Generators of the de Sitter Group for the Hydrogen Atom

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Explicit Hermitian operator functions of **q** and **p** are constructed for the generators of the de Sitter group $O(4,1)$ on the bound-state wave functions for the hydrogen atom. This is done for each of the one-parameter family of irreducible unitary representations of $O(4,1)$ in which the irreducible representations of the four-dimensional rotation group $O(4)$ correspond to the degeneracy subspaces of the bound-state energy levels. The commutation relations and the values of the invariants which label the representation of $O(4,1)$ are verified by direct operator calculations.

I. INTRODUCTION

The hydrogen atom provides a dynamically nontrivial example of a system described by a group larger than the invariance group of the Hamiltonian.[1] The bound states of the hydrogen atom span a single irreducible unitary representation of the de Sitter group $O(4,1)$. This group has ten generators $M_{\alpha\beta}=-M_{\beta\alpha}$, for $\alpha, \beta=0, 1, 2, 3, 4$, satisfying the commutation relations

$$[M_{\alpha\beta},M_{\gamma\delta}]=i(g_{\alpha\delta}M_{\beta\gamma}-g_{\alpha\gamma}M_{\beta\delta}+g_{\beta\gamma}M_{\alpha\delta}-g_{\beta\delta}M_{\alpha\gamma}) \quad (1)$$

with $g_{\alpha\beta}=0$ except for $g_{00}=1$ and $g_{11}=g_{22}=g_{33}=g_{44}=-1$. The angular momentum and the Lenz vector provide representations

$$M_{jk}=\epsilon_{jkl}L_l=q_jp_k-q_kp_j$$
$$M_{j4}=K_j=|2H|^{-1/2}[q_j/r+(\tfrac{1}{2})\epsilon_{jkl}(L_kp_l-p_kL_l)] \quad (2)$$

for $j, k, l=1, 2, 3$, for six of the generators.[2] These are Hermitian operators which commute with the Hamiltonian

$$H=p^2/2-1/r.$$

On the bound-state subspace they satisfy the commutation relations (1) and generate a unitary representation of the four-dimensional rotation group $O(4)$. This subgroup of $O(4,1)$ is the invariance group of H for the bound states[2,3]; its representation is irreducible on the subspace spanned by the bound states for any one energy eigenvalue.

The irreducible unitary representations of $O(4)$ are labeled by two invariants, which for the generators (2) are

$$\tfrac{1}{2}M_{jk}M_{jk}=L^2+K^2=-1-(2H)^{-1}$$

and

$$\tfrac{1}{8}\epsilon_{jklm}M_{jk}M_{lm}=\mathbf{L}\cdot\mathbf{K}=0 \quad (3)$$

with each repeated index j, k, l, m implying a sum from 1 to 4. Thus, if we knew no more about the hydrogen atom than can be learned from the $O(4)$ generators (2), we could deduce that each bound-state energy eigenvalue E of H corresponds to one of the values

$$-1-(2E)^{-1}=4j(j+1) \quad (4)$$

for $j=0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$ which are allowed for the first of the two $O(4)$ invariants (3) when the second is zero.[4,5] But we would not know that there actually is an eigenvalue of H corresponding to each of these allowed values. Nor would we know that for each eigenvalue the subspace of eigenvectors does not support more than one multiple of the irreducible unitary representation of $O(4)$ specified by the invariants.

Interest in the larger group $O(4,1)$ is due to the fact[6,7] that it has a one-parameter family of inequivalent irreducible unitary representations in each of which the irreducible representations of the subgroup $O(4)$ correspond to the hydrogen-atom bound states. These are the irreducible unitary representations labeled by a positive value and zero, respectively, for the two invariants

$$-\tfrac{1}{2}g_{\alpha\gamma}g_{\beta\delta}M_{\alpha\beta}M_{\gamma\delta}$$

and

$$-g_{\mu\nu}w_\mu w_\nu, \quad (5)$$

where

$$w_\mu=\tfrac{1}{8}\epsilon_{\mu\alpha\beta\gamma\delta}M_{\alpha\beta}M_{\gamma\delta}$$

