

Current Operators and Majorana Equation for the Hydrogen Atom from Dynamical Groups*

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(Received 28 November 1966)

It is proved that the dipole operator in the hydrogen atom is the product of an element in the Lie algebra and of a group element of the conformal group $O(4,2)$. A relativistic wave equation containing the total momentum only is set up which describes the internal structure of the system purely group theoretically and gives the correct mass spectrum. The diagonalization of this equation determines a new basis of states in which the dipole operator is simply an element of the Lie algebra. The angle of transformation to the new basis is evaluated to be $\theta = 2 \tanh^{-1}(1 - \epsilon/n)$, or, $\theta = \log(2n/\epsilon)$, where n is the principal quantum number and ϵ is essentially the fine-structure constant.

I. CURRENT OPERATORS IN $O(4,2)$

IN a recent paper¹ an irreducible unitary representation of the conformal group $O(4,2)$ was constructed on the Hilbert space of bound-state wave functions of the H atom. First of all we now give a realization of this representation in terms of boson creation and annihilation operators which will be useful in the following. In this representation the wave functions in parabolic coordinates are identified as

$$|n, n_1, n_2\rangle = [n_1!(n_2+m)!n_2!(n_1+m)!]^{-1/2} \times a_1^{\dagger n_1+m} a_2^{\dagger n_1} b_1^{\dagger n_1+m} b_2^{\dagger n_2} |0\rangle, \text{ for } m > 0 \quad (1.1)$$

and the generators L_{ab} of $O(4,2)$ as

$$\begin{aligned} L_{ij} &= \frac{1}{2}(a^\dagger \sigma_k a + b^\dagger \sigma_k b); \quad i, j, k \text{ cyclic,} \\ L_{i4} &\equiv M_i = -\frac{1}{2}(a^\dagger \sigma_i a - b^\dagger \sigma_i b), \\ L_{i5} &= -\frac{1}{2}(a^\dagger \sigma_i C b^\dagger - a C \sigma_i b), \\ L_{45} &= (1/2i)(a^\dagger C b^\dagger - a C b), \\ L_{i6} &= (1/2i)(a^\dagger \sigma_i C b^\dagger + a C \sigma_i b), \\ L_{46} &= \frac{1}{2}(a^\dagger C b^\dagger + a C b), \\ L_{56} &= \frac{1}{2}(a^\dagger a + b^\dagger b + 2) \equiv N. \end{aligned} \quad (1.2)$$

Here σ are the Pauli matrices, $C = i\sigma_2$, L_{ij} is the angular momentum, M_i the Lenz vector, and N gives the principal quantum number n .

In I it was shown that the dipole operator x when applied to states $|n, n_1, n_2\rangle$ can be written in terms of the $O(4,2)$ generators as

$$\begin{aligned} x_i &= D_{N/(N-1)} \frac{1}{2} (L_{i5} - iL_{i6}) \frac{(N+1)^2}{N} + L_{i4} \\ &+ D_{N/(N+1)} \frac{1}{2} (L_{i5} + iL_{i6}) \frac{(N-1)^2}{N}, \end{aligned} \quad (1.3)$$

where D_a is defined as the dilatation operator

$$D_a f(x) = f(ax). \quad (1.4)$$

* Research supported by the U. S. Air Force Office of Scientific Research, Office of Aerospace Research, U. S. Air Force, under AFOSR Grant No. AF-AFOSR-30-65.

¹ A. O. Barut and Hagen Kleinert, Phys. Rev. 156, 1541 (1967); hereafter referred to as I.

For the calculation of $D_{N/(N\pm 1)}$ we used the position representation of the wave functions and the question remained whether and how such a typically spatial operation could be cast into a group operation.

