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GROUP PROPERTIES OF RADIAL WAVEFUNCTIONS (*)

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Résumé. — Le groupe non-compact O (2, 1) est utilisé pour les fonctions d'ondes radiales hydrogénoïdes : on peut montrer que ces fonctions forment les bases des représentations des dimensions infinies de l'algèbre de O (2, 1). On trouve également que \( r^s \) et \( r^{-s} \) (\( s \) positif) se transforment dans cette algèbre comme des tenseurs. L'analyse des éléments de matrice de \( r^s \) et \( r^{-s} \) montre que le théorème de Wigner-Eckart est valable pour ce groupe et que les coefficients de Clebsch-Gordan correspondants sont proportionnels aux coefficients de Clebsch-Gordan du groupe \( R(3) \) qui sont très bien connus. Cette proportionnalité fournit des explications simples des règles de sélection, trouvées par Pasternack et Sternheimer, sur les éléments de matrice radiaux hydrogénoïdes. On démontre par ailleurs que les éléments diagonaux hydrogénoïdes de \( r^s \) et \( r^{-s} \) sont proportionnels à des symboles \( 3 - j \).

Abstract. — The non-compact group O (2, 1) is used in an investigation of hydrogenic radial wavefunctions. These radial functions are shown to form bases for infinite dimensional representations of the algebra of O (2, 1). It is found that \( r^s \) and \( r^{-s} \) (\( s \) positive) transform as tensors with respect to this algebra. Analysis of matrix elements of \( r^s \) and \( r^{-s} \) shows that the Wigner-Eckart theorem is valid for this group and that the pertinent Clebsch-Gordan coefficients are proportional to the familiar \( R(3) \) Clebsch-Gordan coefficients. This proportionality provides simple explanations of the selection rules for hydrogenic radial matrix elements noted by Pasternack and Sternheimer, and the proportionality of hydrogenic expectation values of \( r^s \) and \( r^{-s} \) to \( 3 - j \) symbols.

1. Introduction. — Although the hydrogen atom has been studied in great detail for many years, many of its properties are not yet fully understood. For example, several years ago it was noted by Pasternack and Sternheimer [1] that hydrogenic radial matrix elements satisfy certain selection rules:

\[
\int \frac{R_{nl} R_{nl'}}{r^s} \; dr = 0 \quad s = 2, 3, ..., |l - l'| + 1.
\]

where the radial wavefunction is \( R_{nl}/r \). In addition, expectation values of powers of \( r \) calculated with hydrogenic functions [2] can be seen to be proportional to \( 3 - j \) symbols in which \( l \) plays the part of the angular momentum, and the principal quantum number, \( n \), plays the part of a magnetic quantum number, e. g.

\[
<1/r^s>_{nl} = \frac{Z^s(3 n^2 - l(l + 1))}{2 n^s(l + \frac{1}{2})(l + \frac{1}{2})(l + 1)} \frac{1}{(l - \frac{1}{2})}
\]

which is clearly proportional [3] to the \( 3 - j \) symbol

\[
\begin{pmatrix}
  l & 2 & l \\
  n & 0 & n
\end{pmatrix}
\]

That properties of the radial function such as these are not well understood emphasizes the lack of interest which has traditionally been shown in this portion of the total wavefunction. The atomic physicist has concentrated his attention on the angular portion of the wavefunction, the spherical harmonics. Group theory has been vigorously applied to this study of angular wavefunctions, and has proved to be invaluable [4]. The high-energy theorist, on the other hand, has been interested in the group properties of the entire wavefunction of the hydrogen atom, and so has considered this atom in the light of such groups as O(4), O(4, 1) and O(4, 2) [5], [6], [7].

In the commonly used central field model of the atom, one considers separately the radial and angular parts of the wavefunction. Thus, a study of the group properties of the radial functions alone is of great interest to the atomic theorist. In the remainder of this paper, we propose to carry out such a study for the hydrogen atom. Application to other systems will be discussed in the final section.