and each repeated index $\alpha, \beta, \gamma, \delta, \mu, \nu$ implies a sum from 0 to 4, with $\epsilon_{\mu\alpha\beta\gamma\delta}$ being totally antisymmetric, and $\epsilon_{01234}=1$.[7] Any one of these irreducible unitary representations of $O(4,1)$ provides a complete group-theoretic description of the hydrogen-atom bound states. It provides an answer to the questions mentioned above which are not answered by studying the generators (2) of $O(4)$: for each energy eigenvalue, the irreducible unitary representation of $O(4)$ which characterizes the subspace spanned by the bound-state eigenvectors of H occurs once and only once in the

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[1] A. O. Barut, P. Budini, and C. Fronsdal, Proc. Roy. Soc. **A291**, 106 (1966); E. C. G. Sudarshan, N. Mukunda, L. O'Raifeartaigh, Phys. Letters, **19**, 322 (1965); N. Mukunda, L. O'Raifeartaigh, and E. C. G. Sudarshan, Phys. Rev. Letters **15**, 1041 (1965). See also I. A. Malkin and V. I. Man'ko JETP Pis'am V Redaktsiyu **2**, 230 (1965) [English transl.: JETP Letters **2**, 146 (1965)], who prefer a larger group.

[2] V. Bargmann, Z. Physik. **99**, 576 (1936).

[3] V. Fock, Z. Physik **98**, 145 (1935).

[4] W. Pauli, Z. Physik **36**, 336 (1926).

[5] The operators $\mathbf{J}_1=\frac{1}{2}(\mathbf{L}+\mathbf{K})$ and $\mathbf{J}_2=\frac{1}{2}(\mathbf{L}-\mathbf{K})$ commute with each other, and each satisfies angular-momentum commutation relations. Therefore $\mathbf{J}_1^2$ and $\mathbf{J}_2^2$ are invariants which must have values $j_1(j_1+1)$ and $j_2(j_2+1)$ for an irreducible representation. If $\mathbf{J}_1^2-\mathbf{J}_2^2=\mathbf{L}\cdot\mathbf{K}$ is zero, then $j_1=j_2=j$ and $\mathbf{L}^2+\mathbf{K}^2=2(\mathbf{J}_1^2+\mathbf{J}_2^2)$ has the value (4).

[6] L. H. Thomas, Ann. Math. **42**, 113 (1941).

[7] T. D. Newton, Ann. Math. **51**, 730 (1950).

irreducible unitary representation of $O(4,1)$. This makes us curious about the generators $M_{0\alpha}$ which do not commute with H and which have not been understood as physical quantities like the generators (2) of $O(4)$. Bacry[8] solved the Poisson bracket relations to find expressions for these generators in classical mechanics; Bander and Itzykson,[9] Han [10] and Budini[11] have found a representation for them on the Hilbert space of square-integrable functions on Fock's unit four-sphere[3]; but explicit expressions for the generators $M_{0\alpha}$ as functions of operators $\mathbf{q}$ and $\mathbf{p}$ on ordinary hydrogen-atom wave functions have been unknown.

II. STATEMENT OF RESULTS

Using Thomas' formulas for the matrix elements,[6] and working with hydrogen-atom wave functions in parabolic coordinates, we have constructed the operators[12]

$$M_{0j}=i[T_j^{(+,+)}-T_j^{(+,-)}]\left[1+\frac{Q-2}{N(N+1)}\right]^{1/2}e^{i\theta(N)}$$

$$-i\left[1+\frac{Q-2}{N(N+1)}\right]^{1/2}e^{-i\theta(N)}[T_j^{(-,+)}-T_j^{(-,-)}]$$

$$M_{04}=[T_3^{(+,+)}+T_3^{(+,-)}]\left[1+\frac{Q-2}{N(N+1)}\right]^{1/2}e^{i\theta(N)}$$

$$-\left[1+\frac{Q-2}{N(N+1)}\right]^{1/2}e^{-i\theta(N)}[T_3^{(-,+)}+T_3^{(-,-)}] \quad (6)$$