In this paper we show that the dilatation operator can in fact be expressed as a finite group element in $O(4,2)$ so that the matrix elements of the dipole operators are given by

$$\begin{aligned} \langle n'l'm' | x_i | nlm \rangle &= (i/\omega_{n'n}) (1/n'n) \\ &\times \langle n'l'm' | e^{-i\vartheta_{n'n} L_{45}} L_{i6} | nlm \rangle + \langle n'l'm' | L_{i4} | nlm \rangle, \end{aligned} \quad (1.5)$$

where $\omega_{n'n}$ is the Rydberg frequency for the transition $n \rightarrow n'$,

$$\omega_{n'n} = -\frac{1}{2n^2} + \frac{1}{2n'^2} = \frac{1}{2} \frac{n^2 - n'^2}{n^2 n'^2}, \quad (1.6)$$

and the angle $\vartheta_{n'n}$ of the group transformation is given by

$$\tanh \frac{1}{2} \vartheta_{n'n} = \frac{n-n'}{n+n'}, \quad \text{or } \vartheta_{n'n} = \log \frac{n}{n'}. \quad (1.7)$$

The proof of (1.5) is given in the Appendix. Here we shall discuss the meaning of this equation, its further consequences, and how one can formulate the radiation theory of the hydrogen atom group-theoretically from the beginning.

First of all, if we insert Eq. (1.5) into the quantum equation

$$p_i = i[H, x_i] = i[-(1/2N^2), x_i]$$

and observe that the Lenz vector L_{i4} commutes with H , we find for the momentum operator the simpler expression

$$\langle n'l'm' | p_i | nlm \rangle = \frac{1}{n'n} \langle n'l'm' | e^{-i\vartheta_{n'n} L_{45}} L_{i6} | nlm \rangle. \quad (1.8)$$

All operations on the right-hand side of (1.5) or (1.8) are contained in the group $O(4,2)$. As a consequence the conformal group contains the whole algebra of observables on the Hilbert space of bound-state wave functions and can thus indeed be called the *dynamical group* of the H atom. Because we need the generators L_{45} , L_{i6} , L_{56} of $O(4,2)$ this is in fact a minimal dynamical

group. The states $|nlm\rangle$ themselves form an irreducible representation of the subgroup $O(4,1)$; these are the states in the rest frame.

II. RELATIVISTIC WAVE EQUATION FOR THE HYDROGEN ATOM CONSIDERED AS A COMPOSITE PARTICLE

With Eqs. (1.5) and (1.8) the dynamics is completely formulated in the group-theoretical language as follows: Take the group $O(4,2)$, assign the "particles" to a single irreducible representation of the subgroup $O(4,1)$; the electromagnetic interactions are then described by the currents $e^{i\theta}L_{45}L_{i6}$. We shall see that the last sentence can also be formulated: The electromagnetic interactions are then described by the currents L_{i6} on the mixed states $e^{i\theta}L_{45}|nlm\rangle$. In this way, the position operators of the internal structure of the particle has been eliminated. This is a necessary step if the same formalism is to be applied to particle physics.

The problem that we have to solve now is how to find the above dipole operator if one does not have a Schrödinger equation and a correspondence principle. Can one find a relativistic description of the compound system in terms of its total momentum P_μ such that the internal structure is described purely group-theoretically? Isospin and $SU(3)$ groups seem to be manifestations of internal dynamics. Such a formulation, in special cases, goes back to Majorana² and has been the subject of the dynamical group theory in recent years. The generalization of the Majorana equations has been recently reconsidered by Nambu³ and the present authors.⁴ Nambu's equation does not solve the exact H-atom problem and has some unphysical features. We now want to give a solution to this problem.

We start from the states $|\bar{n}lm\rangle$ which are mixtures of the $O(4,1)$ states. The form of the new states will be determined. The boosted states $|\bar{n}lm; \hat{p}\rangle$ form a reducible representation of the Poincaré group. We then project out definite mass and spin values by the Majorana type equations⁴

$$(i\Gamma^\mu P_\mu + \beta S - \gamma)|\bar{n}lm; \hat{p}\rangle = 0. \quad (2.1)$$

