# Coulomb problem in an angular-momentum basis: An algebraic formulation

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We show that a representation-independent, spectrum-generating algebra for the Coulomb problem in an angular momentum basis can be obtained by quantizing two complex, time-dependent, classical vectors, $\mathbf{D}_c = \mathbf{F}_c + i\mathbf{G}_c$ and $\mathbf{D}_c^*$. The approach is based on an analogy with a treatment of the isotropic harmonic oscillator [A. J. Bracken and H. I. Leemon, J. Math. Phys. **21**, 2170 (1980)], and on work in which classical constants of the motion were quantized to yield shift operators for angular momentum in the Coulomb problem [O. L. de Lange and R. E. Raab, Phys. Rev. A **34**, 1650 (1986)]. By construction $\mathbf{F}_c$ and $\mathbf{G}_c$ are orthogonal to the orbital angular momentum $\mathbf{L}$, their moduli have equal, constant magnitude, and they rotate about $\mathbf{L}$. In this construction we use $\mathbf{A}_c$ (the Laplace-Runge-Lenz vector) and $\mathbf{A}_c \times \hat{\mathbf{L}}$ as basis vectors. $\mathbf{F}_c$ and $\mathbf{G}_c$ contain an undetermined phase factor $\exp(i\delta)$. $\mathbf{D}_c$ and $\mathbf{D}_c^*$ are quantized by requiring that the resulting operators should be shift operators for energy and angular momentum in the bound-state kets $|nlm\rangle$. This determines the operators $\Delta^{\pm}$ corresponding to the classical phase factors $\exp(\pm i\delta)$. In the coordinate and momentum representations of wave mechanics respectively, $\Delta^{\pm}$ are the dilatation operators for coordinate-space and momentum-space wave functions. The shift operators can be factorized to yield 20 abstract operators. Apart from their dependence on $\Delta^{\pm}$ and constants of the motion, ten of these are linear in $\mathbf{p}$, eight are linear in $\mathbf{r}$, and two are quadratic in $\mathbf{r}$. Apart from $\Delta^{\pm}$, these operators can be linearized by replacing constants of the motion with their eigenvalues: In the coordinate and momentum representations of wave mechanics they are first-order differential operators. The shift operators are part of a Hermitian basis for a spectrum-generating algebra which is shown to be $SO(2,1) \oplus SO(3,2)$.

## I. INTRODUCTION

Recently we presented an algebraic treatment of shift operators for angular momentum in the Coulomb problem.[1,2] These operators were derived as quantum-mechanical analogs of certain classical constants of the motion. The purpose of this paper is twofold. Firstly, we extend our previous work to obtain a representation-independent, spectrum-generating algebra for the Coulomb problem in an angular momentum basis. Secondly, the formulation is devised to bring out the analogy with a related problem, namely, an algebraic treatment of the three-dimensional, isotropic harmonic oscillator (hereafter referred to as the oscillator) in an angular momentum basis.

Lie algebras for the Coulomb and the oscillator problems, and the relationship between these systems, have been the subject of numerous studies (see, for example, Kramer and Moshinsky,[3] McIntosh,[4] Englefield,[5] Wybourne,[6] and the references therein). Recently, Bracken and Leemon[7] have presented an algebraic formulation for the harmonic oscillator in an angular momentum basis. This formulation enabled them to identify a previously unrecognized spectrum-generating algebra for the oscillator, namely, $SO(2,1) \oplus SO(3,2)$ [$\simeq Sp(2,R) \oplus Sp(4,R)$]. Their results complement earlier work, for example, the identification of the Lie algebra $Sp(6,R)$ as a spectrum-generating algebra for the oscillator in the basis $H_1, H_2, H_3$ ($H_i = a_i^\dagger a_i$, where $a_i$ are the boson annihilation operators).[8] In Ref. 7, basis operators for a spectrum-generating algebra are derived using the boson operators and the dimension operator. In Appendix A we show that these basis operators can also be constructed by quantizing certain classical vectors for the oscillator. These vectors are orthogonal to the orbital angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, their moduli have equal, constant magnitude and they rotate about $\mathbf{L}$ with $\pm$ times the angular frequency of the oscillator. The basis operators derived in this way contain, as factors, several operators which are related to differential operators obtained by the so-called factorization method for solving the Sturm-Liouville equation.[9]

In this paper we show that a similar analysis can be carried out for the Coulomb problem. In Sec. II we summarize and discuss some previous results. In Sec. III we derive two complex, time-dependent classical vectors for the Coulomb potential [$\mathbf{F}_c$ and $\mathbf{G}_c$, Eqs. (33) and (34)]. By construction, $\mathbf{F}_c$ and $\mathbf{G}_c$ are orthogonal to $\mathbf{L}$ [Eqs. (25) and (26)], their moduli have equal, constant magnitude [Eq. (32)], and they rotate about $\mathbf{L}$ [Eq. (35)]. $\mathbf{F}_c$ and $\mathbf{G}_c$ contain an undetermined phase factor $\exp(i\delta)$. This method of construction is essentially the same as that for the oscillator (Appendix A). However, the resulting vectors $\mathbf{F}_c$ and $\mathbf{G}_c$ are more complicated than those for the oscillator. In Sec. IV we consider the quantization of the vectors $\mathbf{D}_c = \mathbf{F}_c + i\mathbf{G}_c$ and $\mathbf{D}_c^*$. By requiring that the resulting vector operators should be shift operators for energy and angular momentum in the bound-state kets $|nlm\rangle$, we are able to determine quantum-mechanical analogs $\mathbf{D}^{\pm}$ of $\mathbf{D}_c$ and $\mathbf{D}_c^*$. $\mathbf{D}^{\pm}$

