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SYMMETRY PRINCIPLES IN ATOMIC SPECTROSCOPY

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Résumé. — Bien que la théorie des groupes compacts conduise à un élégant formalisme mathématique pour le calcul des propriétés des systèmes à plusieurs électrons, elle ne mène pas à une interprétation physique significative de ces propriétés. On discute l'avantage d'appliquer les groupes non compacts aux systèmes à plusieurs électrons. Comme étude préliminaire, l'algèbre des opérateurs tensoriels de SO(4) est développée en utilisant les coefficients connus du couplage vectoriel de SO(4) qui, à leur tour, sont employés pour étudier la chaîne canonique

$$SO(5) \supset SO(4) \supset SO(3) \supset SO(2)\,,$$

qui donne une réalisation physique dans la symétrie dynamique des états liés de l'atome d'hydrogène. Ces résultats sont étendus aux représentations du groupe non compact de Sitter SO(4, 1) construit dans la base canonique SO(4, 1) ⊃ SO(4) ⊃ SO(3) ⊃ SO(2). La possibilité d'appliquer la théorie des groupes non compacts aux atomes à plusieurs électrons est alors considérée.

Abstract. — It is suggested that while the theory of compact groups leads to an elegant mathematical formalism for calculating the properties of many-electron systems, it does not lead to a physically significant interpretation of these properties. The desirability of applying non-compact groups to many-electron systems is discussed. As a preliminary study the tensor operator algebra of SO(4) is developed using the known SO(4) vector coupling coefficients which in turn are used to study the canonical chain SO(5) ⊃ SO(4) ⊃ SO(3) ⊃ SO(2) which finds a physical realization in the dynamical symmetry of the bound states of the hydrogen atom. These results are then extended to the representations of the non-compact de Sitter group SO(4, 1) constructed in the canonical basis SO(4, 1) ⊃ SO(4) ⊃ SO(3) ⊃ SO(2). The possibility of applying the theory of non-compact groups to many-electron atoms is then considered.

1. **Introduction.** — Racah's applications [1, 2] of compact groups to the theory of complex spectra were largely concerned with the setting up of an elegant mathematical formalism to permit the calculation of the properties of many electron systems. No attempt was made to attach any physical significance to the various groups used in making these calculations. Later work has continued the development of the mathematical formalism [3-5].

Two applications of group theory where physical significance can be attached to the relevant group representations are well-known, namely to the three-dimensional isotropic harmonic oscillator (SU(3)) and to a single charged particle moving in a pure Coulomb potential (SO(4)). In each case the non-relativistic degeneracies of the single particle energy levels can be interpreted in terms of the symmetry properties of the relevant Hamiltonian [6]. The symmetry group SU(3) has been successfully exploited in the case of nuclei even for systems containing more than one nucleon [7].

In the atomic case as soon as more than one electron systems are encountered the SO(4) symmetry of the central Coulomb potential is destroyed by the inter-electron Coulomb repulsion [6, 8]. Thus while SO(4) symmetry is physically significant for the case of the hydrogen atom it does not seem to be relevant to the helium atom and beyond. Attempts to find other examples of approximate symmetries have been relatively unsuccessful. Thus while the states of the $(5\ d + 6\ s)^2$ complex of La II provide a good example of SU_3 symmetry in an atomic problem such an example must be regarded as an accident rather than a general symmetry principle for atomic systems [9].

Thus it would appear that there are relatively few examples where compact groups can be employed in a physically significant manner. Most problems of physical interest must take into account the fact that a given system may exist in an infinity of different states. The irreducible representations of compact groups are all finite dimensional and thus do not supply the possibility of enveloping the infinite dimensional Hilbert space associated with real problems. As an attempt to get out of this demise we are led to explore the properties of non-compact groups which possess infinite dimensional unitary representations. The application of the non-compact de Sitter group SO(4, 1) and the conformal group SO(4, 2) to the hydrogen atom has been remarkably successful [10, 11] in supplying single infinite dimensional unitary representations that have the property of enveloping the eigenfunctions of the complete set of bound states, in the case of SO(4, 1), and the complete set of bound and continuum states in the case of SO(4, 2). In these cases it has been possible to calculate all the relevant physical properties of the hydrogen atom in terms of the matrix elements of the relevant group generators.

It is of considerable interest to explore the possibilities of extending the methods of non-compact groups to many-electron atoms. Here the representations that must be considered are of considerably greater complexity and in this paper we limited our attention to the special case of the representations of the de Sitter group SO(4, 1). The representation theory of the group SO(4, 1) is well-known [12-16]. The traditional approaches to the theory of the de Sitter group have tended to revolve about the exploitation of the basic commutation properties of the group generators following the manner of Thomas [12] and Harish-Chandra [17].