for $j=1, 2, 3$; Q can be any positive number, θ can be any real function (zero, for example), and

$$T_j^{(+,\pm)}=(\tfrac{1}{4})\left(\left[i\mathbf{q}\cdot\mathbf{p}+\bar{N}+1-\frac{1}{\bar{N}+1}r\right]\right.$$

$$\left.\pm\left[\mathrm{i}rp_j+\bar{K}_j-\frac{1}{\bar{N}+1}q_j\right]\right)\left(\frac{\bar{N}}{\bar{N}+1}\right)^{i\mathbf{q}\cdot\mathbf{p}+2}$$

$$T_j^{(-,\pm)}=(\tfrac{1}{4})\left(\left[i\mathbf{q}\cdot\mathbf{p}-\bar{N}+1+\frac{1}{\bar{N}-1}r\right]\right.$$

$$\left.\mp\left[\mathrm{i}rp_j-\bar{K}_j+\frac{1}{\bar{N}-1}q_j\right]\right)\left(\frac{\bar{N}}{\bar{N}-1}\right)^{i\mathbf{q}\cdot\mathbf{p}+2} \quad (7)$$

for $j=1, 2, 3$; $N=|2H|^{-1/2}$ and $\bar{N}$ and $\bar{K}_j$ mean that N and K_j (which commute with each other) are placed to the right of everything else. Different values of Q give inequivalent irreducible unitary representations of $O(4,1)$; Q and zero are the values of the two invariants (5) which label the inequivalent irreducible unitary representations of $O(4,1)$ in which the irreducible representations of $O(4)$ correspond to the hydrogen-atom bound states.[7] Different functions θ give equivalent representations related by unitary operator functions of H; they account for all the unitary transformations which leave the generators (2) of the invariance group unchanged. We have verified by explicit calculation that on the bound-state subspace the operators (6) are Hermitian and that, together with the operators (2), they satisfy the commutation relations (1) and give the values Q and zero for the two invariants (5) of $O(4,1)$. In the classical limit the operators (6) reduce to Bacry's solution of the Poisson bracket relations.[8] These calculations are described in the following sections.

Finally it should be noted that the properties of the operators $M_{0\alpha}$ on the bound-state subspace do not determine these operators uniquely as functions of $\mathbf{q}$ and $\mathbf{p}$. For this it would be necessary to specify the properties desired for these operators on the continuum subspace. Thus, as far as the bound-state subspace is concerned, we may add to the operators $M_{0\alpha}$ given above any functions of $\mathbf{q}$ and $\mathbf{p}$ which have zero projections on the bound-state subspace.

III. METHOD OF CONSTRUCTION

Formulas for matrix elements of the generators $M_{0\alpha}$ are given by Thomas.[6] For the irreducible unitary representations of $O(4,1)$ relevant to the hydrogen atom, these matrix elements are for a basis in which H, L_3, and K_3 are diagonal; the basis vectors are labeled by $j=0, \frac{1}{2}, 1, \frac{3}{2}\cdots$ and $m_1, m_2=-j, -j+1,\cdots j$; the eigenvalues of H are given by (4), and the eigenvalues of L_3 and K_3 are m_1+m_2 and m_1-m_2, respectively. The hydrogen-atom wave functions in parabolic coordinates provide such a basis.[2] In the notation of Schiff,[13] the bound-state wave functions $u_{n_1n_2m}$ of parabolic coordinates are (unnormalized) eigenvectors of H, L_3, and K_3; the eigenvalues of H are $-(2n^2)^{-1}$ with $n=n_1+n_2+|m|+1$, and the eigenvalues of L_3 and K_3 are m and n_1-n_2, respectively. Thus, allowing for normalization constants and phase conventions, we know how the generators $M_{0\alpha}$ should operate on these wave functions. In particular, M_{03} and M_{04} should take a wave function $u_{n_1n_2m}$ to certain linear combinations of the four wave functions $u_{n_1\pm1,n_2,m}$ and $u_{n_1,n_2\pm1,m}$. Since M_{01} and M_{02} can be gotten by rotating M_{03}, the problem is to find operators for raising and lowering n_1 and n_2.