 

contain operators $\Delta^{\pm}$ [Eq. (77)] which correspond to the classical phase factors $\exp(\pm i\delta)$. In the coordinate representation of wave mechanics, $\Delta^{\pm}$ are the well-known "scaling" or "dilatation" operators for coordinate-space wave functions. In the corresponding analysis for the oscillator, $\Delta^{\pm}$ can be set equal to 1 [Eq. (A15)]. $\mathbf{D}^{\pm}$ can be expressed as products of operators which, apart from their dependence on $\Delta^{\pm}$ and constants of the motion ($H$ and $\mathbf{L}^2$), are linear in $\mathbf{p}$ [Eqs. (107) and (108)]. We also derive, by a similar procedure, operators $\tilde{\mathbf{D}}^{\pm}$ [Eqs. (81) and (82)] which consist of factors that are either linear in $\mathbf{r}$ [Eq. (17)] or quadratic in $\mathbf{r}$ [Eqs. (99) and (100)], apart from their dependence on $\Delta^{\pm}$ and constants of the motion. Thus we obtain the 20 abstract operators $\mathbf{U}^{\pm}$, $\mathbf{V}^{\pm}$, $R^{\pm}$, $P^{\pm}$, $Q^{\pm}$, and $\tilde{Q}^{\pm}$ (Sec. IV). If in these operators we replace constants of the motion with their eigenvalues, we obtain 20 operators which are linear in either $\mathbf{p}$ or $\mathbf{r}$ [Eqs. (109)–(112)]. The operators derived in Sec. IV are used in Sec. V to construct a Hermitian basis for a spectrum-generating algebra for the Coulomb problem. This algebra, SO(2,1)⊕SO(3,2), fulfills a similar role to that for the oscillator in Ref. 7.

## II. SHIFT OPERATORS FOR ANGULAR MOMENTUM IN THE COULOMB PROBLEM

We summarize and discuss some previous results, together with modifications which are used in this paper.

In the angular momentum basis the set of commuting observables is the Hamiltonian

$$H=(2M)^{-1}\mathbf{p}^2-kr^{-1}\ , \tag{1}$$

$\mathbf{L}^2$ and $L_z$, and the normalized common eigenvectors are denoted by $|\,nlm\,\rangle$. In the following we assume bound states with energy

$$E=-\hbar^2(2Ma^2n^2)^{-1}\ , \tag{2}$$

where $a=\hbar^2(Mk)^{-1}$ is the Bohr radius if $k=e^2(4\pi\varepsilon_0)^{-1}$.

For the classical motion of a particle in the Coulomb potential, the Laplace-Runge-Lenz vector

$$\mathbf{A}_c=(Mk)^{-1}\mathbf{L}\times\mathbf{p}+r^{-1}\mathbf{r} \tag{3}$$

is a constant of the motion.[10] $\mathbf{A}_c$ is orthogonal to $\mathbf{L}$ and

$$A_c=\left[1+\frac{2HL^2}{Mk^2}\right]^{1/2} \tag{4}$$

is equal to the eccentricity $e$ of the orbit. From the conserved classical vectors

$$\mathbf{C}_c^{\pm}=(1\mp i\hat{\mathbf{L}}\times)\,\mathbf{A}_c\ , \tag{5}$$

we construct the vector operators[1,2]

$$\mathbf{C}^{\pm}=(\,\mathbf{A}\pm i\mathbf{B}^{\pm})(S\pm\tfrac{1}{2})\ , \tag{6}$$

where

$$\mathbf{A}=\tfrac{1}{2}\hbar^{-2}a(\mathbf{L}\times\mathbf{p}-\mathbf{p}\times\mathbf{L})+r^{-1}\mathbf{r}\ , \tag{7}$$

$$\begin{aligned}\mathbf{B}^{\pm}&=\mathbf{A}\times\mathbf{L}[\hbar(S\pm\tfrac{1}{2})]^{-1}\\&=[r^{-1}\mathbf{r}\times\mathbf{L}+\hbar^{-2}a\mathbf{p}L^2][\hbar(S\pm\tfrac{1}{2})]^{-1}\ ,\end{aligned} \tag{8}$$

$$S=(\hbar^{-2}\mathbf{L}^2+\tfrac{1}{4})^{1/2}\ . \tag{9}$$

$\mathbf{A}$ is the Pauli-Lenz operator.[11] $S$ is equal to one half the dimension operator;[12] it is a Hermitian integral operator which satisfies the eigenvalue equation

$$S\,|\,nlm\,\rangle=(l+\tfrac{1}{2})\,|\,nlm\,\rangle\ . \tag{10}$$

In Refs. 1 and 2, $\mathbf{A}\pm i\mathbf{B}^{\pm}$ are derived as quantum-mechanical analogs of $\mathbf{C}_c^{\pm}$ by requiring that the resulting operators be shift operators for angular momentum. The factor $S\pm\frac{1}{2}$ in Eq. (6) has been included to ensure that the coefficients in Eq. (11) below do not involve indeterminate forms. We note that $\mathbf{B}^{\pm}$, unlike $\mathbf{A}$, are not Hermitian. Although Hermitian forms for $\mathbf{B}^{\pm}$ can be derived,[1] Eq. (8) is adequate for our purposes.