In the present paper we give a method of exploring the properties of the de Sitter group that makes full use of the Racah tensor operator algebra. While this approach has a number of novel features no claim can be made for the originality of the final results. The methods used here do, however, give an interesting insight into the properties of non-compact groups and their relationship to compact groups. To make our development possible we first sketch the relevant tensor operator algebra of the group SO(4) and then develop expressions for the reduced matrix elements of the generators of SO(5). The SO(4) vector coupling coefficients are then used to construct the eigenvalues of the two Casimir invariant operators of SO(5). These results are then carried over to the development of the corresponding results for the de Sitter group SO(4, 1).

2. **Tensor Operator Algebra of SO (4).** — The basic theory of the group SO(4) has been outlined by Pauli [18] and Biedenharn [19] and here we follow the notation of Biedenharn. The group generators may be represented in terms of the components of the tensor operators $\mathbf{L}^{(1)}$ and $\mathbf{A}^{(1)}$ where $\mathbf{L}^{(1)}$ is the usual angular momentum vector and $\mathbf{A}^{(1)}$ the Runge-Lenz vector. The irreductible representations of SO(4) may be labelled by a pair of integers or half-integers $[pq]$ such that $p \geqslant |q| \geqslant 0$ and q may be positive or negative.

Biedenharn [19] has utilized the local isomorphism of the group SO(4) with the group SO(3) × SO(3) to obtain the SO(4) vector coupling coefficients for those representations in which the subgroup SO(3) is diagonal. Thus the complete coupling coefficients for the canonical chain SO(4) ⊃ SO(3) ⊃ SO(2) are known. Biedenharn's result may be written as

$$< [p_1\, q_1]\, j_1\, m_1 [p_2\, q_2]\, j_2\, m_2 \mid [p_1\, q_1]\, [p_2\, q_2]\, ; [p_{12}\, q_{12}]\, J_{12}\, M_{12} > = (-1)^{J_{12}-M_{12}} \begin{pmatrix} j_1 & J_{12} & j_2 \\ m_1 & -M_{12} & m_2 \end{pmatrix} \times$$

$$\times [(p_{12}+q_{12}+1)(p_{12}-q_{12}+1) \times (2j_1+1)(2j_2+1)(2J_{12}+1)]^{1/2}$$

(condt)

$$\begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p_{12}+q_{12}) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p_{12}-q_{12}) \\ j_1 & j_2 & J_{12} \end{Bmatrix}. \quad (1)$$

It is useful to be able to construct tensor operators $\mathbf{T}^{[pq]K}$ that have well-defined transformation properties not only with respect to SO(3) and SO(2) but also SO(4). Using the Wigner-Eckart theorem [3] we have

$$\left\langle \alpha_1 [p_1\, q_1]\, J_1\, M_1 \left| T^{[pq]}{}^{K}_{Q} \right| \alpha_2 [p_2\, q_2]\, J_2\, M_2 \right\rangle = (-1)^{J_1-M_1} \begin{pmatrix} J_1 & K & J_2 \\ -M_1 & Q & M_2 \end{pmatrix} \times$$

$$\times < \alpha_1 [p_1\, q_1]\, J_1 || T^{[pq]K} || \alpha_2 [p_2\, q_2]\, J_2 > . \quad (2)$$

The reduced matrix element on the right-hand-side may now be written as

$$< \alpha_1 [p_1\, q_1]\, J_1 || T^{[pq]K} || \alpha_2 [p_2\, q_2]\, J_2 > = [(2K+1)(2J_1+1)(2J_2+1)]^{1/2} \times$$

$$\times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p+q) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p-q) \\ J_1 & J_2 & K \end{Bmatrix}$$

$$\times < \alpha_1 [p_1\, q_1] || T^{[pq]} || \alpha_2 [p_2\, q_2] > \quad (3)$$

where we have absorbed a factor $[p_1 + q_1 + 1]^{1/2}$ in our definition of the SO(4) reduced matrix elements so that later equations assume a more symmetrical form.

The evaluation of the reduced matrix elements of coupled products of SO(4) symmetrized operators may be effected by use of the Innes-Ufford identity [20] or by the diagrammatic methods of Jucys et al. [21] to give the result

$$< \alpha_1[p_1\, q_1]\, J_1 \,||\, \{ T^{[p_3 q_3]}\, U^{[p_4 q_4]} \}\, [pq]\, K \,||\, \alpha_2[p_2\, q_2]\, J_2 > =$$

$$= (-1)^{p_1+p_2+p}[(2K+1)(p+q+1)(p-q+1)(2J_1+1)(2J_2+1)]^{1/2} \sum_{\alpha_5[p_5 q_5]} \times$$

$$\times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p+q) \\ \frac{1}{2}(p_4+q_4) & \frac{1}{2}(p_3+q_3) & \frac{1}{2}(p_5+q_5) \end{Bmatrix} \begin{Bmatrix} \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p-q) \\ \frac{1}{2}(p_4-q_4) & \frac{1}{2}(p_3-q_3) & \frac{1}{2}(p_5-q_5) \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p+q) \\ \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p-q) \\ J_1 & J_2 & K \end{Bmatrix}$$

$$\times < \alpha_1[p_1\, q_1] \,||\, T^{[p_3 q_3]} \,||\, \alpha_5[p_5\, q_5] > < \alpha_5[p_5\, q_5] \,||\, U^{[p_4 q_4]} \,||\, \alpha_2[p_2\, q_2] > . \quad (4)$$