2. The Group Algebra. — We find that our study can be carried out using a three-dimensional algebra composed of the operators \( J_+ \), \( J_- \), and \( J_3 \), having the commutators

\[
\begin{align*}
[J_3, J_+] &= \pm J_3 \\
[J_+, J_-] &= 2 J_3.
\end{align*}
\]

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The desired realization of these operators in two variables \((r, z)\) is given by [8]
\[
J_3 = -i \frac{\partial}{\partial r} \\
J_- = e^{i \alpha} \left( z \frac{\partial}{\partial z} \mp i \frac{\partial}{\partial r} \mp \frac{z}{2} \right).
\]
\[
(2)
\]

Bases for representations of this algebra can be formed by the functions
\[
f_{n\ell} = \left[ \frac{(n - l - 1)! (2 l + 1)}{(n + l)! 2 \pi} \right]^{\frac{1}{2}} \times \times e^{i n r} e^{-z^2 / 2} L^{l+1}_{n-l-1}(z)
\]
where \(L^k\) is the Laguerre polynomial of Morse and Feshbach [9]. This function is simply related to hydrogenic radial functions by
\[
\langle f_{n\ell} | r \rangle = e^{i n r} \left( \frac{2 l + 1}{2 \pi} \right)^{\frac{1}{2}} \left( \frac{n}{2} \right)^{\frac{1}{2}} R_{n\ell},
\]
where \(Ze\) is the charge of the nucleus.

Using (2) and (3), one obtains
\[
J_3 f_{n\ell} = n f_{n\ell} \\
J_- f_{n\ell} = \pm \left[ \pm (n \mp l) (n \pm l + 1) \right]^{\frac{1}{2}} f_{n\ell \pm 1}
\]
The Casimir operator for this algebra, which is given by \(G = J_+ J_- + J_3^2 - J_3\), can be shown, using (2) and (5), to satisfy the relationship
\[
G f_{n\ell} = \left( \frac{2}{3} \frac{d^2}{dr^2} + 2n - \frac{z^2}{\ell} \right) f_{n\ell} = l(l + 1) f_{n\ell}.
\]
Using (5), one finds that
\[
J_- f_{n\ell} = 0,
\]

implying that the basis has a lower bound when
\[
n = \ell = l + 1.
\]
There is, however, no upper bound, since \(J_+ f_{n\ell} \neq 0\) for all \(n \gg \ell\); the representation is thus infinite dimensional. It is also clearly irreducible. This algebra is thus the complexification of an algebra isomorphic to the algebras of the three-dimensional non-compact groups (e.g., SU(1, 1), O(2, 1)). Operators very similar to these have, in fact, been used by Barut and Kleinert [5] in a study of a subgroup of \(O(4, 2)\), an \(O(2, 1)\) group which they called the «transition group» of the hydrogen atom. As we shall see later, the algebra of Barut and Kleinert [5] does not appear to be useful in the context of the problem we wish to consider.

Finally, we define a Hilbert space as the space of functions \(f_{n\ell}\) with inner product
\[
(f_{n\ell} | f_{n'\ell'}) = \int f_{n\ell}^* f_{n'\ell'} d\Omega,
\]
where \(d\Omega = z^{-2} dr \cdot dz\). One can easily show that, in this space, the \(f_{n\ell}\) are orthonormal
\[
(f_{n\ell} | f_{n'\ell'}) = \delta(l, l') \delta(n, n') .
\]
Using (2), (6) and integrating by parts, one obtains
\[
(f_{n\ell} | J_3 f_{n'\ell'}) = (J_3 f_{n\ell} | f_{n'\ell'}) ,
\]
\[
(f_{n\ell} | J_- f_{n'\ell'}) = -(J_- f_{n\ell} | f_{n'\ell'}) .
\]
These results imply that the representations of \(O(2, 1)\), formed by the states \(f_{n\ell}\) are unitary [10]. We shall refer to irreducible representations of this type as \(D_{n\ell}^{+}\).

3. Operators. — We wish to consider matrix elements of operators of the type \(r^{-k} e^{i \alpha} (= T_{k}^{(q)})\) and \(r^k e^{i \alpha} (= P_{k}^{(q)})\), where \(k \geq 0\) and integer in both cases. The manner in which these operators transform with respect to the operations of the group is determined by their commutators with the group algebra:
\[
[J_\pm, T_{q}^{(k)}] = -(k \mp q) T_{q}^{(k)}
\]
\[
[J_3, T_{q}^{(k)}] = q T_{q}^{(k)}
\]
\[
[J_\pm, P_{q}^{(k)}] = (k \pm q) P_{q}^{(k)}
\]
\[
[J_3, P_{q}^{(k)}] = q P_{q}^{(k)} .
\]