The two vector operators $\mathbf{C}^{\pm}$ yield the six shift operations

$$C_k^{\pm}\,|\,nlm\,\rangle=\alpha_k^{\pm}(l,m)\beta^{\pm}(n,l)\,|\,n,l\pm1,m+k\,\rangle\ , \tag{11}$$

where $k=\pm1$ or 0, $C_{\pm1}=C_x\pm iC_y$, $C_0=C_z$, and

$$\alpha_0^{\pm}(l,m)=[(l-m+\tfrac{1}{2}\pm\tfrac{1}{2})(l+m+\tfrac{1}{2}\pm\tfrac{1}{2})]^{1/2}\ , \tag{12}$$

$$\alpha_{+1}^{\pm}(l,m)=\mp[(l\pm m+\tfrac{1}{2}\pm\tfrac{1}{2})(l\pm m+\tfrac{1}{2}\pm\tfrac{3}{2})]^{1/2}\ , \tag{13}$$

$$\alpha_{-1}^{\pm}(l,m)=\pm[(l\mp m+\tfrac{1}{2}\pm\tfrac{1}{2})(l\mp m+\tfrac{1}{2}\pm\tfrac{3}{2})]^{1/2}\ , \tag{14}$$

$$\beta^{\pm}(n,l)=\left[\frac{l+\frac{1}{2}}{l+\frac{1}{2}\pm1}[1-n^{-2}(l+\tfrac{1}{2}\pm\tfrac{1}{2})^2]\right]^{1/2}\ . \tag{15}$$

Equations (11)–(15) can be obtained from Eqs. (10), (11), (28), and (29), of Ref. 1, after noting the different choice of basis kets used here (see Appendix B).

The operators $\mathbf{C}^{\pm}$ defined by Eqs. (6)–(9) are complicated: Apart from their dependence on $\mathbf{L}^2$, they are quadratic functions of the momentum operator $\mathbf{p}$ and they are also nonlinear functions of the position operator $\mathbf{r}$. Simpler structures for $\mathbf{C}^{\pm}$ can be obtained by suitable factorizations. These are[13]

$$\mathbf{C}^{\pm}=\hbar^{-2}a\mathbf{U}^{\pm}R^{\pm} \tag{16}$$

and

$$\mathbf{C}^{\pm}=\pm i\tfrac{1}{2}\hbar^{-2}a\mathbf{V}^{\pm}P^{\pm}\ , \tag{17}$$

where

$$\mathbf{U}^{\pm}=\pm ir^{-1}\mathbf{r}\times\mathbf{L}+\hbar r^{-1}\mathbf{r}(S\pm\tfrac{1}{2})\ , \tag{18}$$

$$R^{\pm}=\pm ir^{-1}\mathbf{r}\cdot\mathbf{p}(S\pm\tfrac{1}{2})-\hbar^{-1}\mathbf{L}^2r^{-1}+\hbar a^{-1}\ , \tag{19}$$

$$\mathbf{V}^{\pm}=\pm i\mathbf{p}^{-1}\mathbf{p}\times\mathbf{L}+\hbar p^{-1}\mathbf{p}(S\pm\tfrac{1}{2})\ , \tag{20}$$

$$\begin{aligned}P^{\pm}=&\mp i\hbar^{-1}p^{-1}\mathbf{r}\cdot\mathbf{p}(\mathbf{p}^2-2MH)+p^{-1}(\mathbf{p}^2+2MH)(S\pm\tfrac{1}{2})\\&\mp2p^{-1}(p^2-2MH)\ .\end{aligned} \tag{21}$$

Apart from their dependence on constants of the motion, $\mathbf{U}^{\pm}$ and $R^{\pm}$ are linear in $\mathbf{p}$, while $\mathbf{V}^{\pm}$ and $P^{\pm}$ are linear in $\mathbf{r}$. For the purpose of operating on eigenkets, the factors in $\mathbf{C}^{\pm}$ can be linearized by replacing $H$ and $\mathbf{L}^2$ with their eigenvalues. Thus

$$\mathbf{C}^{\pm}\,|\,nlm\,\rangle=\hbar^{-2}a\mathbf{U}_l^{\pm}R_l^{\pm}\,|\,nlm\,\rangle \tag{22}$$

and

$$\mathbf{C}^{\pm} \mid nlm \rangle = \pm i\tfrac{1}{2}\hbar^{-2} a \mathbf{V}_l^{\mp} P_{nl}^{\pm} \mid nlm \rangle , \tag{23}$$

where $\mathbf{U}_l^{\mp}$, $R_l^{\pm}$, $\mathbf{V}_l^{\mp}$, and $P_{nl}^{\pm}$ are given by Eqs. (18)–(21) with $\mathbf{L}^2$, $S$, and $H$ replaced by $\hbar^2 l(l+1)$, $l+\frac{1}{2}$, and $E$, respectively. In the coordinate representation of wave mechanics, $\mathbf{U}_l^{\mp}$ and $R_l^{\pm}$ are first-order differential operators which act on the angular and radial parts, respectively, of the coordinate-space wave function. In the momentum representation of wave mechanics $\mathbf{V}_l^{\mp}$ and $P_{nl}^{\pm}$ are the corresponding first-order differential operators for the momentum-space wave function. For additional discussion of these operators see Ref. 13.

In Ref. 1 we attempted to obtain an invariance algebra by modifying the operators $\mathbf{C}^{\pm}$ so that the factors $\beta^{\pm}$ are removed from Eq. (11). While this procedure is satisfactory for kets with $l < n-1$ in Eq. (11), some of the commutation relations of the Lie algebra SO(3,2) discussed in Ref. 1 are not satisfied when $\mathbf{C}^{\pm}$ act on kets with $l = n-1$. We show below that this difficulty can be avoided by including shift operators for energy in the basis operators: SO(3,2) is then obtained as a subalgebra of a spectrum-generating algebra (Sec. V).

## III. CLASSICAL VECTORS

In this section we derive complex, time-dependent, classical vectors for the Coulomb potential which are suitable for constructing quantum-mechanical basis operators of a spectrum-generating algebra. By analogy with the oscillator (Appendix A), we require that the moduli of these vectors should (i) be orthogonal to $\mathbf{L}$, (ii) rotate about $\mathbf{L}$, and (iii) have constant, equal magnitude. For the oscillator the construction of the appropriate vectors is straightforward (Appendix A); for the Coulomb potential the procedure is less obvious.