Comparison of Eqs (3) and (4) gives the additional result

$$< \alpha_1[p_1\, q_1] \,||\, \{ T^{[p_3 q_3]}\, U^{[p_4 q_4]} \}\, [pq] \,||\, \alpha_2[p_2\, q_2] > = (-1)^{p_1+p_2+p} \sqrt{(p+q+1)(p-q+1)} \sum_{\alpha_5[p_5 q_5]} \times$$

$$\times \begin{Bmatrix} \frac{1}{2}(p_1+q_1) & \frac{1}{2}(p_2+q_2) & \frac{1}{2}(p+q) \\ \frac{1}{2}(p_4+q_4) & \frac{1}{2}(p_3+q_3) & \frac{1}{2}(p_5+q_5) \end{Bmatrix} \begin{Bmatrix} \frac{1}{2}(p_1-q_1) & \frac{1}{2}(p_2-q_2) & \frac{1}{2}(p-q) \\ \frac{1}{2}(p_4-q_4) & \frac{1}{2}(p_3-q_3) & \frac{1}{2}(p_5-q_5) \end{Bmatrix}$$

$$\times < \alpha_1[p_1\, q_1] \,||\, T^{[p_3 q_3]} \,||\, \alpha_5[p_5\, q_5] > < \alpha_5[p_5\, q_5] \,||\, U^{[p_4 q_4]} \,||\, \alpha_2[p_2\, q_2] > . \quad (5)$$

Equations (1) to (5) allow us to factorize out the JM dependence of any SO(4) symmetrized operator leaving us with reduced matrix elements that are independent of any labels associated with the representations of SO(3) and SO(2). To proceed further we must determine the SO(4) reduced matrix elements of the generators of SO(4).

3. **Reduced Matrix Elements for SO(4).** — Butler and Wybourne [22] have shown that the generators of the group O(n) transform according to the [11] representation. In the particular case of SO(4) we find that $\mathbf{L} + \mathbf{A}$ and $\mathbf{L} - \mathbf{A}$ transform as the [11] and [1-1] representations of SO(4) respectively. It is a simple exercise to calculate the diagonal matrix elements of $\mathbf{L}^{(1)}$ and $\mathbf{A}^{(1)}$ [19]. These results may then be compared with Eq. (3) to yield

$$< \alpha_1[p_1\, q_1] \,||\, L + A \,||\, \alpha_2[p_2\, q_2] > =$$
$$= \delta_{\alpha_1\alpha_2}\, \delta_{p_1p_2}\, \delta_{q_1q_2}[(p_1 \pm q_1)(p_1 \pm q_1 + 1) \times$$
$$\times (p_1 \pm q_1 + 2)(p_1 \mp q_1 + 1)]^{1/2} . \quad (6)$$

This result, used in conjunction with eqs (2) and (3), allows the computation of all the matrix elements of the group generators of SO(4) together with those of $\mathbf{L}$ and $\mathbf{A}$ separately.

4. **Algebra of SO(5).** — We now consider the enlargement of the algebra of SO(4) to that of SO(5). The infinitesimal operators $J_{\lambda\mu}$ of SO(5) may be defined in terms of five real variables x_i ($i = 1, 2, ..., 5$) as [2]

$$J_{\lambda\mu} = i \left\{ x_\mu \frac{\partial}{\partial x_\lambda} - x_\lambda \frac{\partial}{\partial x_\mu} \right\}$$

where $J_{\lambda\mu} = -J_{\mu\lambda}$. The basic commutator may be written as

$$[J_{\lambda\mu}, J_{\sigma\rho}] = i\{\delta_{\lambda\sigma} J_{\mu\rho} + \delta_{\lambda\rho} J_{\sigma\mu} + \delta_{\mu\sigma} J_{\rho\lambda} + \delta_{\mu\sigma} J_{\lambda\sigma}\} . \quad (7)$$