It is convenient to also define states \(G_{k\ell}q\) and \(H_{k\ell}q\) which satisfy the relations
\[
J_\pm G_{k\ell}q = -(k \mp q) G_{k\ell \pm 1}
\]
\[
J_3 G_{k\ell}q = q G_{k\ell}q
\]
\[
J_\pm H_{k\ell}q = (k \pm q) H_{k\ell \pm 1}
\]
\[
J_3 H_{k\ell}q = q H_{k\ell}q .
\]

The transformation properties of the quantity produced by the action of \(T_{q}^{(k)}\) on \(f_{n\ell}\) are then the same as the transformation properties of the product
\[
G_{k\ell}q f_{n\ell} .
\]
A corresponding relationship holds, of course, between \(P_{q}^{(k)} f_{n\ell}\) and \(H_{k\ell} f_{n\ell}\). If the Wigner-Eckart theorem holds in this space, therefore, we can study the effects of operators by carrying out a more straightforward investigation of the coupling of two states. In following this procedure we are, of course, imitating the traditional techniques used in \(R(3)\). We shall assume that the Wigner-Eckart theorem is valid for this non-compact group; this assumption will later be shown to be consistent with our results.

One notes immediately that the states \(G_{k\ell}q\) form a representation of the algebra which is not fully reducible. However, one can form an irreducible representation in the subspace with \(|q| \leq k\). We shall henceforth consider only this subspace, and shall denote
GROUP PROPERTIES OF RADIAL WAVEFUNCTIONS

C4-19

this $2k + 1$ dimensional representation by $\mathcal{D}(k)$. One can also form a (not-fully) reducible representation using the states $\mathcal{H}_k$. Irreducible representations can, in this case, be formed in the subspaces with $|q| \geq k$.

However, we shall find it convenient to deal with the entire reducible representation, which we denote as $\mathcal{D}_k$. A representation of $O(2, 1)$ can be unitary only if, among other things, the eigenvalues of $J_+$, $J_-$, and $J_0$ are real and negative definite [10]. Clearly, this is not the case for representations having as bases either $\mathcal{H}_k$ or $\mathcal{H}_k$ with $|q| \leq k$. Thus neither $\mathcal{D}(k)$ nor $\mathcal{D}_k$ is unitary. This result is in agreement with that of Barut and Fronsdal [10], who found no finite dimensional unitary representations of $O(2, 1)$ (except for the trivial 1-dimensional representation).

4. The Product Representation $\mathcal{D}(k) \times \mathcal{D}_l^+$

We now consider the product representation

$$\mathcal{D}(k) \times \mathcal{D}_l^+, \tag{80}$$

with basis formed by the functions $G_{kl}/l_0$. We must first decompose this product representation into irreducible representations of the algebra (2). By considering the possible eigenvalues of $J_0$, one finds immediately that

$$\mathcal{D}(k) \times \mathcal{D}_l^+ = \sum_{l' = l-k}^{l+k} \mathcal{D}_{l'}^+ \quad l \geq k$$

$$= 2 \sum_{l' = -k}^{k-l} \mathcal{D}_{l'}^+ + \sum_{l' = k-l}^{k+l} \mathcal{D}_{l'}^+ + \sum_{l' = 0}^{k-l-1} \mathcal{D}(l') \quad k \geq l. \tag{11}$$

In order to carry out any actual calculations, of course, we must obtain the Clebsch-Gordan coefficients for this decomposition. In the general case, these coefficients will be difficult to find because of the complexity of (11) when $k \geq l$. We shall see, however, that we can restrict ourselves to the range $l' \geq |k - l|$ for the purposes of this problem; in this range, the coefficients can be obtained in a straightforward manner using the techniques of Racah [11].

Before proceeding, it is advantageous to renormalize the states $G_{kl}$ such that the new states, called $g_{kl}$, satisfy the equations

$$J_ \pm g_{kl} = [(k \mp q) (k \pm q + 1)]^{1/2} g_{k\pm 1}$$

$$J_0 g_{kl} = (k - l) g_{kl}. \tag{12}$$

We can also renormalize our operators in order to keep the transformation properties of the states and operators the same. The renormalized operators, $t_q^{(l)}$, can be written as

$$t_q^{(l)} = (-1)^l k! [(k - q)! (k + q)!]^{-1/2} T_q^{(l)}. \tag{13}$$

One can easily verify that these operators satisfy the commutation relations

$$[J_+ t_q^{(k)}, t_{-q}^{(l)}] = [(k \mp q) (k \pm q + 1)]^{1/2} t_{q\pm 1}^{(k)}$$

$$[J_0 t_q^{(k)}, t_{-q}^{(l)}] = q t_q^{(k)}. \tag{14}$$

With the definition (12), one has

$$(g_{kl'}, | J_\pm | g_{kl}) = (J_\mp g_{kl'}, | g_{kl}) \tag{15}$$

which again emphasizes that the $g_{kl}$ do not form a unitary representation of the algebra.