From the discussion in Sec. II it is clearly desirable to have the Laplace-Runge-Lenz vector $\mathbf{A}_c$ and an orthogonal vector,

$$\mathbf{B}_c = \mathbf{A}_c \times \hat{\mathbf{L}} , \tag{24}$$

appear as variables in the time-dependent vectors. Thus we choose the constants of the motion $\mathbf{A}_c$ and $\mathbf{B}_c$ as "basis vectors," and define

$$\mathbf{F}_c = (f\,\mathbf{A}_c + g\mathbf{B}_c)e^{i\delta} \tag{25}$$

and

$$\mathbf{G}_c = \mathbf{F}_c \times \hat{\mathbf{L}} = (-g\,\mathbf{A}_c + f\mathbf{B}_c)e^{i\delta} , \tag{26}$$

where $\delta$, $f$, and $g$ are real functions of $\mathbf{r}$ and $\mathbf{p}$. Let $\mathbf{X}$ denote the modulus

$$\mathbf{X} = e^{-i\delta}\mathbf{F}_c \quad \text{or} \quad e^{-i\delta}\mathbf{G}_c . \tag{27}$$

Then

$$\mathbf{X}^2 = (f^2+g^2)\,\mathbf{A}_c^2 \tag{28}$$

will be constant if $f^2+g^2$ is constant. From Eq. (1) and the relation $\mathbf{p}^2 = r^{-2}[\mathbf{L}^2 + (\mathbf{r}\cdot\mathbf{p})^2]$, we have the identity

$$-2MH(r+\tfrac{1}{2}kH^{-1})^2 + (\mathbf{r}\cdot\mathbf{p})^2 = -\tfrac{1}{2}Mk^2H^{-1} - L^2 . \tag{29}$$

This suggests the ansatz

$$f = (-2MH)^{1/2}(r+\tfrac{1}{2}kH^{-1}) , \tag{30}$$

$$g = \mathbf{r}\cdot\mathbf{p} . \tag{31}$$

[The alternative choice for the relative sign of $f$ and $g$ leads to $\dot{\mathbf{X}} = -\boldsymbol{\omega}\times\mathbf{X}$ instead of Eq. (35) below.] From Eqs. (28)–(31) and (4),

$$\mathbf{X}^2 = -\frac{Mk^2}{2H}\left[1+\frac{2HL^2}{Mk^2}\right]^2 = L^2e^4(1-e^2)^{-1} , \tag{32}$$

where $e$ is the eccentricity of the orbit. From Eqs. (25), (26), (30), and (31),

$$\mathbf{F}_c = [(-2MH)^{1/2}(r+\tfrac{1}{2}kH^{-1})\,\mathbf{A}_c + (\mathbf{r}\cdot\mathbf{p})\mathbf{B}_c]e^{i\delta} \tag{33}$$

and

$$\mathbf{G}_c = [-(\mathbf{r}\cdot\mathbf{p})\,\mathbf{A}_c + (-2MH)^{1/2}(r+\tfrac{1}{2}kH^{-1})\mathbf{B}_c]e^{i\delta} . \tag{34}$$

From the time derivative of Eqs. (27), (33), (34), and with $dr/dt = (Mr)^{-1}\mathbf{r}\cdot\mathbf{p}$ and $d(\mathbf{r}\cdot\mathbf{p})/dt = 2H + kr^{-1}$, it follows that

$$\dot{\mathbf{X}} = \boldsymbol{\omega}\times\mathbf{X} , \tag{35}$$

where

$$\boldsymbol{\omega} = (-2MH)^{1/2}(Mr)^{-1}\hat{\mathbf{L}} . \tag{36}$$

Thus the moduli of the complex vectors $\mathbf{F}_c$ and $\mathbf{G}_c$ have constant, equal magnitude and rotate with angular velocity $\boldsymbol{\omega}$.

The corresponding analysis of the oscillator is similar though less involved [Appendix A, Eqs. (A1)–(A5)]. For the oscillator, it turns out that a phase factor in $\mathbf{F}_c$ and $\mathbf{G}_c$ is unnecessary (Appendix A); for the Coulomb potential this phase factor is essential (Sec. IV). Whereas the vectors $\mathbf{F}_c$ and $\mathbf{G}_c$ for the oscillator rotate with the angular velocity of the particle, the corresponding angular velocity for the Coulomb problem differs from that of the particle and is not constant [Eq. (36)]. Its average value can be calculated with the aid of the virial theorem:

$$\langle \omega \rangle = (-2MH)^{3/2}(M^2k)^{-1} \tag{37}$$

$$= 2\pi T^{-1} , \tag{38}$$

where $T$ is the period of the motion. For the oscillator, the difference between adjacent energy levels is $\hbar^{-1}$ times the constant angular frequency of the oscillator. For the Coulomb potential, the difference between adjacent levels is

$$E_{n+1} - E_n \approx \hbar(M^2k)^{-1}(-2ME_n)^{3/2} \tag{39}$$

if $n \gg 1$. If $\langle \omega_n \rangle$ denotes the value of $\langle \omega \rangle$ when $H = E_n$ in Eq. (37), it is evident that

$$\hbar\langle \omega_n \rangle \approx E_{n+1} - E_n \tag{40}$$

when $n \gg 1$.

