}}|n_1+1, n_2+1, M-1\rangle && \text{for } M>0 \\
\bar{q}_{\frac{1}{2}}|n_1, n_2, M\rangle &= \left(\frac{xn_1n_2}{n(n-1)}\right)^{\frac{1}{2}}|n_1-1, n_2-1, M-1\rangle \\
&\qquad +\left(\frac{x(n_1-M+1)(n_2-M+1)}{n(n+1)}\right)^{\frac{1}{2}}|n_1, n_2, M-1\rangle && \text{for } M\leqslant 0.
\end{aligned}
\tag{66}
$$

These operators presumably have a direct physical interpretation in terms of the hydrogenic wavefunctions. They could, in principle, be written down in terms of the angular momentum and Runge–Lenz operators and, thereby, be expressed as differential operators in terms of the space coordinates. The authors intend to investigate these possibilities further and hope to publish their results in due course.

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