We now proceed to determine the coefficients $B(kq, ln | l' n')$

which appear in the expansion

$$| F_{ln} = \sum_{l,n} B(kq, ln | l' n') g_{kl} f_{ln} \tag{16}$$

where the states $F_{ln}$ form a unitary basis for $\mathcal{D}_l^+$, i.e.

$$J_\pm F_{ln} = \pm \left[ (n' \mp l') (n' \pm l' \pm 1) \right]^{1/2} F_{ln \pm 1}$$

$$J_0 F_{ln} = n' F_{ln'}, \tag{17}$$

$$J_\pm | F_{ln} = \delta(l, l') \delta(n, n'),$$

and $l' \geq |l - k|$. This final condition assures the simple form of (16).

The calculation proceeds in a straightforward manner: we first operate on both sides of (16) with $J_-$ and obtain the recursion relation

$$-[(k - q) (k + q + 1)]^{1/2} B(kq - 1, ln | l' n') +$$

$$+[(n - l) (n + l + 1)]^{1/2} B(kq, ln + 1 | l' n') =$$

$$= [n' - l' - 1] (n' + l') B(kq, ln | l' n' - 1). \tag{18a}$$

Operation on both sides of (16) with $J_+$ leads to another set of recursion relations:

$$[(k - q + 1) (k + q)]^{1/2} B(kq + 1, ln | l' n') +$$

$$+[(n - l - 1) (n + l + 1)]^{1/2} B(kq, ln - 1 | l' n') =$$

$$= [n' - l' + 1] (n' + l') B(kq, ln | l' n' + 1). \tag{19a}$$

In order to avoid square roots, we define a new variable $f(q, n, n')$:

$$B(kq, ln | l' n') = (-1)^{l+1+l'} [(k - q)! (k + q)!$$

$$\times (l + n)! (l' + n')! (n - l - 1)! (n' - l' - 1)!]^{1/2} \times f(q, n, n'). \tag{20}$$

Eq. (18a) then becomes

$$(n' + l') (n' - l' - 1) f(q, n, n' - 1) =$$

$$= -f(q + 1, n, n') f(q, n + 1, n' - 1) \tag{18b}$$

and (19a) becomes

$$f(q, n, n' + 1) =$$

$$= (k - q + 1) (k + q) f(q - 1, n, n') +$$

$$+ (n - l - 1) (n + 1) f(q, n - 1, n'). \tag{19b}$$

When $n' = l' + 1 = n'$, (18b) becomes

$$f(q + 1, n, n') = f(q, n + 1, n'). \tag{20b}$$
\[ f(q, n, n') = \frac{(k+q)!}{(k-l'+n-l-1)!} \frac{(n+l)!(n-l-1)!}{(n-l'-1-i)!} \times (n'-l'+1+i)! \frac{(n-q)!}{(n-l'-1-i)!} \times (n-l'-1-i)! \]

where we have also used the obvious equality \( n + n = n' \).

Because of the difference between (8) and (15), the expansion coefficients for the bras will not be the same as the expansion coefficients for the kets obtained above. We must therefore consider the coefficients \( A(kq, ln | l' n') \) which appear in the expansion

\[ (F_{l'n'}) = \sum_{k,n} A(kq, ln | l' n') (g_{lk}) | f_{ln} \].

These coefficients can be obtained by operating on both sides of (22) with the operators \( (J_{z}^{+})^{p} \) following the procedure given above. If we impose one further condition, that is,

\[ B(kk, ll + 1 | k + l k + l + 1) = A(kk, ll + 1 | k + l k + l + 1) = 1, \]

we find the different coefficients are simply related by

\[ B(kq, ln | l' n') = (-1)^{l'+q} A(kq, ln | l' n'). \]

The inverse transformations, that is, expansions of the product \( (g_{lk}) | f_{ln} \), cannot be so easily carried out because of the complexity of the second of eq. (11). We shall not consider these inverse transformations any further.