We may introduce sets of tensor operators such that

$$J_0^{(1)} = J_{12} \qquad J_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}}(J_{23} \pm iJ_{31}) \quad (8a)$$

$$A_0^{(1)} = J_{43} \qquad A_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}}(J_{41} \pm iJ_{42}) \quad (8b)$$

$$B_0^{(1)} = J_{35} \qquad B_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}}(J_{15} \pm iJ_{25}) \quad (8c)$$

$$S_0^{(0)} = iJ_{45} .$$

The tensor operator component $J_0^{(1)}$ provides the generator of SO(2) while the components of $\mathbf{J}^{(1)}$ generate the algebra of SO(3). The tensor operators $\mathbf{J}^{(1)}$ and $\mathbf{A}^{(1)}$ may be used together to construct the SO(4) algebra [4, 8, 22]. Adding the tensor operator $\mathbf{B}^{(1)}$ and the scalar operator $S_0^{(0)}$ to $\mathbf{J}^{(1)}$ and $\mathbf{A}^{(1)}$ allows us to enlarge the SO(4) algebra to that of SO(5), and thus complete the canonical chain

$$SO(5) \supset SO(4) \supset SO(3) \supset SO(2) . \quad (9)$$

The matrix elements of $\mathbf{J}^{(1)}$ and $\mathbf{A}^{(1)}$ are already found and it remains to obtain expressions for those of $\mathbf{B}^{(1)}$ and $S_0^{(0)}$. As noted earlier, the generators $\mathbf{J}^{(1)}$ and $\mathbf{A}^{(1)}$ together span the [11] and [1-1] representations of SO(4) while the new generators $\mathbf{B}^{(1)}$ and $S_0^{(0)}$ that enlarge the canonical chain transform as the [10] representation of SO(4).

The eigenvalues of $S_0^{(0)}$ and $B_\rho^{(1)}$ acting on a ket $|\gamma[pq]\,Jm\rangle$ may be readily found to be

$$S_0^{(0)}|\gamma[pq]\,JM\rangle = \frac{1}{\sqrt{2}}\sum_{[p'q']}(-1)^{(p+p'+q-q'+2J+1)/2}\times$$
$$\times\begin{Bmatrix} J & \frac{1}{2}(p+q) & \frac{1}{2}(p-q) \\ \frac{1}{2} & \frac{1}{2}(p'-q') & \frac{1}{2}(p'+q') \end{Bmatrix}$$
$$\times\langle\gamma[p'q']\,||\,S^{[10]}\,||\,\gamma[pq]\rangle\,|\gamma[p'q']\,JM\rangle \tag{10}$$

and

$$B_\lambda^{(1)}|\gamma[pq]\,JM\rangle =$$
$$=\sum_{[p'q']}\sum_{J'M'}(-1)^{J'-M'}[3(2J+1)(2J'+1)]^{1/2}\times$$
$$\times\begin{pmatrix} J' & 1 & J \\ -M' & \rho & M \end{pmatrix}\begin{Bmatrix} \frac{1}{2}(p+q) & \frac{1}{2} & \frac{1}{2}(p'+q') \\ \frac{1}{2}(p-q) & \frac{1}{2} & \frac{1}{2}(p'-q') \\ J & 1 & J' \end{Bmatrix}$$
$$\times\langle\gamma[p'q']||B^{[10]}||\gamma[pq]\rangle|\gamma[p'q']\,J'M'\rangle \tag{11}$$

where we make use of eqs (2) and (3). Since $\mathbf{B}^{(1)}$ and $S_0^{(0)}$ are group generators of SO(5) their reduced matrix elements must be diagonal in the auxiliary quantum numbers γ which presumably may later be identified with the labels of SO(5) representations.

Noting the commutation relation

$$[A_0^{(1)}, S_0^{(0)}] = -B_0^{(1)}$$

readily leads to the identity

$$\langle\gamma[p'q']\,||\,S^{[10]}\,||\,\gamma[pq]\rangle =$$
$$= -\langle\gamma[p'q']\,||\,B^{[10]}\,||\,\gamma[pq]\rangle \tag{12}$$

while application of the Wigner-Eckart theorem to the conjugate reduced matrix elements leads directly to the result that

$$\langle\gamma[pq]\,||\,B^{[10]}\,||\,\gamma[p'q']\rangle =$$
$$=(-1)^{p-p'}\langle\gamma[p'q']\,||\,B^{[10]}\,||\,\gamma[pq]\rangle^{*}. \tag{13}$$

We now endeavour to find formulae giving the explicit dependence upon $[pq]$ of the reduced matrix elements, initially using the result

$$[B_0^{(1)}, S_0^{(0)}]\,|\gamma[pq]\,JM\rangle = A_0^{(1)}\,|\gamma[pq]\,JM\rangle\,. \tag{14}$$

Explicit evaluation of the relevant vector coupling coefficients leads to the two identities

$$\langle\gamma[p\pm 1, q\pm 1]\,||\,B^{[10]}\,||\,\gamma[p\pm 1, q]\rangle\times$$
$$\times\langle\gamma[p\pm 1, q]\,||\,B^{[10]}\,||\,\gamma[pq]\rangle$$
$$=\langle\gamma[p\pm 1, q\pm 1]\,||\,B^{[10]}\,||\,\gamma[p, q\pm 1]\rangle\times$$
$$\times\langle\gamma[p, q\pm 1]\,||\,B^{[10]}\,||\,\gamma[pq]\rangle \tag{15}$$

and

$$\langle\gamma[p\pm 1, q\mp 1]\,||\,B^{[10]}\,||\,\gamma[p\pm 1, q]\rangle\times$$
$$\times\langle\gamma[p\pm 1, q]\,||\,B^{[10]}\,||\,\gamma[pq]\rangle$$
$$=\langle\gamma[p\pm 1, q\mp 1]\,||\,B^{[10]}\,||\,\gamma[p, q\mp 1]\rangle\times$$
$$\times\langle\gamma[p, q\mp 1]\,||\,B^{[10]}\,||\,\gamma[pq]\rangle$$

