New vector operators for the nonrelativistic Coulomb problem

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The purpose of this paper is to obtain a Lie algebra with the property that suitable linear combinations of its basis operators are ladder operators for the quantum number l in the eigenkets $|nlm\rangle$ of the nonrelativistic Coulomb problem. By analogy with the way in which the Pauli-Lenz operator $\mathbf{A}$ is constructed from the classical Laplace-Runge-Lenz vector $\mathbf{A}_c$, we deduce a new Hermitian vector operator $\mathbf{B}$ as a quantum-mechanical analog of a conserved classical vector $\mathbf{B}_c$ which is orthogonal to $\mathbf{A}_c$ and the orbital angular momentum $\mathbf{L}$, and has the property $B_c=A_c$. Apart from a standard modification, $\mathbf{B}\to\mathbf{B}_c$ as $\hbar\to 0$. We show that the combination $\mathbf{A}+i\mathbf{B}$ provides abstract ladder operators for the quantum numbers l, and l and m, and we calculate the coefficients for these transformations. The operators $\mathbf{L}$ and $\mathbf{B}$ are a basis for a Lie algebra which is the same as that of $\mathbf{L}$ and $\mathbf{A}$, namely, O(4). The Hermitian operators H, B_z, and L_z are a set of commuting operators and we determine the corresponding eigenvalues and eigenkets. Finally we show that the ten operators $\mathbf{A}$, $\mathbf{B}$ (both suitably modified), $\mathbf{L}$, and $(\hbar^{-2}\mathbf{L}^2+\frac{1}{4})^{1/2}$ can be combined to form a Hermitian basis for a Lie algebra, the de Sitter algebra O(3,2).

I. INTRODUCTION

It is well known that the classical dynamics of a particle in a central potential admits constants of the motion additional to the energy E and the angular momentum $\mathbf{L}$.[1–4] If the potential allows periodic motion then there exists a conserved vector which is an algebraic function of the position and momentum vectors $\mathbf{r}$ and $\mathbf{p}$. A familiar example is the nonrelativistic Coulomb problem, for which the conserved vector is

$$\mathbf{A}_c=(Mk)^{-1}\mathbf{L}\times\mathbf{p}+r^{-1}\mathbf{r}\ . \tag{1}$$

where M is the mass of the particle and k is the constant in $\mathbf{F}=-kr^{-3}\mathbf{r}$.

This so-called Laplace-Runge-Lenz vector provides a simple solution for the classical motion: the eccentricity of the orbit is equal to A_c and the radius vector to the aphelion of the orbit is parallel to $\mathbf{A}_c$. Of course, the existence of the conserved vectors $\mathbf{L}$ and $\mathbf{A}_c$ is related to the symmetry inherent in the Coulomb problem and, in fact, the six quantities $\mathbf{L}$ and $[Mk^2/2(|E|)]^{1/2}\mathbf{A}_c$ are generators of a symmetry group. If $E<0$ this group is isomorphic to the Lie group SO(4)—the orthogonal group of rotations in four dimensions.[5]

The quantum-mechanical version of the nonrelativistic Coulomb problem can be treated in a similar manner by introducing a Hermitian vector operator which is a quantum-mechanical analog of (1), namely, the Pauli-Lenz vector:[6–9]

$$\mathbf{A}=(-2Ma^2\hbar^{-2}H)^{-1/2}\left[\frac{a}{2\hbar^2}(\mathbf{L}\times\mathbf{p}-\mathbf{p}\times\mathbf{L})+r^{-1}\mathbf{r}\right], \tag{2}$$

where $H=(2M)^{-1}(\mathbf{p}^2-2\hbar^2a^{-1}r^{-1})$ and $a=\hbar^2/Mk$ is the Bohr radius if $k=e^2(4\pi\epsilon_0)^{-1}$. Here and in what follows it is assumed that bound states are being considered. Use of the two constants of the motion $\mathbf{L}$ and $\mathbf{A}$ provides a derivation of the Bohr formula for E by general algebraic methods (Pauli[6]). As in the classical case $\mathbf{L}$ and $\mathbf{A}$ generate a symmetry group which is isomorphic to SO(4).[10]

An important property of these generators is that they can be used to construct ladder operators for certain energy eigenkets. For example, if $|Epm\rangle$ is a ket for the commuting operators H,A_z,L_z then the ladder operators for p and m consist of appropriate linear combinations of $\mathbf{L}$ and $\mathbf{A}$. These operators map $|Epm\rangle$ onto adjacent kets such as $|E,p+1,m+1\rangle$ [see Eqs. (19) and (20) below]; thus, starting with any one of these kets it is possible to reach all of them by using the ladder operators. There are many other examples of ladder operators which consist of linear combinations of the generators of a group, and the construction and properties of these operators have been the subject of numerous studies (see, for example, Englefield[11] and Wybourne[12] and the references therein).