Define

$$\mathbf{D}_c = \mathbf{F}_c + i\mathbf{G}_c \ . \tag{41}$$

Then Eqs. (33) and (34) yield

$$\mathbf{D}_c = Q_c^+ \mathbf{C}_c^+ \tag{42}$$

and

$$\mathbf{D}_c^* = Q_c^- \mathbf{C}_c^- \ , \tag{43}$$

where

$$Q_c^\pm = [\mp i\mathbf{r}\cdot\mathbf{p} + (-2MH)^{1/2}(r + \tfrac{1}{2}kH^{-1})]e^{\pm i\delta} \tag{44}$$

and $\mathbf{C}_c^\pm$ are given in Eq. (5). The factors in square brackets in Eq. (44) are linear in $\mathbf{p}$ and nonlinear in $\mathbf{r}$, apart from their dependence on $H$. In view of the comments in Sec. II, it is also desirable to obtain alternatives to Eqs. (42)–(44) in which these factors are linear in $\mathbf{r}$ and nonlinear in $\mathbf{p}$. This can be achieved by using Eq. (1) to eliminate $r$ in favor of $\mathbf{p}^2$ in Eq. (30), and proceeding as before. This yields the desired vectors

$$\tilde{\mathbf{D}}_c = \tilde{Q}_c^+ \mathbf{C}_c^+ \tag{45}$$

and

$$\tilde{\mathbf{D}}_c^* = \tilde{Q}_c^- \mathbf{C}_c^- \ , \tag{46}$$

where

$$\tilde{Q}_c^\pm = [\mp i\mathbf{r}\cdot\mathbf{p} + 2Mk(-2MH)^{1/2}(\mathbf{p}^2 - 2MH)^{-1} - Mk(-2MH)^{-1/2}]e^{\pm i\delta} \tag{47}$$

and $\mathbf{C}_c^\pm$ are given in Eq. (5).

Equations (44) and (47) contain unknown phase factors, for example, those of $\mathbf{F}_c$ and $\mathbf{G}_c$ [Eqs. (25) and (26)]. Also, it is clear that in the above $\mathbf{D}_c$ and $\tilde{\mathbf{D}}_c$ are determined only to within a factor which is a constant of the motion. These undetermined quantities could be specified by consideration of a noninvariance algebra for the classical motion.[14] However, Eqs. (42)–(47) are sufficient for our purposes: The operators corresponding to the phase factors in Eqs. (44) and (47) can be determined by requiring that quantization of $\mathbf{D}_c$ and $\tilde{\mathbf{D}}_c$ should yield shift operators for energy [see Sec. IV]; similarly, the role of any constant factor in $\mathbf{D}_c$ and $\tilde{\mathbf{D}}_c$ is best seen in the algebra of quantum-mechanical analogs of these vectors [see Sec. V].

## IV. OPERATORS

We wish to convert the classical vectors $\mathbf{D}_c$, $\mathbf{D}_c^*$, $\tilde{\mathbf{D}}_c$, and $\tilde{\mathbf{D}}_c^*$, obtained in Sec. III, into quantum-mechanical shift operators for energy and angular momentum. Although the classical vectors involve undetermined phase factors, we shall see that Eqs. (42)–(47) contain sufficient information to make possible the desired quantizations.

Consider first $\mathbf{D}_c$ and $\mathbf{D}_c^*$. From Eqs. (42)–(44) we construct the operators

$$\mathbf{D}^+ = \mathbf{C}^+ Q^+ \ , \tag{48}$$

$$\mathbf{D}^- = Q^- \mathbf{C}^- \ , \tag{49}$$

where $\mathbf{C}^\pm$ are given by Eqs. (6)–(9), and

$$Q^\pm = \mp i\mathbf{r}\cdot\mathbf{p}\Delta^\pm + \hbar a^{-1} r\Delta^\pm Y^\pm - \hbar\Delta^\pm Z^\pm \ . \tag{50}$$

Here $Y^\pm$ and $Z^\pm$ are constants of the motion: They are functions only of

$$N = \hbar a^{-1}(-2MH)^{-1/2} \ , \tag{51}$$

such that as $\hbar \to 0$,

$$Y^\pm \to N^{-1} \ , \tag{52}$$

$$Z^\pm \to N \ . \tag{53}$$

The operators $\Delta^\pm$ correspond to the phase factors in Eq. (44); $\Delta^\pm$ and their classical limits are calculated below [Eqs. (77) and (78)]. In writing down Eq. (50) we have adopted a specific ordering of operators: Functions of the Hamiltonian are placed to the right, followed by $\Delta^\pm$. This ordering simplifies the subsequent calculations.

From Eqs. (48), (49), and (11), $\mathbf{D}^\pm$ will be shift operators for angular momentum provided

$$[L_i, Q^\pm] = 0 \ , \tag{54}$$

and hence

$$[L_i, \Delta^\pm] = 0 \ . \tag{55}$$

Apart from their dependence on $\mathbf{r}$ and $\mathbf{p}$, $\Delta^\pm$ may also depend explicitly on $H$, $\mathbf{L}^2$, and $L_z$. Because the latter do not commute with $\mathbf{r}$ and $\mathbf{p}$, it is advantageous to define operators $\Delta_{nlm}^\pm$ which are independent of $H$, $\mathbf{L}^2$, and $L_z$, and which satisfy

$$\Delta_{nlm}^\pm \,|\, nlm\rangle = \Delta^\pm \,|\, nlm\rangle \ . \tag{56}$$

For convenience of notation we denote $\Delta_{nlm}^\pm$ by $\Delta_n^\pm$. The effect of $Q^\pm$ on $|\, nlm\rangle$ is the same as that of the operator

$$Q_n^\pm = \mp i\mathbf{r}\cdot\mathbf{p}\Delta_n^\pm + \hbar a^{-1} r\Delta_n^\pm Y_n^\pm - \hbar\Delta_n^\pm Z_n^\pm \ . \tag{57}$$

The operators $\Delta_n^\pm$, $Y_n^\pm$, $Z_n^\pm$, and $\Delta^\pm$ are determined below by requiring that $\mathbf{D}^\pm$, and hence $Q^\pm$, be shift operators for energy.