Use of eq. (13) then leads to the two identities

$$|\langle\gamma[p+1, q+1]\,||\,B^{[10]}\,||\,\gamma[p+1, q]\rangle|^2 =$$
$$=|\langle\gamma[p, q+1]\,||\,B^{[10]}\,||\,\gamma[pq]\rangle|^2 = f(q) \tag{16a}$$

and

$$|\langle\gamma[p+1, q+1]\,||\,B^{[10]}\,||\,\gamma[p, q+1]\rangle|^2 =$$
$$=|\langle\gamma[p+1, q]\,||\,B^{[10]}\,||\,\gamma[pq]\rangle|^2 = f(p) \tag{16b}$$

The above identities are entirely equivalent to those found by Kemmer, Pursey and Williams [23] who exploit the isomorphism between SO(4) and SU(2) × SU(2). While their method has a number of important simplifying features we have deliberately avoided it so as to give a prototype calculation for later extension to more complex cases where simplifying isomorphisms are absent.

Equations (16*a*) and (16*b*) may be solved inductively following the method of Kemmer et al [23] to give

$$f(p) + f(q) = -\tfrac{1}{4}(p+q+2)(p-q+1)\times$$
$$\times\left[(p+q+2)^2 + (p-q+1)^2 + 2\gamma\right] \tag{17a}$$

and consequently,

$$f(p) = -\tfrac{1}{2}\{(p+\tfrac{3}{2})^2[(p+\tfrac{3}{2})^2+\gamma]+\delta\} \tag{17b}$$

and

$$f(q) = \tfrac{1}{2}\{(q+\tfrac{1}{2})^2[(q+\tfrac{1}{2})^2+\gamma]+\delta\}\,. \tag{17c}$$

The unitarity of the representations of compact groups ensures that for a given irreducible representation of SO(5) p and q have upper bounds k and l respectively such that $f(k) = f(l) = 0$ and hence

$$\gamma = -(k+\tfrac{3}{2})^2 - (l+\tfrac{1}{2})^2 \tag{18a}$$

and

$$\delta = (k+\tfrac{3}{2})^2(l+\tfrac{1}{2})^2\,. \tag{18b}$$

Using these results in eqs (17*b*) and (17*c*) then gives

$$f(p)=\tfrac{1}{2}(k-p)(k+p+3)(p-l+1)(p+l+2) \tag{19a}$$

and

$$f(q)=\tfrac{1}{2}(k-q+1)(k+q+2)(l-q)(l+q+1) \tag{19b}$$

Noting the reality of the reduced matrix elements of $\mathbf{B}^{(1)}$ we may fix our phases so that the square roots of $f(p)$ and $f(q)$ are positive and label the irreducible representations of SO(5) by the pair of positive integers or half integers, $[k\ l]$.

It is apparent from eqs (10) and (11) that $\mathbf{B}^{(1)}$ and $S^{(0)}$ play the role of ladder operators stepping up or down p or q by one unit at a time. Under the restriction SO(5) → SO(4) we find that the irreducible representations $[kl]$ of SO(5) decompose into the set of irreducible representations $[pq]$ of SO(4) such that

$$k \geqslant p \geqslant l \geqslant | q | \geqslant 0 , \qquad (20)$$

with each representation of SO(4) occurring just once. In particular we note that under SO(5) $\rightarrow$ SO(4) we have

$$[n-1,0] \rightarrow [n-1,0] + [n-2,0] + \cdots + [00] \qquad (21)$$

Thus we may use a single representation $[n-1, 0]$ of SO(5) to envelope all the eigenfunctions of the bound states of a hydrogen atom up to those of principal quantum number n. Since the representations of compact groups are all finite dimensional we cannot expect a single representation of SO(5) to envelope all the eigenfunctions of the bound states of the hydrogen atom. As is well-known we must go over to the non-compact group SO(4, 1) to accomplish this task. Before investigating SO(4, 1) we first consider the construction of the Casimir invariant operators of SO(5).

5. **Casimir Invariants of SO(5).** — The representations of SO(5) may be equivalently labelled by the eigenvalues of two Casimir invariant operators that commute with all the infinitesimal operators of SO(5). One is a quadratic function and the other a quartic function of the group generators.