However, for the kets $|Elm\rangle$ of the commuting operators H, L^2, L_z a linear combination of generators of SO(4) cannot, in general, map $|Elm\rangle$ onto a ket with l changed by ± 1. Instead an indirect sequence of transformations represented by a nonlinear function of L_i and A_i must be used for this purpose (Sec. II). This contrasts with the ladder operators $L_\pm=L_x\pm iL_y$ for m, with the ladder operators for the energy eigenvalue and with the examples referred to above.

These remarks suggest that the theory of ladder operators for the quantum number l of the kets $|Elm\rangle$ for the Coulomb problem is incomplete. The present paper is intended to remedy this situation: we show that by considering additional operators to the generators of SO(4) one can obtain ladder operators for l. In Sec. II we summarize some useful properties of the Pauli-Lenz vector $\mathbf{A}$.

Then in Sec. III we derive a new Hermitian vector operator **B** which in linear combination with **A** yields ladder operators for l, and l and m. The coefficients for these transformations are calculated. In Sec. IV it is shown that **L** and **B** are a basis for the Lie algebra O(4). The operators H, B_z, L_z are a set of commuting operators and we determine the corresponding eigenvalues and eigenkets. The enlarged set of ten operators **L**, **A**, **B**, and $(\hbar^{-2}\mathbf{L}^2+\frac{1}{4})^{1/2}$ can be combined to form a Hermitian basis for a Lie algebra. This is found to be the de Sitter algebra O(3,2) (Sec. V).

II. PROPERTIES OF THE PAULI-LENZ VECTOR

We give a brief review of some well-known properties of the Pauli-Lenz vector which are of use in this paper.

The commutators

$$[L_i,L_j]=i\hbar\epsilon_{ijk}L_k\ , \tag{3}$$

$$[L_i,A_j]=i\hbar\epsilon_{ijk}A_k\ , \tag{4}$$

and

$$[A_i,A_j]=i\hbar^{-1}\epsilon_{ijk}L_k\ , \tag{5}$$

show that the Hermitian operators **L** and **A** are a basis for the Lie algebra O(4); the corresponding symmetry group is SO(4). The Casimir operators

$$C_1=\hbar^{-2}\mathbf{L}^2+\mathbf{A}^2\ , \tag{6}$$

$$C_2=\mathbf{L}\cdot\mathbf{A} \tag{7}$$

can also be written

$$C_1=-(2Ma^2\hbar^{-2}H)^{-1}-1 \tag{8}$$

and

$$C_2=0\ . \tag{9}$$

From Eq. (4), **A** is a vector operator and according to the Wigner-Eckart theorem

$$A_\pm\,|\,Elm\,\rangle=\pm[(l\mp m)(l\mp m-1)]^{1/2}a_l\,|\,E,l-1,m\pm1\,\rangle \pm[(l\pm m+1)(l\pm m+2)]^{1/2} \times a_{l+1}\,|\,E,l+1,m\pm1\,\rangle\ , \tag{10}$$

and

$$A_z\,|\,Elm\,\rangle=(l^2-m^2)^{1/2}a_l\,|\,E,l-1,m\,\rangle -[(l+1)^2-m^2]^{1/2}a_{l+1}\,|\,E,l+1,m\,\rangle\ , \tag{11}$$

where $A_\pm=A_x\pm iA_y$ and $a_l=-[l(2l+1)]^{-1/2}\times\langle E,l-1||A||E,l\rangle$. Here and in what follows the kets are chosen in such a way that

$$\langle E,l+1||A||E,l\rangle =[(2l+1)/(2l+3)]^{1/2}\langle E,l||A||E,l+1\rangle\ . \tag{12}$$

This choice is the same as that of Bohm[13] but differs from that of Biedenharn and Louck.[14]

Use of Eqs. (5), (10), and (11) shows that the coefficient a_l must satisfy the finite-difference equation

$$(2l+3)a_{l+1}^2-(2l-1)a_l^2=1\ .$$

This can be rewritten as

$$[4(l+1)^2-1]a_{l+1}^2-(4l^2-1)a_l^2=2l+1\ ,$$

from which it is obvious that $(4l^2-1)a_l^2=l^2-n^2$, where n is independent of l but otherwise is arbitrary. Thus

$$a_l=i\left[\frac{n^2-l^2}{4l^2-1}\right]^{1/2}\ . \tag{13}$$

The possible values of n can be calculated as in Bohm.[13] Alternatively they may be obtained from the coefficients of the ladder operators for l which are derived in this paper: from Eqs. (37) and (39) below it is clear that for physical eigenkets l must have a maximum value of $n-1$. Thus $n=1,2,3,\ldots$. From Eqs. (6), (10), (11), and (13)

$$C_1\,|\,Elm\,\rangle=(n^2-1)\,|\,Elm\,\rangle\ . \tag{14}$$

Equations (8) and (14) yield eigenvalues $E=-(2Ma^2\hbar^{-2}n^2)^{-1}$.