Here Γ_μ is the four-vector generator in $O(4,2)$ which can be chosen as

$$\Gamma^\mu = (L_{i6}, L_{56}), \quad (2.2)$$

S is the remaining scalar (under the Poincaré group) generator

$$S = L_{46}, \quad (2.3)$$

and β and γ are functions of the Poincaré invariants. We determine the new states $|\bar{n}lm\rangle$ by the requirement that in the rest frame Eq. (2.1) is diagonal and the rest states $|nlm\rangle$ have the mass m . If we apply a group

transformation to (2.1) in order to diagonalize it we get

$$\begin{aligned} e^{i\theta_n L_{45}} [i\Gamma^0 P_0 + \beta S - \gamma] e^{-i\theta_n L_{45}} \\ = m [\cosh\theta_n - (\beta/m) \sinh\theta_n] N \\ + m [(\beta/m) \cosh\theta_n - \sinh\theta_n] - \gamma = 0. \end{aligned}$$

This expression is diagonal; if we choose

$$\tanh\theta_n = \beta/m, \quad \tanh\frac{1}{2}\theta_n = \frac{\beta/m}{[1 - (\beta/m)^2]^{1/2}}, \quad (2.4)$$

then the function $\gamma(m)$ is determined from the mass spectrum to be

$$\gamma(m) = mN[1 - (\beta/m)^2]^{1/2}. \quad (2.5)$$

Thus the new states in Eq. (2.1) are given by

$$|\bar{n}lm\rangle = e^{-i\theta_n L_{45}} |nlm\rangle. \quad (2.6)$$

The constant β will be chosen in such a way that the matrix elements of the current of Eq. (2.1), namely

$$\begin{aligned} \langle \bar{n}'l'm' | J_i | \bar{n}lm \rangle \\ = (e/n n') \langle \bar{n}'l'm' | L_{i6} | \bar{n}lm \rangle \\ = (e/n n') \langle n'l'm' | e^{i\theta_n' L_{45}} L_{i6} e^{-i\theta_n L_{45}} | nlm \rangle, \end{aligned} \quad (2.7)$$

coincides with our Eq. (1.8). This equation is more symmetric than (1.8). But because L_{45} commutes with L_{i6} the exponential factor is $e^{i(\theta_n' - \theta_n)L_{45}}$. If we now choose

$$\beta = m^2 = 1 - (\epsilon^2/n^2) \quad (2.8)$$

then

$$\tanh\frac{1}{2}\theta = \frac{m}{1 + (1 - m^2)^{1/2}} = \frac{m}{1 + \epsilon/n} \cong 1 - \epsilon/n.$$

Hence

$$\tanh\frac{1}{2}(\theta_{n'} - \theta_n) \cong (n - n')/(n + n') = -\tanh\frac{1}{2}\theta_{n',n} \quad (2.9)$$

and Eq. (2.7) is identical with (1.8).

Thus Eq. (2.1) describes the internal structure of the system group-theoretically at least up to dipole approximation. It is important to note that the current operators are simple generators of the Lie algebra, L_{i6} , not with respect to physical states, but with respect to "rotated" states $|\bar{n}lm\rangle$, whereas for $|nlm\rangle$ we have to use the "rotated" currents $e^{i\theta_n L_{45}} |nlm\rangle$. Because the group is noncompact, the transformation is hyperbolic. The angle θ measures the deviation of the actual mass of the hydrogen atom compared to the mass of the free proton and electron. Another way of putting these results is the following: If we keep the form of the currents fixed then the electromagnetic interactions *mix* the original states $|nlm\rangle$ into $|\bar{n}lm\rangle$ up to dipole approximation; the system is now in a state which is a superposition of all states $|nlm\rangle$.

Equation (2.1) is relativistic, but in order that it should describe the real relativistic hydrogen atom, spin must be introduced as well as the correct form of the boosting operations.

² E. Majorana, Nuovo Cimento **9**, 335 (1932).

³ Y. Nambu, Progr. Theoret. Phys. (Kyoto) **37**, 368 (1966).

⁴ A. O. Barut and Hagen Kleinert, Phys. Rev. (to be published).