Finally, using eqs (16), (22) and (23) we obtain the orthogonal relationships

\[ \sum_{k,n} A(kq, ln | l' n') A(kq, ln | l'' n'') (-1)^{l'+q} = \delta(l', l'') \delta(n', n''). \]

We see that the inverse transformation to the \( A's \) is not obtained simply by taking the conjugate transpose. This result demonstrates that the transformations are not unitary — a result of the representation \( \delta(k) \) not being unitary itself.

We can use eq. (24) to obtain the constant \( B \). Using (20) and (21) to obtain \( A(kq, ln | l' n') \), specializing to the case \( n' = n' \), and writing \( n = l' + 1 - q \), we have

\[ \frac{1}{(2l'+1)!} \sum_{q} [(k-q)!/(k+q)! (l+l'+1-q)! \times (l'-l-q)!] B^2 = 1. \]

This sum can be easily carried out using the techniques described in Appendix I of Edmonds [3]. One obtains

\[ B = \left[ \sum_{p} (-1)^{p} \right] \frac{(k-q)!}{(k+q)!} \frac{(l+l'+1-q)!}{(l+l'-1-q)!} \times (l'-l-q)! B^2 = 1. \]

Finally, before writing out the complete coupling coefficient, it is convenient to change the summation parameter in (21) using the technique of Racah [11] and Edmonds [3] (p. 45). We write

\[ \sum_{l} \frac{(k+n-l'-1-1)!}{(k-n-l'-1-i)!} \times (n-l'-1-i)! \times (n-l'-1-i)! \times (n-l-i)! \times (n-l'-1-i)! \times (n-l-i)! \times (n-l-i)! \times (n-l-i)! \times \frac{(k-q)!}{(k+q)!} \times \frac{(l+l'+1-q)!}{(l+l'-1-q)!} \times (l'-l-q)! B^2 = 1. \]

Collecting all of these results, we have

\[ A(kq, ln | l' n') = (-1)^{k+q} A(l', l', k) \times \]

\[ \sum_{p} (-1)^{p} \times \frac{(n'+l'+1)!}{(l+n)!} \frac{(l+l'+1)!}{(l+l'-1-q)!} \times (l'+l'-1-q)! \times (l'-l-q)! \times (k-q)! \times \frac{(n'+l'+1-q)!}{(l+n)!} \times \frac{(l+l'+1-q)!}{(l+l'-1-q)!} \times (l'-l-q)! B^2 = 1. \]

5. The Coefficients \( A(kq, ln | l' n') \). — Before proceeding to the calculation of matrix elements, let us consider the coefficients derived in the previous section. It is convenient at this point to rewrite (26) in terms of binomial coefficients

\[ A(kq, ln | l' n') = (-1)^{k+q} A(l', l', k) \times \]

\[ \sum_{p} (-1)^{p} \times \frac{(n'+l'+1)!}{(l+n)!} \frac{(l+l'+1)!}{(l+l'-1-q)!} \times (l'+l'-1-q)! \times (l'-l-q)! \times (k-q)! \times \frac{(n'+l'+1-q)!}{(l+n)!} \times \frac{(l+l'+1-q)!}{(l+l'-1-q)!} \times (l'-l-q)! B^2 = 1. \]

In order for (28) to be equal to (26), we must assume for the moment that the binomial coefficient \( \binom{n}{r} \) is
defined only for \( n \geq 0 \). We can also write the \( R(3) \) Clebsch-Gordan coefficient obtained by Wigner \[12\] in terms of binomial coefficients
\[
(kq, \ln | l' n'\rangle) = (-1)^{k+q} A(l, l', k) \times
\frac{(l-n)! (l'+n')! (k-q)! (2 l'+1)!}{(k+q)! (l+n)! (l'-n')}^{1/2}
\times \sum_p (-1)^{p+k+q} \binom{l'-n'+q}{k-q} \binom{k+n'+l'-p}{l'+n'} \binom{l+n}{p}
\]
with the same assumption being made for the binomial coefficients. In this case, of course,
\[
| n | \leq l \quad \text{and} \quad | n' | \leq l'.
\]

The Clebsch-Gordan coefficients given above for \( O(2, 1) \) and \( R(3) \) are clearly closely related. The most obvious difference between the two coefficients lies in the first binomial coefficient in each summation.