The operators H,A_z,L_z are also a commuting set with kets $|\,npm\,\rangle$. These can be expanded:

$$|\,npm\,\rangle=\sum_l D_l\,|\,nlm\,\rangle\ . \tag{15}$$

From (14) and (15)

$$C_1\,|\,npm\,\rangle=(n^2-1)\,|\,npm\,\rangle\ . \tag{16}$$

Define

$$\mathbf{X}^\pm=\tfrac{1}{2}(\mathbf{A}\pm\hbar^{-1}\mathbf{L}) \tag{17}$$

and

$$X_\pm^+=X_x^+\pm iX_y^+,\quad X_\pm^-=X_x^-\pm iX_y^-\ .$$

Then from the commutators

$$[H,X_\pm^+]=[H,X_\pm^-]=0\ ,$$
$$\hbar^{-1}[L_z,X_\pm^+]=[A_z,X_\pm^+]=\pm X_\pm^+\ , \tag{18}$$
$$\hbar^{-1}[L_z,X_\pm^-]=-[A_z,X_\pm^-]=\pm X_\pm^-\ ,$$

it follows that $X_\pm^+$ and $X_\pm^-$ are ladder operators for p and m in the kets $|\,npm\,\rangle$. The coefficients for these transformations follow from expectation values such as

$$\langle X_\mp^+X_\pm^+\rangle=\langle(\mathbf{X}^+)^2-(X_z^+)^2\mp X_z^+\rangle =\tfrac{1}{4}[n^2-(m+p\pm1)^2]\ ,$$

where in the last step $(\mathbf{X}^+)^2=\frac{1}{4}C_1$ and Eq. (16) have been used. Thus

$$X_\pm^+\,|\,npm\,\rangle=\tfrac{1}{2}[n^2-(m+p\pm1)^2]^{1/2}\,|\,n,p\pm1,m\pm1\,\rangle \tag{19}$$

and

$$X_\pm^-\,|\,npm\,\rangle=\tfrac{1}{2}[n^2-(m-p\pm1)^2]^{1/2}\,|\,n,p\mp1,m\pm1\,\rangle\ . \tag{20}$$

Equations (19) and (20) can also be obtained by using the theory of the coupling of two angular momenta.[14]

It is apparent that to transform the ket $|nlm\rangle$ into a neighboring ket such as $|n,l+1,m\rangle$ by using the generators of SO(4), one must apply a nonlinear function of these generators, for example, $L_-^{l-m+1}A_+L_+^{l-m}$ [see Eqs. (10) and (45)]. This procedure differs from the usual ladder operation such as that for m and p in Eqs. (19) and (20) or the eigenvalue l of the kets $|nlm\rangle$ for the three-dimensional isotropic harmonic oscillator.

III. LADDER OPERATORS FOR l

It has been known since the work of Fock[8] and Bargmann[9] that if a classical system possesses constants of the motion whose Poisson brackets define a Lie algebra, it is possible, at least for the simplest systems, to find quantum-mechanical operators whose commutation brackets serve the same purpose. Furthermore, as the example of the isotropic harmonic oscillator illustrates, linear combinations of these operators should yield ladder operators.

For our purpose it is instructive to compare the Coulomb problem and the three-dimensional isotropic harmonic oscillator. The classical dynamics of each system possesses both SO(4) and SU(3) symmetry: the generators of SO(4) are the six conserved quantities **L** and a Laplace-Runge-Lenz vector $\mathbf{A}_c$, whereas the generators of SU(3) are the eight conserved quantities **L** and a symmetric, traceless second-rank tensor T_{ij} (Fradkin[2]). The tensor T_{ij} for the classical Coulomb problem is rather complicated and therefore the quantum-mechanical treatment employs the operator analogs of **L** and $\mathbf{A}_c$. For the oscillator the opposite is true and hence for the quantum-mechanical oscillator it is conventional to use **L** and T_{ij}.[15,16] In the classical dynamics $\mathbf{A}_c$ specifies a single symmetry axis of the elliptical orbit for the Coulomb problem, whereas for the oscillator T_{ij} specifies (via its eigenvectors) the two orthogonal symmetry axes of the elliptical orbit.[17] In the quantum theory of the oscillator a suitable linear combination of the generators of SU(3) (the quadrupole tensor operator) yields ladder operators for l, and l and m in the basis $|nlm\rangle$;[12,18] however, no linear combination of the generators of SO(4) will yield ladder operators for l in the Coulomb basis $|nlm\rangle$.