The quadratic invariant I_2 must be a scalar under SO(4) and its subgroups and be constructed from second degree products of the group generators of SO(5). Remembering that under SO(4) $\mathbf{B}^{(1)}$ and $S^{(0)}$ together transform as the [10] representation we have from eqs (2) to (4)

$$< \alpha[pq] \, JM \mid \{ \mathbf{B}^{[10]} \, \mathbf{B}^{[10]} \}^{[00]0}_{0} \mid \alpha'[p' \, q'] \, J' \, M' > =$$
$$= \delta_{\alpha\alpha'} \, \delta_{pp'} \, \delta_{qq'} \, \delta_{JJ'} \, \delta_{MM'} [f(p) + f(q) +$$
$$+ f(p-1) + f(q-1)] / 2(p+q+1)(p-q+1)$$

which from eq. (17a) becomes

$$< \alpha[pq] \, JM \mid \{ \mathbf{B}^{[10]} \, \mathbf{B}^{[10]} \}^{[00]0}_{0} \mid \alpha[pq] \, JM > =$$
$$= -\frac{\gamma}{2} - \frac{5}{4} - \frac{1}{2} [p(p+2) + q^2] . \qquad (22)$$

But for SO(4) we have the Casimir invariant $2F = (\mathbf{J}^2 + \mathbf{A}^2)$ which has eigenvalues $p(p+2) + q^2$ and hence

$$I_2 = 2F + 2 \{ \mathbf{B}^{[10]} \, \mathbf{B}^{[10]} \}^{[00]0}_{0} \qquad (23)$$

is a Casimir invariant of SO(5) with eigenvalues

$$I_2 \mid \alpha[pq] \, JM > = (-\tfrac{5}{2} - \gamma) \mid \alpha[pq] \, JM > \qquad (24)$$

where γ is as given in eq. (18a). We note that eq. (23) may be equivalently written as

$$2 I_2 = \mathbf{J}^2 + \mathbf{A}^2 + \mathbf{B}^2 - \mathbf{S}^2 \qquad (25)$$

and in terms of the $[kl]$ representation of SO(5) has the eigenvalues

$$I_2 \mid \alpha[kl] \, [pq] \, JM > =$$
$$= [k(k+3) + l(l+1)] \mid \alpha[kl] \, [pq] \, JM > . \qquad (26)$$

The construction of the fourth-order Casimir invariant I_4 is somewhat more tedious. We proceed by constructing fourth order operators out of **J**, **A** and **B** which are scalars under SO(4) $\supset$ SO(3) $\supset$ SO(2). Since under SO(4) we have $[11] \times [1 \, -1] = [20]$ and $[10] \times [10] \supset [20]$ we may start by considering the matrix elements of the fourth-order scalar operator

$$< \alpha[pq] \, JM \mid \{ [(\mathbf{J} + \mathbf{A})^{[11]} (\mathbf{J} - \mathbf{A})^{[1-1]}]^{[20]} \times$$
$$\times [\mathbf{B}^{[10]} \, \mathbf{B}^{[10]}]^{[20]} \}^{[00]0}_{0} \mid \alpha[pq] \, JM > \qquad (27)$$

which is obviously diagonal in the

$$\mathrm{SO}(5) \supset \mathrm{SO}(4) \supset \mathrm{SO}(3) \supset \mathrm{SO}(2)$$

canonical chain. Use of eq. (2) followed by eq. (4) and explicit evaluation of the relevant $3n-j$ symbols yields eq. (27) as

$$= < \alpha[pq] \mid\mid [(\mathbf{J} + \mathbf{A})^{[11]} (\mathbf{J} - \mathbf{A})^{[1-1]}]^{[20]} \mid\mid \alpha[pq] > \times$$
$$\times < \alpha[pq] \mid\mid [\mathbf{B}^{[10]} \, \mathbf{B}^{[10]}]^{[20]} \mid\mid \alpha[pq] > \times$$
$$\times \{ 3(p^2 - q^2 + 2p + 1) \}^{-1} . \qquad (28)$$

The reduced matrix elements may then be evaluated using eq. (5) followed by eq. (6) and eqs (16a) and (16b) to give eq. (28) as

$$= - \{ (p+q)(p-q) f(p) +$$
$$+ (p+q+2)(p-q+2) f(p-1)$$
$$- (p+q)(p-q+2) f(q)$$
$$- (p-q)(p+q+2) f(q-1) \} \times$$
$$\times \{ 12(p^2 - q^2 + 2p + 1) \}^{-1} . \qquad (29)$$

The above result may then be simplified using eqs (17b) and (17c) to give eq. (29) as

$$= \frac{1}{96} (16 \delta + 4 \gamma + 8 \gamma [p(p+2) + q^2] +$$
$$+ [8 p^4 + 8 q^4 + 32 p^3 + 36 p^2 - 12 q_2 + 8 p + 1]) . \qquad (30)$$