However, if we recall that the binomial coefficient \( \binom{n}{r} \) is defined for negative \( n \), and is given by \[3\]
\[
\binom{n}{r} = (-1)^r \binom{r-n-1}{r},
\]
we see that these two binomial coefficients can be expressed in terms of the same algebraic product, with one being defined for \( l' - n' + \rho \geq 0 \), the other for \( l' - n' + \rho \leq 0 \). That is
\[
\binom{l'-n'+\rho}{k-q} = (l'-n'+\rho) (l'-n'+\rho-1) \ldots (l'-n+\rho-k+1)
\]
\[l'-n'+\rho \geq 0\]
and
\[
(-1)^{k+q} \binom{k+n'-l'-1-\rho}{k-q} = (k+n'-l'-1-\rho) \ldots (n'-l'-\rho) (-1)^{k+q}
\]
\[l'-n'+\rho \leq 0\]
Thus, we see that each term in the sum over \( \rho \) is algebraically the same function of \( l', n', k, q, l \) and \( n \) for both coefficients.

The remaining difference between the coefficients lies in the square root multiplying the summation. As we shall see in the next section, our only interest lies in the coefficient \( A(k0, \ln | l' n\rangle) \). In this case, one can easily show that the radical appearing in the \( O(2, 1) \) coefficient differs from the radical in the \( R(3) \) coefficient by a factor of \((l'-l)^{1/2}\).

We have the very interesting result, therefore, that
\[
A(k0, \ln | l' n\rangle)
\]
and \((k0, \ln | l' n\rangle)\) are given by the same algebraic functions of the variables \( k, l, n, \) and \( l' \). This can be a very valuable relationship, for there exist several tables of \( R(3) \) Clebsch-Gordan and \( 3 - l' \) symbols \[3, 13\] in which \( k \) has been fixed at some numerical value, and the resulting coefficient is given as a function of \( l, n, \) and \( l' \) only. These tables can be used directly as a source of the coefficients \( A(k0, \ln | l' n\rangle) \) through use of the relation
\[
A(k0, \ln | l' n\rangle) = a(k0, \ln | l' n\rangle)
\]
where \( a = 1 \) if \( l - l' \) is even, \(-i\) if \( l - l' \) is odd. Equation \(30\) is valid, of course, only if the algebraic forms of both coefficients are involved.

6. Matrix Elements of \( t_q^{(k)} \).—If the Wigner-Eckart theorem does indeed hold in this space, we should find that the matrix element
\[
(f_{l' q} | t_q^{(k)} | f_{l n})
\]
where \( l', k, \) and \( l \) satisfy triangular conditions, is proportional to the coefficient \( A(kq, \ln | l' n\rangle) \). We can easily show that this proportionality does, indeed, exist. This can be shown by considering a matrix element of the commutator \([J_+ , t_q^{(k)}]\) ; one obtains the relationship
\[
\pm \left[ (n' \pm l') (n' + l' + 1) \right]^{1/2} (f_{l' n' + l' + 1} | t_q^{(k)} | f_{l n}) = \\
\pm \left[ (k \pm q) (k \pm q + 1) \right]^{1/2} (f_{l' q} | t_q^{(k)} | f_{l n})
\]
where \( \pm (n \mp l) (n \pm l + 1) \right]^{1/2} (f_{l' q} | t_q^{(k)} | f_{l n \pm 1})
\]
and
\[31\]
where the top sign results from the commutator \( [J_+, t_q^{(k)}] \), the bottom from the commutator with \( J_- \). Clearly, these recursion relations will be satisfied if
\[
(f_{l' q} | t_q^{(k)} | f_{l n}) = A(kq, \ln | l' n\rangle) (l' \| t_q^{(k)} \| l) \quad \text{if}
\]

\[32\]
where \( l' \| t_q^{(k)} \| l \) is a reduced matrix element which is independent of \( q, n, \) and \( n' \).

Using \(4\), \(3\), and \(32\), we can write the matrix element of \( 1/r^k \) evaluated with hydrogenic functions in the form
\[
\int_0^\infty R_m R_{m'} \frac{d r}{r^k} = \\
= (2 Z/n)^k \frac{1}{2n[(2 l + 1)(2 l' + 1)]^{1/2}} (f_{l' q} | t_q^{(k-2)} | f_{l n})
\]
\[33\]
where \( k = 2 \leq | l + l' | \).

The selection rules noted by Pasternack and Sternheimer \[1\] are seen to be a natural consequence of the equality \(33\) : the coefficient \( A(k - 2 \ 0, \ln | l' n|) \) vanishes unless \( k - 2 \leq | l - l' | \). In addition, the discussion of the previous section.
taken in conjunction with (33), makes obvious the proportionality of expectation values of $1/r^k$ to $3 - j$ symbols (Sec. 1).