A clue on how to proceed is provided by considering an obvious operator analog of the factor in square brackets in Eq. (44), namely, $\mp i\mathbf{r}\cdot\mathbf{p} + \hbar a^{-1} rN^{-1} - \hbar N$. It is straightforward to show that

$$[H, \mp i\mathbf{r}\cdot\mathbf{p} + \hbar a^{-1} rN^{-1} - \hbar N] = \pm\hbar^2(Ma)^{-1} r^{-1}[\mp i\mathbf{r}\cdot\mathbf{p} + \hbar a^{-1} rN^{-1} - \hbar(N \pm 1)]N^{-1} \ . \tag{58}$$

Thus for

$$T_n^\pm = \mp i\mathbf{r}\cdot\mathbf{p} + \hbar a^{-1} rn^{-1} - \hbar(n \pm 1) \ , \tag{59}$$

it follows from Eq. (58) that

$$[H,T_n^{\pm}]\,|\,nlm\,\rangle=\pm\hbar^2(Man)^{-1}r^{-1}T_n^{\pm}\,|\,nlm\,\rangle\ . \quad (60)$$

$Q_n^{\pm}$ can be expressed in terms of $T_n^{\pm}$,

$$Q_n^{\pm}=\Delta_n^{\pm}T_n^{\pm}\pm i[\Delta_n^{\pm},\mathbf{r}\cdot\mathbf{p}]-\hbar a^{-1}\Delta_n^{\pm}rn^{-1}+\hbar a^{-1}r\Delta_n^{\pm}Y_n^{\pm}-\hbar\Delta_n^{\pm}[Z_n^{\pm}-(n\pm1)]\ . \quad (61)$$

From Eqs. (60), (61), and the commutator

$$[H,\Delta_n^{\pm}T_n^{\pm}]=[H,\Delta_n^{\pm}]T_n^{\pm}+\Delta_n^{\pm}[H,T_n^{\pm}]\ , \quad (62)$$

we find

$$HQ_n^{\pm}\,|\,nlm\,\rangle=(E_{n\pm1}Q_n^{\pm}+\Omega^{\pm})\,|\,nlm\,\rangle\ , \quad (63)$$

where $E_n$ is given by Eq. (2), and

$$\Omega^{\pm}=(H-E_{n\pm1})\left\{\pm i[\Delta_n^{\pm},\mathbf{r}\cdot\mathbf{p}]-\hbar a^{-1}\left[\Delta_n^{\pm}\frac{r}{n}-\frac{r}{n\pm1}\Delta_n^{\pm}\right]+\hbar a^{-1}r\Delta_n^{\pm}[Y_n^{\pm}-(n\pm1)^{-1}]-\hbar\Delta_n^{\pm}[Z_n^{\pm}-(n\pm1)]\right\}$$
$$+\left\{\hbar^2(Ma)^{-1}(n\pm1)^{-1}\left[\Delta_n^{\pm}\frac{n}{r}-\frac{n\pm1}{r}\Delta_n^{\pm}\right]+(2M)^{-1}\left[\mathbf{p}^2\Delta_n^{\pm}-\left[\frac{n}{n\pm1}\right]^2\Delta_n^{\pm}\mathbf{p}^2\right]\right\}T_n^{\pm}\ . \quad (64)$$

In Eq. (64) we have added and subtracted $\hbar a^{-1}r\Delta_n^{\pm}(n\pm1)^{-1}$. In Eqs. (61), (63), and (64), $n>1$ in $Q_n^-$ and $\Omega^-$; $Q_1^-$ is considered separately below. From Eq. (63), $Q_n^{\pm}$ will be shift operators for energy if $\Omega^{\pm}=0$. By inspection, each of the quantities in square brackets in Eq. (64) will be zero if

$$\Delta_n^{\pm}F(\mathbf{r},\mathbf{p})=F\left[\frac{n}{n\pm1}\mathbf{r},\frac{n\pm1}{n}\mathbf{p}\right]\Delta_n^{\pm}\ , \quad (65)$$

$$Y_n^{\pm}=(n\pm1)^{-1}\ , \quad (66)$$

$$Z_n^{\pm}=n\pm1\ . \quad (67)$$

Thus from Eqs. (61) and (57)

$$Q_n^{\pm}=\Delta_n^{\pm}T_n^{\pm} \quad (68)$$

$$=\mp i\mathbf{r}\cdot\mathbf{p}\Delta_n^{\pm}+\hbar a^{-1}r\Delta_n^{\pm}(n\pm1)^{-1}-\hbar\Delta_n^{\pm}(n\pm1) \quad (69)$$

are shift operators for energy provided $\Delta_n^{\pm}$ satisfies Eq. (65). For the special case of $Q_1^-$,

$$Q_1^-=T_1^-=i\mathbf{r}\cdot\mathbf{p}+\hbar a^{-1}r \quad (70)$$

has the desired effect,

$$Q_1^-\,|\,100\rangle=0\ . \quad (71)$$

[Equation (71) follows from[13] $R^+\,|\,100\rangle=0$ and Eq. (19).] From Eqs. (50) and (69),

$$Q^{\pm}=\mp i\mathbf{r}\cdot\mathbf{p}\Delta^{\pm}+\hbar a^{-1}r\Delta^{\pm}(N\pm1)^{-1}-\hbar\Delta^{\pm}(N\pm1)\ , \quad (72)$$

provided $Q^-$ does not act on $|\,100\rangle$, in which case

$$Q^-=i\mathbf{r}\cdot\mathbf{p}+\hbar a^{-1}r\ . \quad (73)$$

From Eqs. (54) and (63) the shift operations are

$$Q^{\pm}\,|\,nlm\,\rangle=\gamma^{\pm}(n,l)\,|\,n\pm1,l,m\,\rangle\ . \quad (74)$$

If $\Delta_n^{\pm}$ are unitary, it is shown in Appendix C that

$$\gamma^{\pm}(n,l)=\hbar\left[\frac{n\pm1}{n}[n(n\pm1)-l(l+1)]\right]^{1/2}\ . \quad (75)$$

Unitary operators which satisfy Eq. (65) are

$$\Delta_n^{\pm}=\left[\frac{n}{n\pm1}\right]^{i\hbar^{-1}\mathbf{r}\cdot\mathbf{p}+3/2}\ . \quad (76)$$