[8] H. Bacry, Nuovo Cimento **41**, A222 (1966).
[9] M. Bander and C. Itzykson (to be published).
[10] M. Y. Han, Nuovo Cimento (to be published).
[11] P. Budini (to be published).
[12] A set of operators $M_{0\alpha}$ has been constructed from wave functions in spherical coordinates by R. Musto, Phys. Rev. (to be published). We get the same operators for each value of his label q by setting $Q=2-q(q+1)$. Thus positive Q correspond to $1>q\geqslant-\frac{1}{2}$ and $q=-\frac{1}{2}+ih$ for positive h. Musto emphasizes also the representations for positive integers q. A representation of this type is irreducible on the subspace spanned by the bound states for $n>q$. [The square-root factors in (6) are zero for $N=q$. This prevents the operators $M_{0\alpha}$ from connecting the subspace for $n>q$ to the subspace for $n\leqslant q$.] Positive Q label representations of Newton's Class I and positive integers q label representations of Newton's Class II (Ref. 7).

[13] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., pp. 87–89.

Of the operators (7), $T_3^{(+,+)}$ and $T_3^{(-,-)}$ are raising and lowering operators respectively for n_1, and $T_3^{(+,-)}$ and $T_3^{(-,+)}$ are raising and lowering operators, respectively, for n_2. The main factors for raising and lowering n_1, for example, are derived from the presence in $u_{n_1n_2m}$ of an associated Laguerre polynomial $L_{n_1+|m|}{}^{|m|}(\xi/n)$ with ξ being one of the parabolic coordinates.[13]

The factors $(\bar{N}/\bar{N}\pm1)^{i\mathbf{q}\cdot\mathbf{p}}$ are dilation operators. They scale the coordinates of the wave functions from $\mathbf{x}$ to $[n/(n\pm1)]\mathbf{x}$. For example, they take ξ/n to $\xi/(n\pm1)$ in the associated Laguerre polynomial. They are obtained from the scaling operation

$$f(a\mathbf{x})=a^{\mathbf{x}\cdot\nabla}f(\mathbf{x})$$

for a positive number a by substituting the operator N for its eigenvalue n. To be in a position to operate directly on its eigenfunctions, N must be placed to the right of all other operators. This is indicated by the bar.

The recurrence relations and differential equations satisfied by the associated Laguerre polynomials imply that[14]

$$L_{n_1+1+|m|}{}^{|m|}(s)=\frac{n_1+|m|+1}{n_1+1}\times\left(s\frac{d}{ds}+n_1+|m|+1-s\right)L_{n_1+|m|}{}^{|m|}(s)$$

$$L_{n_1-1+|m|}{}^{|m|}(s)=(n_1+|m|)^{-2}\left(s\frac{d}{ds}-n_1\right)L_{n_1+|m|}{}^{|m|}(s).$$

Operators for raising and lowering n_1 in the index of the associated Laguerre polynomial are obtained by substituting the operators $\bar{N}$, $\bar{L}_3$, and $\bar{K}_3$ for their respective eigenvalues $n_1+n_2+|m|+1$, m, and n_1-n_2. Since N, L_3, and K_3 commute with each other, there is no problem in placing operators to the right in a position to operate on their eigenfunctions. This is indicated again by bars.

Neither the dilation operators nor the raising and lowering operators for the indices are unique, since their properties are required only on a particular set of functions. To the latter, for example, we could add the differential operator which annihilates the associated Laguerre polynomials. Once these choices are made, however, operators (6) and (7) are obtained from the matrix elements by putting the various parts together, taking account of normalization constants and the various factors of the wave functions. At this stage we did not bother with phase factors. The most general phase factors, involving the arbitrary function θ, were determined in the verification procedure.

[14] Similar raising and lowering operators were constructed by E. Schrödinger, Proc. Roy. Irish Acad. **A46**, 9 (1940), and L. Infeld and T. E. Hull, Rev. Mod. Phys. **23**, 21 (1951).