7. Matrix Elements of $P_{q}^{(k)}$. — The product representation $\mathcal{D}_k \times \mathcal{D}_k^*$ cannot be decomposed into irreducible representations as simply as was the product representation $\mathcal{D}(k) \times \mathcal{D}_k^*$ (eq. (11)). The added complexity in this case arises because $\mathcal{D}_k$ is itself not irreducible. It therefore seems simplest to consider directly reducible representations as simply as was the product

Proceeding as in the previous section, we consider matrix elements of the commutators $[J_±, P_q^{(k)}]$; the resulting equations are

$$[n' \pm l'] (n' \mp l' \mp 1)]^{\frac{1}{2}} (f_{\nu', \pm 1} | P_q^{(k)} | f_{\nu}) =$$

$$= \pm (k \pm q) (f_{\nu', | P_q^{(k)} | f_{\nu}}) +$$

$$+ [(n \mp l) (n \pm l \pm 1)]^{\frac{1}{2}} (f_{\nu', | P_q^{(k)} | f_{\nu \pm 1}})$$

(34)

where, again, the top sign refers to the commutator with $J_+$, the lower, to the commutator with $J_-$. Let us now define the coefficient $g(q, n, n')$, by the equation

$$g(q, n, n') = \int (f_{\nu', | P_q^{(k)} | f_{\nu}})$$

$$\times [(l + n)! (l' + n')! (n - l - 1)! (n' - l - 1)!]^{-\frac{1}{2}}$$

(35)

where $b = (k + q - 1)!$ if $-k < q$

$\quad b = (-q - k)! (-1)^{k+q}$ if $-k > q$.

Inserting (35) into (34), we obtain the recursion relations

$$(n' + l') (n' - l' - 1) g(q, n, n' - 1) =$$

$$= -g(q + 1, n, n') + g(q, n + 1, n')$$

$$g(q, n, n' + 1) =$$

$$= (k - q) (k + q - 1) g(q - 1, n, n') +$$

$$+ (n + l) (n - l - 1) g(q, n - 1, n')$$

(36)

valid for all $q$. These recursion relations can be seen to be exactly equivalent to those satisfied by $f'(q, n, n')$ (eqs 18b and 19b) if we replace $k$ by $k + 1$. That is, if $t^{(k)}$ is defined as a « tensor » of rank $k$ with respect to this algebra, $P^{(k)}$ transforms like a « tensor » of rank $k - 1$. We therefore define the tensor operator $p^{(k)}$ by

$$p^{(k)} = P^{(k+1)} = r^{k+1} e^{imt}.$$  

(37)

It is difficult to obtain a general expression for $g(q, n, n')$ valid for all $q$; it is, however, clear that $g(0, n, n)$ must be equal to $f(0, n, n)$ to within a factor depending only on $k$, $l$, and $l'$. Using (21), therefore, we find that we can write

$$(f_{\nu', | P_0^{(k)} | f_{\nu}}) = C(k0, ln | l', n) (l' \parallel p^{(k)} \parallel l)_2$$  

(38)

where $(l' \parallel p^{(k)} \parallel l)_2$ is independent of $n$, and

$$C(k0, ln | l', n) =$$

$$= [n + l)! (n - l - 1)! (n - l' - 1)! (l' + n)!]^{\frac{1}{2}} \times$$

$$\times \sum \frac{(k - l' + n - 1)!}{(k - n + l' + 1)! (n + l - 1)! (l' + n - 1 - l)!}.$$  

(39)

The coefficient $C(k0, ln | l', n)$ has, of course, the same dependence on $n$ as has $A(k0, ln | f' m)$. There is in this case, however, no triangular limitation on $k$, $l$, and $l'$.

Using (4), (37), and (38), we can write matrix elements of $r^k$ evaluated with hydrogenic functions in the form

$$\int R_{l'} R_{n} r^k dr =$$

$$= (n/2 Z)^k \frac{1}{2 n[(2 l + 1)(2 l' + 1)]^{\frac{1}{2}}} (f_{\nu', | p^{(k+1)} | f_{\nu}})$$

$$= (n/2 Z)^k \frac{C(k + 1, 0, ln | l', n)}{2 n[(2 l + 1)(2 l' + 1)]^{\frac{1}{2}}} (l' \parallel p^{(k+1)} \parallel l)_2.$$  

(40)

The discussion of section 5, in conjunction with (40), makes obvious the proportionality of expectation values of $r^k$ to $3 - j$ symbols in which $n$ plays the part of a magnetic quantum number.