This comparison suggests that for the Coulomb problem we introduce a vector constant of the motion which is orthogonal to both the Laplace-Runge-Lenz vector Eq. (1) and the angular momentum vector. With cylindrical coordinates such that $\mathbf{L}=(0,0,L_z)$, Eq. (1) can be written $\mathbf{A}_c=(A_r,A_\phi,0)$ where $A_r=1-(\mathbf{L}^2/Mk)r^{-1}$ and $A_\phi=(L/k)\dot{r}$. Thus we consider the conserved vector

$$\mathbf{B}_c=(A_\phi,-A_r,0)\,. \tag{21}$$

Then

$$\mathbf{L}\cdot\mathbf{B}_c=0\,,$$
$$\mathbf{A}_c\cdot\mathbf{B}_c=0\,, \tag{22}$$
$$B_c=A_c=\left[1+\frac{2\mathbf{L}^2E}{Mk^2}\right]^{1/2},$$
$$\mathbf{A}_c\times\mathbf{B}_c=-\left[1+\frac{2\mathbf{L}^2E}{Mk^2}\right]\hat{\mathbf{L}}\,.$$

Equation (21) can be written explicitly:

$$\mathbf{B}_c=\left[\frac{1}{r}\mathbf{r}\times\mathbf{L}+\frac{1}{Mk}\mathbf{p}\mathbf{L}^2\right]\frac{1}{L}\,. \tag{23}$$

A straightforward though tedious calculation yields the Poisson brackets

$$\{L_i,B_j'\}=\epsilon_{ijk}B_k'\,,$$

and

$$\{B_i',B_j'\}=\epsilon_{ijk}L_k\,,$$

where $\mathbf{B}'=[-Mk^2/(2E)]^{1/2}\mathbf{B}_c$ and $E<0$. Thus for bounded motion **L** and **B**$'$ are generators of a symmetry group SO(4).

Although in the classical problem $\mathbf{B}_c$ provides the same information as $\mathbf{A}_c$, we shall show that some useful new quantum-mechanical operators can be obtained from $\mathbf{B}_c$. From Eq. (23) we construct an abstract Hermitian operator

$$\mathbf{B}=\tfrac{1}{2}[\mathbf{F}G(\mathbf{L}^2)+G(\mathbf{L}^2)\mathbf{F}^\dagger]\,, \tag{24}$$

where

$$\mathbf{F}=(-2Ma^2\hbar^{-2}H)^{-1/2}\left[\frac{1}{r}\mathbf{r}\times\mathbf{L}+\frac{a}{\hbar^2}\mathbf{p}\mathbf{L}^2\right], \tag{25}$$

G is a Hermitian operator whose functional dependence on $\mathbf{L}^2$ is determined below [Eq. (44)], and $a=\hbar^2/Mk$. The operator $(-H)^{-1/2}$ is introduced in Eq. (25) for the same reason that it is included in the Pauli-Lenz vector Eq. (2), namely, to obtain operators which are a basis for a Lie algebra (Sec. IV). For the Pauli-Lenz vector the classical limit of $(-2Ma^2\hbar^{-2}H)^{1/2}\mathbf{A}$ is $\mathbf{A}_c$; to obtain a classical limit for $(-2Ma^2\hbar^{-2}H)^{1/2}\mathbf{B}$ equal to $\mathbf{B}_c$ will require

$$G(\mathbf{L}^2)\to(\mathbf{L}^2)^{-1/2} \tag{26}$$

as $\hbar\to 0$. [The expression we derive for G does have this limit—see Eq. (44).] The operator **B** is not a unique quantum-mechanical analog of the classical vector $\mathbf{B}_c$ because $\mathbf{L}^2$ does not commute with $\mathbf{r}\times\mathbf{L}$ and **p**. However, the form Eq. (24) is sufficient for our purposes. We note that the operators **A** and **B** are related: use of the identity $\mathbf{F}=\mathbf{A}\times\mathbf{L}$ shows that Eq. (24) can also be written

$$\mathbf{B}=\tfrac{1}{2}[(\mathbf{A}\times\mathbf{L})G(\mathbf{L}^2)-G(\mathbf{L}^2)(\mathbf{L}\times\mathbf{A})]\,.$$

It is straightforward to show that $[H,\mathbf{F}]=0$. Using this and the relations $\mathbf{L}\times\mathbf{r}=-\mathbf{r}\times\mathbf{L}+2i\hbar\mathbf{r}$ and $[\mathbf{L}^2,\mathbf{p}]=2i\hbar(\mathbf{p}\times\mathbf{L}-i\hbar\mathbf{p})$, one obtains $\mathbf{F}^\dagger=\mathbf{F}-2i\hbar\mathbf{A}$. Thus Eq. (24) can be written

$$\mathbf{B}=\tfrac{1}{2}[\mathbf{F}G(\mathbf{L}^2)+G(\mathbf{L}^2)\mathbf{F}-2i\hbar G(\mathbf{L}^2)\mathbf{A}]\,. \tag{27}$$

Clearly $[H,\mathbf{B}]=0$.