Clearly the matrix elements of the invariant operator I_4 cannot depend on p and q and hence a term must be added to the operator in eq. (27) to cancel the additional terms in eq. (30). A convenient choice for I_4 is

$$I_4 = \Xi - F(2F - 2 - I_2) + G^2 \qquad (31)$$

where

$$\Xi = 6 \{ [(\mathbf{J} + \mathbf{A})^{[11]} (\mathbf{J} - \mathbf{A})^{[1-1]}]^{[20]} \times$$
$$\times [\mathbf{B}^{[10]} \, \mathbf{B}^{[10]}]^{[20]} \}^{[00]0}_{0} \qquad (32)$$

and G is the second invariant of SO(4) with eigenvalues $q(p+1)$. We now have the eigenvalues of I_4 as being just

$$\delta = \frac{\gamma}{4} + \frac{1}{16} . \qquad (33)$$

In the $[kl]$ representation of SO(5) we find

$$I_4 \mid \alpha[kl]\,[pq]\,JM > = (k+1)(k+2)\,l(l+1) \mid \alpha[kl]\,[pq]\,JM > . \quad (34)$$

We note that I_4 is an invariant of SO(5) and as such can differ from the conventional fourth-order Casimir operator [2] by at most a scale factor and an additive constant. We may, if desired, use the eigenvalues of I_2 and I_4 to label the different irreducible representations of SO(5). The results we have obtained here are not significantly different from those found by Kemmer et al. [23].

6. **Algebra of the de Sitter group SO (4,1).** — The de Sitter group SO(4, 1) finds a realization as the ten-parameter group of transformation matrices that acting on the five variables w, x, y, z and t holds invariant the indefinite quadratic form

$$w^2 + x^2 + y^2 + z^2 - t^2 . \quad (35)$$

Then ten infinitesimal operators of SO (4,1) satisfy the commutation relations

$$[J_{\lambda\mu}, J_{\sigma\rho}] = i\{ g_{\lambda\rho} J_{\mu\sigma} + g_{\lambda\sigma} J_{\rho\mu} + g_{\mu\sigma} J_{\lambda\rho} + g_{\mu\rho} J_{\sigma\rho} \} \quad (36)$$

where $g_{\alpha\beta} = 0$ except for $g_{11} = g_{22} = g_{33} = g_{44} = -1$ and $g_{55} = 1$.

We can define a set of tensor operators $\mathbf{J}^{(1)}$, $\mathbf{A}^{(1)}$, $\mathbf{B}^{(1)}$ and $\mathbf{S}^{(0)}$ exactly as in eqs (8*a*) to (8*c*). The components of the tensor operators $\mathbf{J}^{(1)}$ and $\mathbf{A}^{(1)}$ satisfy the same commutation relations as for SO(4) and may be used as the generators of SO(4). The commutators involving the components of $\mathbf{J}^{(1)}$ or $\mathbf{A}^{(1)}$ with those of $\mathbf{B}^{(1)}$ or $\mathbf{S}^{(0)}$ also remain unchanged. However, we now find that the commutators for the components of $\mathbf{B}^{(1)}$ and $\mathbf{S}^{(0)}$ occur with the opposite sign to those for SO(5). Thus we may carry over much of the theory developed for SO(5) to SO(4, 1) with only some minor, though significant, changes.

In going from SO(5) ⊃ SO(4) ⊃ SO(3) ⊃ SO(2) to SO(4, 1) ⊃ SO(4) ⊃ SO(3) ⊃ SO(2) we find that eqs (12) and (13) remain unchanged while the sign on the right-hand-side of eq. (14) is reversed. This has the nett effect of changing the sign of eqs (17*a*) to (17*c*) to give

$$f(p) + f(q) = + \tfrac{1}{4}(p+q+2)(p-q+1) \times \left[(p+q+2)^2 + (p-q+1)^2 + 2\gamma\right] \quad (37a)$$

$$f(p) = + \tfrac{1}{2}\{ (p+\tfrac{3}{2})^2 [(p+\tfrac{3}{2})^2 + \gamma] + \delta \} \quad (37b)$$

and

$$f(q) = - \tfrac{1}{2}\{ (q+\tfrac{1}{2})^2 [(q+\tfrac{1}{2})^2 + \gamma] + \delta \} . \quad (37c)$$

The matrix elements given in eqs (22) and (30) change sign, as a consequence of the sign change in $f(p)$ and $f(q)$, and the two group invariants for SO(4, 1) become

$$I_2 = 2\{ \mathbf{B}^{[10]} \mathbf{B}^{[10]} \}^{[00]0}_{0} - 2F \quad (38)$$

and

$$I_4 = \Xi - F(2F - I_2 - 2) + G^2 \quad (39)$$

with eigenvalues of $\frac{5}{2} + \gamma$ and $-\delta - \frac{\gamma}{4} - \frac{1}{16}$ respectively.