APPENDIX: PROOF OF EQ. (1.5) AND IDENTIFICATION OF THE "TRANSITION GROUP" $O(2,1)$

If one inserts intermediate states into (1.3) and observes that $L_{i5} \mp iL_{i6}$ raises (lowers) n by one unit, one obtains

$$\begin{aligned} \langle n'l'm' | x_i | nlm \rangle &= \langle n'l'm' | D_{(n+1)/n} | n+1, l'm' \rangle \\ &\times \langle n+1, l', m' | L_{i5} - iL_{i6} | nlm \rangle [(n+1)^2/2n] \\ &+ \langle n'l'm' | D_{(n-1)/n} | n-1, l', m' \rangle \\ &\times \langle n-1, l', m' | L_{i5} + iL_{i6} \rangle [(n-1)^2/2n] \\ &+ \langle n'l'm' | L_{i4} | nlm \rangle. \end{aligned} \quad (A1)$$

Hence we have only to find group theoretical expressions for the matrix elements of $D_{(n\pm 1)/n}$. In I, Eqs. (26) and (27), we expressed this matrix elements in terms of the integrals over hypergeometric functions:

$$\begin{aligned} \langle n'lm | D_{(n\pm 1)/n} | n\pm 1, lm \rangle &(n\pm 1)^2/n \\ &= [n(n\pm 1)]^{1/2} d_{n\pm 1, l; n', l^{n, n'}}, \end{aligned} \quad (A2)$$

$$\begin{aligned} d_{n, l; n', l^{\tau\tau'}} &= \left(\frac{nn'}{\tau\tau'}\right)^{3/2} \frac{N_{nl}N_{n'l}}{\tau^{l'}\tau'^{l'}} \\ &\times g_{2l+1}^{(1,0)}\left(n_r, \frac{2}{\tau}; n_r', \frac{2}{\tau'}\right), \end{aligned} \quad (A3)$$

$$N_{nl} = \frac{2^{l+1}}{n^2(2l+1)!} \left[\frac{(n+l)!}{n_r!} \right]^{1/2}, \quad (A4)$$

$$\begin{aligned} g_{\rho}^{(\sigma, \tau)}(n_r, k; n_r', k') &= \int_0^{\infty} e^{-\frac{1}{2}(k+k')\xi} \xi^{\rho+\sigma} \\ &\times F(-n_r, \rho+1, k\xi) F(-n_r', \rho+1-\tau, k'\xi). \end{aligned} \quad (A5)$$

These integrals have been evaluated by Gordon⁵ recursively with the result

$$\begin{aligned} g_{2l+1}^{(1,0)}(n_r, k; n_r', k') &= -\frac{4}{k'^2 - k^2} (kr - k'r') \\ &\times g_{2l+1}^{(0,0)}(n_r, k; n_r', k'), \\ g_{2l+1}^{(0,0)}(n_r, k; n_r', k') &= \frac{(2l+1)!^2 n_r!}{(n-n')!(l+n')! (kk')^{l+1}} \\ &\times v^{l+1} u^{n-n'} F(-n_r', n+1+l, \\ &1+n-n', u^2), \\ u &= \frac{k'-k}{k'+k}, \quad v = 2 \frac{(kk')^{1/2}}{k'+k}. \end{aligned} \quad (A6)$$

For $n < n'$ one has to exchange n and n' in (A6) and

$u \rightarrow -u$. If we use the identity

$$F(a, b, c; z) = \frac{1}{(1-z)^2} F\left(a, c-b, c; \frac{z}{z-1}\right)$$

and

$$\sinh \frac{1}{2}\vartheta = \frac{u}{(1-u^2)^{1/2}}, \quad \cosh \frac{1}{2}\vartheta = \frac{1}{(1-u^2)^{1/2}},$$

to rewrite $g_{2l+1}^{(1,0)}$ in (A6) and define the functions

$$\begin{aligned} \mathcal{U}_{nn', l+1}(\vartheta) &\equiv \Theta_{nn'} (\cosh \frac{1}{2}\vartheta)^{-(n+n')} (\sinh \frac{1}{2}\vartheta)^{(n-n')} \\ &\times F(-n_r', -n'-l, 1+n-n', -\sinh^2(\frac{1}{2}\vartheta)) \end{aligned}$$

with

$$\Theta_{nn'} = \frac{1}{(n-n')!} \left[\frac{n_r!(n+l)!}{n_r'!(n'+l)!} \right]^{1/2} \quad (A7)$$