IV. VERIFICATION

It is possible to work directly with the operator expressions (6) and (7) for the $M_{0\alpha}$ and, for example, verify that on the bound-state subspace they satisfy the commutation relations (1). Evidently M_{04} commutes with $\mathbf{L}$, and the operators M_{0j} for $j=1, 2, 3$ satisfy the commutation relations of a vector with $\mathbf{L}$. It is necessary to verify in addition only the three commutation relations

$$\begin{aligned}[M_{34},M_{40}]&=iM_{03}\\ [M_{03},M_{34}]&=iM_{40}\\ [M_{03},M_{40}]&=iM_{34}\end{aligned}\qquad(8)$$

as the remaining commutation relations can be shown to follow from these by use of the Jacobi identity.

The first two of the relations (8) follow immediately once we prove that on the bound-state subspace[15] the $T_j^{(\ ,\ )}$ are raising and lowering operators for N and M_{j4}:

$$\begin{aligned}NT_j^{(\pm,\ )}&=T_j^{(\pm,\ )}(N\pm1)\\ M_{j4}T_j^{(\ ,\pm)}&=T_j^{(\ ,\pm)}(M_{j4}\pm1)\end{aligned}\qquad(9)$$

for $j=1, 2, 3$. The first of the relations (9) follows, in turn, from the demonstration that for bound states[15]

$$\begin{aligned}-(1/2N^2)T_j^{(\pm,\ )}&=HT_j^{(\pm,\ )}\\ &=T_j^{(\pm,\ )}H(N/(N\pm1))^2\\ &=T_j^{(\pm,\ )}[-1/2(N\pm1)^2]\end{aligned}\qquad(10)$$

for $j=1, 2, 3$. To prove (10) one simply calculates the commutator of H and $T_j^{(\pm,\ )}$ and appropriately rearranges terms. The only novel feature arises in taking H through the scaling operators; for example

$$H\left(\frac{\bar{N}}{\bar{N}+1}\right)^{i\mathbf{q}\cdot\mathbf{p}}=\left[\frac{-1}{2(\bar{N}+1)^2}-\left(\frac{1}{\bar{N}+1}\right)\frac{1}{r}\right]\left(\frac{\bar{N}}{\bar{N}+1}\right)^{i\mathbf{q}\cdot\mathbf{p}}.\qquad(11)$$

The calculation of the second of the relations (9) then proceeds in a similar fashion. The third of the commutation relations (8) follows from the properties

$$\begin{aligned}&[T_j^{(\pm,+)},T_j^{(\pm,-)}]=0,\\ &16T_j^{(\pm,+)}T_j^{(\mp,-)}=L_j^2-(N\pm K_j\mp1)^2,\\ &16T_j^{(\mp,-)}T_j^{(\pm,+)}=L_j^2-(N\pm K_j\pm1)^2,\end{aligned}$$

for $j=1, 2, 3$, which can be verified by direct substitution.

Verification that the values of the invariants (5) for this representation are Q and zero, respectively,

[15] On the bound-state subspace $N=(-2H)^{-1/2}$ and $H=-(2N^2)^{-1}$. Our operator algebra is done with these relations. The algebraic manipulations of this section (but not the proof of Hermiticity) are then valid for positive as well as negative H. However with this definition of N the formulas (6) and (7) do not give well-defined operators $M_{0\alpha}$ on the subspace for positive H. A useful feature of this operator algebra is its invariance under $N\rightarrow-N$.

presents no new problems. It is easy to see that

$$L_jM_{j4}=0\,,\qquad L_jM_{0j}=0\,,$$
$$L_iM_{40}=\epsilon_{ijk}M_{0j}M_{k4}\qquad \text{for } i=1,2,3\,,$$

where sums over j, $k=1$, 2, 3 are understood, and from these that the second invariant vanishes. In calculating the first invariant another useful property of the $T_j^{(\ ,\ )}$ is

$$8(T_j^{(\pm,+)}T_j^{(\mp,+)}+T_j^{(\pm,-)}T_j^{(\mp,-)})=2L^2+1-N^2+K_j^2-L_j^2$$

for $j=1$, 2, 3.