8. Reduced Matrix Elements. — In order to fully utilize (33) and (40), one must be able to evaluate the reduced matrix elements $(l' \parallel r^{(k)} \parallel l)_2$ and

$$\int R_{l'} R_{n} r^{k} dr.$$  

The traditional method for determining reduced matrix elements is to find one easily evaluated matrix elements, and to extract from that matrix element the reduced matrix element. This is the procedure we shall follow here.

We assume, first, that $l' \geq l$. Matrix elements in which the bra is the state $(f_{ll'} + 1)$ are easily evaluated, since

$$f_{ll' + 1} = e^{i(l' + 1)\tau} r^{l' + 1} [2 \pi(2 l')!]^{-\frac{1}{2}}.$$  

The matrix element

$$\int R_{l'} R_{n} r^{(k)} | f_{ll'} + 1\rangle$$

then becomes simply an integral over one Laguerre polynomial. Such an integral can be carried out in a very straightforward fashion using the generating function for Laguerre polynomials [9]

$$e^{-1/t} \sum_{a=0}^{n} \frac{r^a}{(n + a)!} P_n^{(k)}(x).$$  

(30)
The same statements apply equally well, of course, to the matrix element

\[ \langle r_{r+1} \mid p_0^{(k)} \mid l_{r+1} \rangle . \]

Finally, the coefficients \( A(k0, l_0' + 1 \mid l' l_0' + 1) \) and \( C(k0, l_0' + 1 \mid l' l_0' + 1) \) are easily obtained from (26) and (39). Using the calculated matrix elements and these coefficients in eqs (32) and (38) allows one to make the identifications

\[ (l' \parallel l') = (-1)^k \left[ \frac{(l + l' + 1) (l + l' + k)! (l' + k)!}{(l + k + 1) (l + k + l' + 1)! (l' + k + l)!} \right]^{1/2} \]

and

\[ (l' \parallel l_2) = (-1)^{l' - l} \left[ \frac{(l + l' + 1) (l + l' + k)! (l' + k)!}{k (l' - l)!} \right]^{1/2} \]

These results can now be used with (33) and (40) to obtain matrix elements of any power of \( r \).

9. Discussion. — We have shown that hydrogen-like radial functions can be used to form bases for representations of the non-compact group \( O(2, 1) \). Powers of the radius were found to transform simply with respect to the group algebra. The Clebsch-Gordan coefficients for a particular product representation were determined, and matrix elements of powers of the radius were shown to be simply expressible in terms of these coefficients. The coefficients themselves were discussed, and found to be very similar to the familiar \( R(3) \) Clebsch-Gordan coefficients. In this way, we have been able to explain in a new and interesting manner many of the properties of hydrogenic radial wavefunctions. We must note, however, that the reduction of the Kronecker product of a unitary and a non-unitary representation is very complicated and much work remains to be done in this area.

Our discussion was concerned with functions which have as a variable \( r \). Hydrogenic functions have, of course, the variable \( r/n \). We were limited, therefore, to considering matrix elements diagonal in \( n \). Barut and Kleinert [5] have discussed an algebra which actually has as a basis the hydrogenic radial functions. Their algebra differs from ours, basically, by the inclusion of a dilatation operator \( D_r \), which has the property

\[ D_r f(r) = f(ar) . \]

Unfortunately, powers of \( r \) do not transform so nicely with respect to this algebra as they do with respect to the algebra discussed in this work. Nevertheless, future work must consider matrix elements off-diagonal in \( n \).

Questions of possible application of group theoretical techniques to the radial functions of more complicated atoms naturally arise. Two possible approaches to this more complicated problem would appear promising. First, it is known that many properties of atoms can be reasonably well predicted using the hydrogenic functions as a first order approximation to the real wavefunctions. One has, for example, the work of Layzer [14] in this area; and one might attempt a fresh look at Layzer's techniques and results using a group theoretical approach. A second avenue of investigation would be a search for approximate potentials such that the radial equation could be written in terms of a Casimir operator for some group. The same general approach as carried out above could then be carried out for the group of the new potential. However, whatever approach turns out to be the best, the suggestions that both the radial and angular wavefunctions can be studied using group theory opens many fascinating avenues of conjecture.

References

[8] MILLER (W.), Lie Theory and Special Functions, 1968, Academic Press, New York, has considered an algebra closely related to the one discussed in this paper.