We now consider the effect of the abstract operators **F** and **B** on the kets $|nlm\rangle$. For the choice of kets implicit in Eq. (12) it can be shown that

$$F_\pm \,|\, nlm\rangle = \pm i\hbar(l+1)[(l\mp m)(l\mp m-1)]^{1/2}a_l \,|\, n,l-1,m\pm 1\rangle$$
$$\mp i\hbar l[(l\pm m+1)(l\pm m+2)]^{1/2}a_{l+1}\,|\, n,l+1,m\pm 1\rangle \;, \tag{28}$$

and

$$F_z \,|\, nlm\rangle = i\hbar(l+1)(l^2-m^2)^{1/2}a_l\,|\, n,l-1,m\rangle + i\hbar l[(l+1)^2-m^2]^{1/2}a_{l+1}\,|\, n,l+1,m\rangle \;, \tag{29}$$

where $F_\pm = F_x \pm iF_y$ and a_l is given by Eq. (13). The proof of Eqs. (28) and (29) is given in the Appendix. Using Eqs. (27), (10), (11), (28), and (29), we find

$$B_\pm \,|\, nlm\rangle = \pm\tfrac{1}{2}i\hbar[(l+1)G_l+(l-1)G_{l-1}][(l\mp m)(l\mp m-1)]^{1/2}a_l\,|\, n,l-1,m\pm 1\rangle$$
$$\mp\tfrac{1}{2}i\hbar[(l+2)G_{l+1}+lG_l][(l\pm m+1)(l\pm m+2)]^{1/2}a_{l+1}\,|\, n,l+1,m\pm 1\rangle \tag{30}$$

and

$$B_z \,|\, nlm\rangle = \tfrac{1}{2}i\hbar[(l+1)G_l+(l-1)G_{l-1}](l^2-m^2)^{1/2}a_l\,|\, n,l-1,m\rangle$$
$$+\tfrac{1}{2}i\hbar[(l+2)G_{l+1}+lG_l][(l+1)^2-m^2]^{1/2}a_{l+1}\,|\, n,l+1,m\rangle \;, \tag{31}$$

where G_l is the eigenvalue in

$$G(\mathbf{L}^2)\,|\, nlm\rangle = G_l\,|\, nlm\rangle \;. \tag{32}$$

If G_l satisfies the finite-difference equation

$$(l+1)G_l+(l-1)G_{l-1} = 2\hbar^{-1} \;, \tag{33}$$

Eqs. (30) and (31) become

$$B_\pm \,|\, nlm\rangle = \pm i[(l\mp m)(l\mp m-1)]^{1/2}a_l\,|\, n,l-1,m\pm 1\rangle \mp i[(l\pm m+1)(l\pm m+2)]^{1/2}a_{l+1}\,|\, n,l+1,m\pm 1\rangle \;, \tag{34}$$

and

$$B_z \,|\, nlm\rangle = i(l^2-m^2)^{1/2}a_l\,|\, n,l-1,m\rangle + i[(l+1)^2-m^2]^{1/2}a_{l+1}\,|\, n,l+1,m\rangle \;. \tag{35}$$

Now define the abstract operator

$$\mathbf{C} = \frac{i}{2}(\mathbf{A}+i\mathbf{B}) \;. \tag{36}$$

Then Eqs. (10), (11), (13), (34), and (35) yield

$$C_\pm \,|\, nlm\rangle = \mp\left[\frac{[n^2-(l+1)^2](l\pm m+1)(l\pm m+2)}{(2l+1)(2l+3)}\right]^{1/2}|\, n,l+1,m\pm 1\rangle \;, \tag{37}$$

$$C_\pm^\dagger \,|\, nlm\rangle = \mp\left[\frac{(n^2-l^2)(l\pm m-1)(l\pm m)}{(2l-1)(2l+1)}\right]^{1/2}|\, n,l-1,m\mp 1\rangle \;, \tag{38}$$

$$C_z \,|\, nlm\rangle = \left[\frac{[n^2-(l+1)^2](l+m+1)(l-m+1)}{(2l+1)(2l+3)}\right]^{1/2}|\, n,l+1,m\rangle \;, \tag{39}$$

$$C_z^\dagger \,|\, nlm\rangle = \left[\frac{(n^2-l^2)(l^2-m^2)}{(2l-1)(2l+1)}\right]^{1/2}|\, n,l-1,m\rangle \;. \tag{40}$$

Thus we have shown that the combination, Eq. (36), of the Pauli-Lenz operator and the operator defined by Eq. (24) yields ladder operators for l, and l and m, provided the operator $G(\mathbf{L}^2)$ in Eq. (24) has eigenvalues which satisfy Eq. (33). Now the solution to Eq. (33) is

$$G_l = 2\hbar^{-1}[2l+1+(-1)^l]^{-1} \;. \tag{41}$$

Therefore consider the Hermitian operator

$$S = (\hbar^{-2}\mathbf{L}^2+\tfrac{1}{4})^{1/2} \;, \tag{42}$$

which provides an explicit representation for the parity operator

$$P = e^{i\pi(S-1/2)} \tag{43}$$

and which also occurs in the scattering operator for the Coulomb problem.[19] From Eqs. (32), (41), (42), and (43) we find the nonsingular operator

$$G(\mathbf{L}^2) = [\hbar(S+\tfrac{1}{2}P)]^{-1} \;. \tag{44}$$

We note that the classical limit of Eq. (44) yields Eq. (26). In what follows Eq. (44) is assumed.