we obtain finally

$$d_{n, l; n', l^{\tau\tau'}} = \left(\frac{\tau\tau'}{nn'}\right)^{1/2} \left(\frac{n'}{\tau'} - \frac{n}{\tau}\right) \frac{1}{\sinh \vartheta_{\tau'\tau}} \mathcal{U}_{nn', l+1}(\vartheta_{\tau'\tau}), \quad (A8)$$

where the angle $\vartheta_{\tau'\tau}$ is determined by

$$\sinh \frac{1}{2}\vartheta_{\tau'\tau} = \frac{\tau - \tau'}{2(\tau\tau')^{1/2}}, \quad \cosh \frac{1}{2}\vartheta_{\tau'\tau} = \frac{\tau + \tau'}{2(\tau\tau')^{1/2}}.$$

In particular then Eq. (A2) becomes

$$\begin{aligned} \langle n'lm | D_{(n\pm 1)/n} | n\pm 1, lm \rangle &\frac{(n\pm 1)^2}{n} \\ &= \mp \frac{1}{\sinh \vartheta_{n'n}} \mathcal{U}_{n\pm 1, n', l+1}(\vartheta_{n'n}). \end{aligned} \quad (A9)$$

There is a good reason of introducing the functions $\mathcal{U}_{nn'}$ in (A7). Consider the noncompact group generators $K_1 = L_{45}, K_2 = -L_{46}$ and $K_3 = L_{56} = N$ of $O(4,2)$. They form the algebra of $O(2,1)$ subgroup. The action

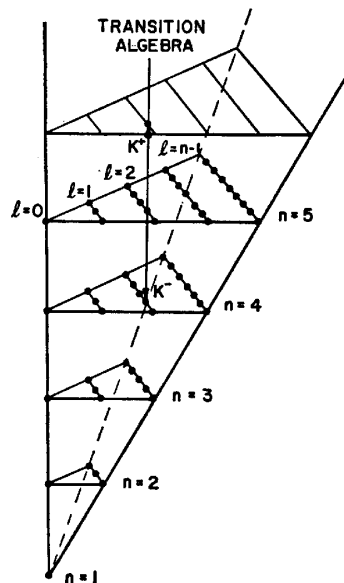


FIG. 1. Weight diagram for the triangular representation of $O(4,1)$. Every vertical line is a representation of the transition subgroup K , an $O(2,1)$ subgroup of the conformal group $O(4,2)$ generated by $L_{45}, -L_{46}, L_{56}$.

⁵ W. Gordon, Ann. Phys. (N. Y.) 2, 1031 (1929).

of the raising and lowering operators $K^\pm = K_1 \pm K_2$ is $\Delta l = 0$, $\Delta m = 0$, and $\Delta n = \pm 1$, and is shown on the weight diagram in Fig. 1. The states $|nlm\rangle$, for fixed l and m , form therefore a basis for an irreducible representation D_+^ϕ of this $O(2,1)$, the transition group,⁴ characterized by the lowest eigenvalue of $K_3 = N$ which is clearly $n = l + 1$. The matrix elements for D_+ of the finite $O(2,1)$ transformations are given by⁶

$$e^{-i\vartheta K_1} |n'lm\rangle = |nlm\rangle \mathcal{U}_{nn',l+1}(\vartheta), \quad (\text{A10})$$

⁶ V. Bargmann, Ann. Math. 48, 568 (1947).

where $\mathcal{U}_{nn',l+1}$ is precisely the function introduced in (A7). Equation (A10) has been proved in Ref. 4. Therefore (A9) becomes

$$\begin{aligned} \langle n'lm | D_{(n\pm 1)/n} | n\pm 1, lm \rangle & \frac{(n\pm 1)^2}{n} \\ & = \mp \frac{1}{\sinh \vartheta_{n'n}} \langle n'lm | e^{-i\vartheta_{n'n} K_1} | n\pm 1, lm \rangle. \end{aligned} \quad (\text{A11})$$

This equation inserted into (A1) gives finally Eq. (1.5). Q.E.D.