That the generators $M_{0\alpha}$ are Hermitian follows from the properties

$$(T_j^{(+,+)})^\dagger=-T_j^{(-,-)}\,,\quad (T_j^{(+,-)})^\dagger=-T_j^{(-,+)}\,,\quad (12)$$

for $j=1$, 2, 3. Our proof of (12) requires some resort to matrix elements. Thus, consider matrix elements of $(T_3^{(+,+)})^\dagger$ between eigenvectors of N, K_3, L_3 labeled by eigenvalues n, k, m. Using our knowledge of the properties of the scaling operators, and of which states are connected by the operators involved, we find that

$$\begin{aligned}\langle n',k',m'|(T_3^{(+,+)})^\dagger|n,k,m\rangle &=\delta_{n',n-1}\delta_{k',k-1}\delta_{m',m}\\ &\times\langle n-1,k-1,m|\left(\frac{N^{\leftarrow}}{N^{\leftarrow}+1}\right)^{-i\mathbf{q}\cdot\mathbf{p}-1}\bigg[i\mathbf{q}\cdot\mathbf{p}+3-N^{\leftarrow}+1\\ &+\frac{1}{N^{\leftarrow}+1}r+irp_3+q_3/r-K_3^{\leftarrow}+\frac{1}{N^{\leftarrow}+1}q_3\bigg]|n,k,m\rangle\\ &=-\delta_{n',n-1}\delta_{k',k-1}\delta_{m',m}\\ &\times\langle n-1,k-1,m|\bigg[i\mathbf{q}\cdot\mathbf{p}+3-\bar N+\frac{1}{\bar N-1}r+irp_3+q_3/r\\ &-\bar K_3+1+\frac{1}{\bar N-1}q_3\bigg]\left(\frac{\bar N}{\bar N-1}\right)^{i\mathbf{q}\cdot\mathbf{p}+1}|n,k,m\rangle\\ &=-\delta_{n',n-1}\delta_{k',k-1}\delta_{m',m}\langle n-1,k-1,m|T_3^{(-,-)}|n,k,m\rangle\\ &=-\langle n',k',m'|T_3^{(-,-)}|n,k,m\rangle\,,\end{aligned}\quad (13)$$

where $N^{\leftarrow}$ and $K_3^{\leftarrow}$ mean that N and K_3 are placed to the left of everything else. The identification of the matrix element in (13) with the matrix element of $T_3^{(-,-)}$ follows from the equivalences

$$\begin{aligned}&(1/(\bar N-1))r\sim 2\bar N-1\,,\quad q_3/r\sim 1\,,\quad i\mathbf{q}\cdot\mathbf{p}\sim\bar N-2\\ &irp_3\sim\bar N-1\,,\quad (1/(\bar N-1))q_3\sim\bar K_3+\bar N-1\,,\end{aligned}\quad (14)$$

where $A\sim B$ means that

$$\langle n-1,k-1,m|A\left(\frac{\bar N}{\bar N+1}\right)^{i\mathbf{q}\cdot\mathbf{p}+1}|n,k,m\rangle=\langle n-1,k-1,m|B\left(\frac{\bar N}{\bar N+1}\right)^{i\mathbf{q}\cdot\mathbf{p}+1}|n,k,m\rangle.$$

The proof of the relations (14) follows by taking the matrix elements of various operator identities such as (11).

Bacry's solutions $B_j=M_{j0}$, for $j=1$, 2, 3, and $S=M_{40}$ of the Poisson bracket relations[8] are obtained by considering (6) and (7) as functions of classical variables $\mathbf{q}$ and $\mathbf{p}$ and taking the limit for large N. For example

$$(N/(N\pm1))^{i\mathbf{q}\cdot\mathbf{p}}\to e^{\mp i\mathbf{q}\cdot\mathbf{p}/N}.$$

It is easy to see that the other factors agree with Bacry's by rearranging a few terms, neglecting occasionally a term of higher order in $1/N$, and adjusting the phase θ.

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