IV. ALGEBRA OF THE OPERATORS L and B

From Eqs. (34), (35), (13), and

$$L_\pm \mid nlm\rangle = \hbar[(l\mp m)(l\pm m+1)]^{1/2} \mid n,l,m\pm 1\rangle , \tag{45}$$

it follows that

$$[L_i,B_j] \mid nlm\rangle = i\hbar\epsilon_{ijk}B_k \mid nlm\rangle$$

and

$$[B_i,B_j] \mid nlm\rangle = i\hbar^{-1}\epsilon_{ijk}L_k \mid nlm\rangle .$$

The action of these commutators on a different basis can be determined by superposition: for example, for the kets $\mid npm\rangle$ of the operators H,A_z,L_z we use the expansion Eq. (15). Thus

$$[L_i,B_j] = i\hbar\epsilon_{ijk}B_k \tag{46}$$

and

$$[B_i,B_j] = i\hbar^{-1}\epsilon_{ijk}L_k , \tag{47}$$

where, as in the theory of the Pauli-Lenz vector, it is implicit that the equations act on a vector space of kets which is an energy eigenspace. [This restriction is required by the inclusion of the operator $(-H)^{-1/2}$ in the definitions Eq. (2) and Eq. (24). In our calculations bound states are assumed.] This method of determining commutation relations is familiar: it occurs, for example, in the theory of a Lie algebra associated with spherical harmonics[11] and in a study of the symmetry algebra associated with a charged particle in a magnetic field.[20] We use the same method in Sec. V.

Equation (46) establishes that **B** is a vector operator while Eqs. (3), (46), and (47) show that the Hermitian operators **L** and **B** are a basis for the Lie algebra O(4). This is an invariance algebra because $[H,\mathbf{L}]=[H,\mathbf{B}]=0$. The Casimir operators are $C_1=\hbar^{-2}\mathbf{L}^2+\mathbf{B}^2$ and $C_2=\mathbf{L}\cdot\mathbf{B}=\mathbf{B}\cdot\mathbf{L}$. From Eqs. (34), (35), (13), and (45) it can be shown that C_1 has eigenvalues n^2-1 while $C_2=0$. Clearly the algebra of **L** and **B** is the same as that of **L** and **A** (see Sec. II).

The Hermitian operators H,B_z,L_z are a commuting set with kets $\mid nqm\rangle$. If we define

$$\mathbf{Y}^\pm = \tfrac{1}{2}(\mathbf{B}\pm\hbar^{-1}\mathbf{L}) , \tag{48}$$

and $Y_\pm^+ = Y_x^+ \pm iY_y^+$, $Y_\pm^- = Y_x^- \pm iY_y^-$, then as in the calculations leading to Eqs. (19) and (20), we find the ladder operators for q and m:

$$Y_\pm^+ \mid nqm\rangle = \tfrac{1}{2}[n^2-(m+q\pm1)^2]^{1/2} \mid n,q\pm1,m\pm1\rangle , \tag{49}$$

$$Y_\pm^- \mid nqm\rangle = \tfrac{1}{2}[n^2-(m-q\pm1)^2]^{1/2} \mid n,q\mp1,m\pm1\rangle . \tag{50}$$

From the coefficients in Eqs. (49) and (50) we obtain the eigenvalues

$$q = n-1, n-2, \ldots, -(n-1)$$

and

$$m = n-\mid q\mid-1, n-\mid q\mid-3, \ldots, -n+\mid q\mid+1 ;$$

or, equivalently, the same formulas with m and q interchanged.

For the ket $\mid n,0,n-1\rangle$ Eqs. (49) and (50) yield

$$Y_+^+ \mid n,0,n-1\rangle = Y_+^- \mid n,0,n-1\rangle = 0 . \tag{51}$$

From Eqs. (34), (13), and (45) it is evident that a normalized solution to Eq. (51) is $\mid n,l=n-1,m=n-1\rangle$. Thus all kets $\mid nqm\rangle$ can be obtained from the single ket $\mid n,l=n-1,m=n-1\rangle$ by applying the ladder operators of Eqs. (49) and (50) and using Eqs. (34), (35), and (45). In the coordinate representation the wave functions calculated in this manner are the Coulomb wave functions in parabolic coordinates. [We note that Eq. (12) is implicit in these calculations.] As is well known, these wave functions span a representation space of the Lie group SO(4).