Thus[15,16]

$$\Delta^{\pm}=\sum_{k=0}^{\infty}\frac{1}{k!}\left[-\frac{i}{\hbar}\right]^k(\mathbf{r}\cdot\mathbf{p}-\tfrac{3}{2}i\hbar)^k[\ln(1\pm N^{-1})]^k\ . \quad (77)$$

We note that, as assumed, $\Delta^{\pm}$ satisfy Eq. (55), and in the classical limit $\Delta^{\pm}$ reduce to the phase factors

$$\Delta_c^{\pm}=\exp[\mp i(-2MH)^{1/2}(Mk)^{-1}\mathbf{r}\cdot\mathbf{p}]\ . \quad (78)$$

The operators $Q_n^{\pm}$ and $Q^{\pm}$ have been derived before. Schrödinger[17] obtained recurrence relations for the radial part of the coordinate-space wave functions in spherical coordinates. By including the "scaling operators" $\Delta_n^{\pm}$ and generalizing Schrödinger's differential forms, Musto[15] obtained the abstract operators Eqs. (68) and (72). A similar treatment, based on recurrence relations for coordinate-space wave functions in parabolic coordinates, has been given by Pratt and Jordan.[16]

For the vector operators $\mathbf{D}^{\pm}$, Eqs. (48), (49), (11), and (74) yield

$$D_k^+\,|\,nlm\,\rangle=\alpha_k^+(l,m)\beta^+(n+1,l)\gamma^+(n,l)\,|\,n+1,l+1,m+k\,\rangle \quad (79)$$

and

$$D_k^-\,|\,nlm\,\rangle=\alpha_k^-(l,m)\beta^-(n,l)\gamma^-(n,l-1)\,|\,n-1,l-1,m+k\,\rangle\ , \quad (80)$$

where the coefficients are given by Eqs. (12)–(15) and (75).

Next, we quantize the vectors $\tilde{\mathbf{D}}_c$ and $\tilde{\mathbf{D}}_c^*$ [Eqs. (45)–(47)]. We write

$$\tilde{\mathbf{D}}^{+}=\mathbf{C}^{+}\tilde{Q}^{+} \tag{81}$$

and

$$\tilde{\mathbf{D}}^{-}=\tilde{Q}^{-}\mathbf{C}^{-} , \tag{82}$$

where $\mathbf{C}^{\pm}$ are given by Eqs. (6)–(9) and $\tilde{Q}^{\pm}$ are to be obtained by quantizing $\tilde{Q}_c^{\pm}$ [Eq. (47)]. This latter quantization is more difficult than that of $Q_c^{\pm}$ because of the term containing $(\mathbf{p}^2-2MH)^{-1}$ in $\tilde{Q}_c^{\pm}$. Therefore, rather than determining $\tilde{Q}^{\pm}$ directly, we first derive operators $\tilde{Q}_n^{\pm}$ which are independent of $H$, and which satisfy

$$\tilde{Q}_n^{\pm}\,|\,nlm\,\rangle=\tilde{Q}^{\pm}\,|\,nlm\,\rangle . \tag{83}$$

To construct $\tilde{Q}_n^{\pm}$ we replace the classical Hamiltonian in Eq. (47) with the eigenvalue $E$ and quantize. The factors in square brackets in Eq. (47) will yield operators which are linear in $\mathbf{r}$. For analyzing the shift properties of such operators we know[13] that it is convenient to use Hylleraas's form of the energy eigenvalue equation, namely,[18]

$$\Lambda_n\,|\,nlm\,\rangle=4\hbar^4a^{-2}\,|\,nlm\,\rangle , \tag{84}$$

where

$$\Lambda_n=\mathbf{r}^2(\mathbf{p}^2-2ME)^2-2i\hbar\mathbf{p}\cdot\mathbf{r}(\mathbf{p}^2-2ME)+4\hbar^2(\mathbf{p}^2-2ME) , \tag{85}$$

and $E$ is given by Eq. (2). Thus, $\tilde{Q}_n^{\pm}$ will be shift operators for energy if

$$\Lambda_{n\pm1}\tilde{Q}_n^{\pm}\,|\,nlm\,\rangle=4\hbar^4a^{-2}\tilde{Q}_n^{\pm}\,|\,nlm\,\rangle . \tag{86}$$

In Eq. (86), $n>1$ in the lowering operation; $\tilde{Q}_1^{-}$ is treated separately below. An indication of how to proceed is provided by considering the effect of $\Lambda_{n\pm1}$ on $\Delta_n$. Using Eqs. (65) and (85), it is straightforward to show that

$$\Lambda_{n\pm1}\Delta_n^{\pm}=\left[\frac{n}{n\pm1}\right]^2\Delta_n^{\pm}\Lambda_n . \tag{87}$$

This result and Eq. (47) suggest that we consider

$$\tilde{Q}_n^{\pm}=\Delta_n^{\pm}[\mp i\mathbf{r}\cdot\mathbf{p}+2\hbar^3a^{-2}(\mathbf{p}^2-2ME)^{-1}\tilde{Y}_n^{\pm}-\hbar\tilde{Z}_n^{\pm}] , \tag{88}$$

where $\Delta_n^{\pm}$ are given by Eq. (76), and $\tilde{Y}_n^{\pm}$ and $\tilde{Z}_n^{\pm}$ are functions only of $n$. With the aid of the commutators

$$[\Lambda_n,\mathbf{r}\cdot\mathbf{p}]=-2i\hbar\Lambda_n[1+4ME(\mathbf{p}^2-2ME)^{-1}]+8\hbar^2ME[\mathbf{r}\cdot\mathbf{p}-i\hbar] \tag{89}$$

and

$$[\Lambda_n,(\mathbf{p}^2-2ME)^{-1}]=-4i\hbar\mathbf{r}\cdot\mathbf{p}+8\hbar^2ME(\mathbf{p}^2-2ME)^{-1}-2\hbar^2 , \tag{90}$$