The irreducible representations of SO(4, 1) may be labelled either by the permissible values of γ and δ or, perhaps more appropriately, by the eigenvalues of I_2 and I_4. The unitary representations of SO(4, 1) are all infinite dimensional and upon restriction to SO(4) yield infinite series of SO(4) representations, each occurring with multiplicity one or zero.

The possible representations of SO(4) contained in a representation of SO(4, 1) are determined by considering the conditions under which $f(p)$ and $f(q)$ are non-negative. The representations of SO(4) will be labelled by the pairs of integers or half integers p and q with $p \geqslant |q| \geqslant 0$. There is no upper bound on p but there are always lower bounds on p and q.

We may classify the different representations of SO(4, 1) by considering the different possible minimum values of p and q and their consequences in eqs (37*a*)-(37*c*). Two distinct series of SO(4, 1) representations arise, those where the eigenvalues of I_2 may assume a continuous range of values and those associated with only discrete values. These two series of representations may be somewhat arbitrarily divided into various classes as has been done, for exemple, by Newton [13]. We obtain the following results.

CONTINUOUS REPRESENTATIONS. — *Class I.*

$$I_2 > 0 \qquad I_4 = 0 \quad (40)$$

where I_2 has a continuous range of values. These representations decompose into the direct sum of the SO(4) representations

$$[00] + [10] + [20] + \cdots + [n\,0] + \cdots . \quad (41)$$

Class III.

$$\left.\begin{aligned} I_2 &= \tfrac{5}{2} - 2(s+\tfrac{1}{2})^2 \\ I_4 &= s(s+1)\,I_2 + s(s+1)(s+2)(s-1) \end{aligned}\right\} s = \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots \quad (42)$$

where I_2 has a continuous range subject to the lower bound restriction. There is a representation for each permissible value of s and I_2 and each representation decomposes into the direct sum of the SO(4) representations

$$\{ [s, -s] + [s, -s+1] + \cdots + [s, s] \} + \{ [s+1, -s] + [s+1, -s+1] + \cdots + [s+1, s] \} + \cdots . \quad (43)$$

DISCRETE REPRESENTATIONS. — *Class II.*

$$\left.\begin{aligned} I_2 &= -(n-1)(n+2) \\ I_4 &= 0 \end{aligned}\right\} n = 1, 2, 3, \ldots \quad (44)$$

There is one representation for each value of n which upon restriction to SO(4) decomposes into the direct sum

$$[n, 0] + [n + 1, 0] + \cdots \quad (45)$$

of SO(4) representations.

Class IV.

$$I_2 = - t(t - 1) - (s - 1)(s + 2) \qquad s = 1/2, 1, 3/2, 2, 5/2, \ldots$$

$$I_4 = - t(t - 1) s(s + 1) \qquad 0 < t \leqslant s . \quad (46)$$

These representations of SO(4, 1) are labelled and distinguished by the various possible pairs of integers or half integers (s, t). Two distinct SO(4, 1) representations arise for each choice of (s, t) and have been designated by Newton [13] as Class IV a and IV b. These representations are distinguished by their different decomposition into the direct sum of SO(4) representations upon the restriction SO(4, 1) → SO(4). For Class IVa we obtain the direct sum of SO(4) representations.

$$\{ [s, -s]+[s, -s+1]+\cdots+[s, -t] \} + \{ [s+1, -s]+[s+1, -s+1]+\cdots+[s+1, -t] \}+\cdots , \quad (47)$$

$$\{ [s, t]+[s, t+1]+\cdots+[s, s] \} + \{ [s+1, t]+[s+1, t+1]+\cdots+[s+1, s] \}+\cdots . \quad (48)$$

It will be noted that the representations in eq. (47) are simply the conjugates of those found in eq. (48).

Our results differ from those of Newton [13] in a number of minor points and are in accord with the amendments of Newton's results published by Dixmeir [15].

Conclusions. — We have developed the algebra of the de Sitter group SO(4, 1) using the tensor operator methods of Racah and the known expressions for the SO(4) vector coupling coefficients. The same method could be readily extended to the groups:

$$SO(4, 1) \supset SO(3, 1), SO(4, 2) \supset SO(2) \times \times SO(3), SO(4, 2) \supset SO(2) \times SO(4)$$

and SO(4, 2) ⊃ SO(3) × SO(2, 1) using the known coupling coefficients. Studies of these series of groups are currently under study.

The use of Gelfand states would give a natural method of extending our results to groups of higher dimensions as has indeed already been considered by Fronsdal [11].

While it is a comparatively simple matter to express the Hamiltonian for a hydrogen atom in terms of group generators of SO(4, 2) and obtain a complete analysis of the hydrogen atom spectrum it is likely to be a far from trivial matter to extend the theory to many-electron systems due to the presence of the Coulomb repulsion terms $\sum_{i<j} e^2/r_{ij}$. Ideally we would like to develop new global quantum numbers for many electron atoms and studies along these lines are currently being undertaken.

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