V. ALGEBRA OF THE OPERATORS L, A, B, AND S

It is of interest to inquire whether some larger set of operators which includes **L**, **A**, and **B** can be a basis for a Lie algebra. From Eqs. (37)–(40) and (45) one finds by using the same method as in Sec. IV that the set of nine operators $C_\pm$, C_z, $C_\pm^\dagger$, $C_z^\dagger$, $L_\pm$, and L_z does not close under commutation.

We recall that the definition of the Pauli-Lenz vector Eq. (2) includes the operator $(-H)^{-1/2}$ to ensure that **A** and **L** are a basis for the algebra O(4). With the same modification in the definition of **B** [see Eqs. (24) and (25)], **B** and **L** are also a basis for the algebra O(4). In the present case to obtain a set of operators which close under commutation we proceed as follows.

First we modify the definitions of **A** and **B**. Let

$$\mathbf{A}' = K\mathbf{A} \tag{52}$$

and

$$\mathbf{B}' = K\mathbf{B} , \tag{53}$$

where

$$K = \left[\frac{-(2Ma^2\hbar^{-2}H)S(S-1)}{(2Ma^2\hbar^{-2}H)(S-\frac{1}{2})^2+1}\right]^{1/2} \tag{54}$$

and **A** and **B** are given by Eqs. (2) and (24). Then for the operator

$$\mathbf{D} = i(\mathbf{A}'+i\mathbf{B}') \tag{55}$$

the results of Sec. III yield

$$D_\pm \mid nlm\rangle = \mp[(l\pm m+1)(l\pm m+2)]^{1/2} \times \mid n,l+1,m\pm1\rangle , \tag{56}$$

$$D_\pm^\dagger \mid nlm\rangle = \mp[(l\pm m-1)(l\pm m)]^{1/2} \times \mid n,l-1,m\mp1\rangle , \tag{57}$$

$$D_z \mid nlm\rangle = [(l+m+1)(l-m+1)]^{1/2} \mid n,l+1,m\rangle , \tag{58}$$

$$D_z^\dagger \mid nlm\rangle = [(l-m)(l+m)]^{1/2} \mid n,l-1,m\rangle \; . \tag{59}$$

Secondly we include in our set of operators the operator S [Eq. (42)]. Thus we consider the ten operators $D_\pm$, D_z, $D_\pm^\dagger$, $D_z^\dagger$, $L_\pm$, L_z, and S, and change to the Hermitian basis $\mathbf{U}=-\frac{1}{2}(\mathbf{D}+\mathbf{D}^\dagger)$, $\mathbf{V}=(i/2)(\mathbf{D}-\mathbf{D}^\dagger)$, $\mathbf{L}$, and S. The 45 commutators which can be formed from these operators can be evaluated using Eqs. (45) and (56)–(59). The results are

$$[L_i,L_j]=i\hbar\epsilon_{ijk}L_k \; , \tag{60}$$

$$[L_i,U_j]=i\hbar\epsilon_{ijk}U_k \; , \tag{61}$$

$$[L_i,V_j]=i\hbar\epsilon_{ijk}V_k \; , \tag{62}$$

$$[L_i,S]=0 \; , \tag{63}$$

$$[U_i,U_j]=-i\hbar^{-1}\epsilon_{ijk}L_k \; , \tag{64}$$

$$[U_i,V_j]=-i\delta_{ij}S \; , \tag{65}$$

$$[U_i,S]=-iV_i \; , \tag{66}$$

$$[V_i,V_j]=-i\hbar^{-1}\epsilon_{ijk}L_k \; , \tag{67}$$

$$[V_i,S]=iU_i \; . \tag{68}$$

These are the same as the commutators which define the Lie algebra O(3,2) (see, for example, Englefield[11]).

From Eqs. (52) and (54) for the modified Pauli-Lenz vector $\mathbf{A}'$ and Eq. (1) for the Laplace-Runge-Lenz vector $\mathbf{A}_c$, we note that the classical limit of $\hbar\mathbf{A}'$ is $L\,\hat{\mathbf{A}}_c$, a vector with magnitude L and pointing to the aphelion of the orbit. Similarly, the classical limit of $\hbar\mathbf{B}'$ is $L\hat{\mathbf{B}}_c$ [see Eqs. (53), (54), and (23)] and $\hbar\mathbf{A}'\times\hbar\mathbf{B}'\to -L\mathbf{L}$.

VI. DISCUSSION

For the bound states of the nonrelativistic Coulomb problem we have introduced a new abstract operator $\mathbf{B}$ which has the following properties:

(i) $\mathbf{B}$ is a conserved, Hermitian, vector operator;

(ii) $\mathbf{L}$ and $\mathbf{B}$ are a basis for an invariance algebra, the Lie algebra O(4):

(iii) H, B_z, L_z are a set of commuting operators: in Sec. IV the eigenvalues of B_z and L_z are determined using suitable ladder operators;

(iv) the combination $\mathbf{A}+i\mathbf{B}$ (where $\mathbf{A}$ is the Pauli-Lenz vector operator) provides ladder operators for the quantum numbers l, and l and m of the eigenkets $\mid nlm\rangle$;

(v) $\mathbf{B}$ is a (nonunique) operator corresponding to a conserved classical vector which is analogous to the Laplace-Runge-Lenz vector;

(vi) the ten operators $\mathbf{A}'$, $\mathbf{B}'$ (modified forms of $\mathbf{A}$ and $\mathbf{B}$), $\mathbf{L}$, and $(\hbar^{-2}\mathbf{L}^2+\frac{1}{4})^{1/2}$ can be linearly combined to yield a Hermitian basis for an invariance algebra, the de Sitter algebra O(3,2);

(vii) the classical limit of $\hbar\mathbf{A}'$ is a vector with magnitude L and directed to the aphelion of the elliptical orbit; the classical limit of $\hbar\mathbf{B}'$ is orthogonal to this and also has magnitude L(specifically, $\hbar\mathbf{A}'\times\hbar\mathbf{B}'\to -L\mathbf{L}$).

APPENDIX

From the definition Eq. (25) and the canonical commutation relations $[p_i,q_j]=-i\hbar\delta_{ij}$, $[p_i,p_j]=[q_i,q_j]=0$, one finds

$$[L_i,F_j]=i\hbar\epsilon_{ijk}F_k \; . \tag{A1}$$

Also $PF_jP^{-1}=-F_j$ where P is the parity operator. Thus $\mathbf{F}$ is a proper vector operator and the Wigner-Eckart theorem yields

$$F_\pm \mid nlm\rangle = \pm[(l\mp m)(l\mp m-1)]^{1/2}c_l \mid n,l-1,m\pm 1\rangle \pm [(l\pm m+1)(l\pm m+2)]^{1/2}d_l \mid n,l+1,m\pm 1\rangle \tag{A2}$$

and

$$F_z \mid nlm\rangle = (l^2-m^2)^{1/2}c_l \mid n,l-1,m\rangle - [(l+1)^2-m^2]^{1/2}d_l \mid n,l+1,m\rangle \; . \tag{A3}$$

We determine the coefficients

$$c_l=-[l(2l+1)]^{-1/2}\langle n,l-1||F||n,l\rangle$$

and

$$d_l=-[(2l+1)(l+1)]^{-1/2}\langle n,l+1||F||n,l\rangle$$

as follows.

Let g be some function of $\mathbf{L}^2$. Then

$$[\mathbf{L}^2,\mathbf{F}g]=-2i\hbar\mathbf{A}\mathbf{L}^2g \; , \tag{A4}$$

where $\mathbf{A}$ is the Pauli-Lenz vector Eq. (2). Also

$$[\mathbf{L}^2,\mathbf{A}]=2\hbar^2\mathbf{A}+2i\hbar\mathbf{F} \; . \tag{A5}$$

So

$$[\mathbf{L}^2,\mathbf{A}+i\mathbf{F}g]=\hbar^2(\mathbf{A}+i\mathbf{F}g)(2+2\hbar^{-1}\mathbf{L}^2g) + 2i\hbar\mathbf{F}(1-\hbar g-\mathbf{L}^2g^2) \; .$$

The second term on the right is zero if

$$g=g_\mu=2\hbar^{-1}[1+(-1)^\mu 2S]^{-1} \; , \tag{A6}$$

where $\mu=0$ or 1 and S is given by Eq. (42). Then

$$[\mathbf{L}^2,\mathbf{A}+i\mathbf{F}g_\mu]=\hbar^2(\mathbf{A}+i\mathbf{F}g_\mu)[1+(-1)^\mu 2S] \; . \tag{A7}$$

Also, from Eqs. (4) and (A1),

$$[L_z,A_j+iF_jg_\mu]=i\hbar\epsilon_{zjk}(A_k+iF_kg_\mu) \; . \tag{A8}$$

From Eqs. (A7) and (A8) it is clear that $A_{\pm}+iF_{\pm}g_{\mu}$ transforms $|\,nlm\,\rangle$ into $|\,n,l+(-1)^{\mu},m\pm 1\rangle$, while $A_z+iF_zg_{\mu}$ transforms $|\,nlm\,\rangle$ into $|\,n,l+(-1)^{\mu},m\,\rangle$.

Using these results, the eigenvalues in

$$g_{\mu}\,|\,nlm\,\rangle = 2\hbar^{-1}[1+(-1)^{\mu}(2l+1)]^{-1}\,|\,nlm\,\rangle\ ,$$

and Eqs. (10), (11), (A2), and (A3), we find

$$c_l = i\hbar(l+1)a_l$$

and

$$d_l = -i\hbar l a_{l+1}\ ,$$

where a_l is given by Eq. (13).

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