and Eq. (87), we find that Eq. (88) will satisfy Eq. (86) if

$$\tilde{Y}_n^{\pm}=\frac{n\mp1}{n^2} , \tag{91}$$

$$\tilde{Z}_n^{\pm}=n . \tag{92}$$

It is apparent from Eq. (88) that

$$[L_i,\tilde{Q}_n^{\pm}]=0 . \tag{93}$$

Thus for

$$\tilde{Q}_n^{\pm}=\Delta_n^{\pm}\tilde{T}_n^{\pm} , \tag{94}$$

where $\Delta_n^{\pm}$ is given by Eq. (76), and

$$\tilde{T}_n^{\pm}=\mp i\mathbf{r}\cdot\mathbf{p}+2\hbar^3a^{-2}(\mathbf{p}^2-2ME)^{-1}(n\mp1)n^{-2}-\hbar n , \tag{95}$$

Eqs. (86) and (93) yield

$$\tilde{Q}_n^{\pm}\,|\,nlm\,\rangle=\tilde{\gamma}^{\pm}(n,l)\,|\,n\pm1,l,m\,\rangle . \tag{96}$$

For the special case of $\tilde{Q}_1^{-}$, it is shown in Appendix C that $\tilde{Q}_1^{-}=\tilde{T}_1^{-}$ has the desired effect,

$$\tilde{Q}_1^{-}\,|\,100\rangle=0 . \tag{97}$$

The coefficients in Eq. (96) are evaluated in Appendix C:

$$\tilde{\gamma}^{\pm}(n,l)=\hbar\left[\frac{n}{n\pm1}[n(n\pm1)-l(l+1)]\right]^{1/2} ,\qquad \tilde{\gamma}^{-}(1,0)=0 . \tag{98}$$

The classical limit of $\tilde{T}_n^{\pm}$ is equal to the factor in square brackets in Eq. (47).

$\tilde{Q}_n^{\pm}$ correspond to abstract operators $\tilde{Q}^{\pm}$. To obtain the latter we cannot simply replace the eigenvalue $E$ with $H$ in Eq. (94) because $H$ does not commute with $\mathbf{r}$ and $\mathbf{p}$. Instead, we use Eqs. (C13) and (C19) to eliminate $(\mathbf{p}^2-2ME)^{-1}$ in Eq. (94), then we rearrange operators using Eq. (65) and replace $E$ with $H$, and $n$ with $N$. This yields

$$\tilde{Q}^{\pm}=\tfrac{1}{2}\hbar^{-1}\mathbf{p}^2\mathbf{r}^2\Delta^{\pm}(N\pm1)^{-1}+\tfrac{1}{2}\hbar a^{-2}\mathbf{r}^2\Delta^{\pm}(N\pm1)^{-3}\mp i\mathbf{r}\cdot\mathbf{p}\Delta^{\pm}[1\mp3(N\pm1)^{-1}]+\hbar\Delta^{\pm}[3(N\pm1)^{-1}-N] , \tag{99}$$

provided $\tilde{Q}^{-}$ does not act on $|\,100\rangle$, in which case

$$\tilde{Q}^{-}=\tfrac{1}{6}\hbar^{-1}\mathbf{p}^2\mathbf{r}^2+\tfrac{1}{6}\hbar a^{-2}\mathbf{r}^2+i\mathbf{r}\cdot\mathbf{p}+\tfrac{3}{2}\hbar \tag{100}$$

and $\tilde{Q}^{-}\,|\,100\rangle=0$. In Eq. (99), $\Delta^{\pm}$ are given by Eq. (77). The effect of $\tilde{Q}^{\pm}$ on $|\,nlm\,\rangle$ is the same as that of $\tilde{Q}_n^{\pm}$, namely,

$$\tilde{Q}^{\pm}\,|\,nlm\,\rangle=\tilde{\gamma}^{\pm}(n,l)\,|\,n\pm1,l,m\,\rangle , \tag{101}$$

where $\tilde{\gamma}^{\pm}(n,l)$ are given by Eq. (98).

Finally, for the vector operators $\tilde{\mathbf{D}}^{\pm}$, Eqs. (81), (82), (11), and (101) yield the shift operations

$$\tilde{D}_k^{+}\,|\,nlm\,\rangle=\alpha_k^{+}(l,m)\beta^{+}(n+1,l)\tilde{\gamma}^{+}(n,l)\,|\,n+1,l+1,m+k\,\rangle \tag{102}$$

and

$$\tilde{D}_k^- \,|\, nlm \rangle = \alpha_k^-(l,m)\beta^-(n,l)\tilde{\gamma}^-(n,l-1)\,|\, n-1,l-1,m+k \rangle \,, \tag{103}$$

where the coefficients are given by Eqs. (12)–(15) and (98).

In the momentum representation of wave mechanics, Eqs. (96) and (97) yield the following recurrence relations for the radial part of the momentum-space wave function:

$$\Delta_n^+ \left[ -p\frac{d}{dp} - 2(n-1)\frac{p_0^2}{n^2p^2+p_0^2} + n - 3 \right] |\, nl \rangle = \left[ \frac{n}{n+1}(n-l)(n+l+1) \right]^{1/2} |\, n+1,l \rangle \,, \tag{104}$$

$$\Delta_n^- \left[ p\frac{d}{dp} - 2(n+1)\frac{p_0^2}{n^2p^2+p_0^2} + n + 3 \right] |\, nl \rangle = \left[ \frac{n}{n-1}(n-l-1)(n+l) \right]^{1/2} |\, n-1,l \rangle \quad (n\neq 1) \,, \tag{105}$$

$$\left[ p\frac{d}{dp} - 4\frac{p_0^2}{p^2+p_0^2} + 4 \right] |\, 10 \rangle = 0 \,, \tag{106}$$

where $p_0 = \hbar a^{-1}$. The solution to Eqs. (104)–(106) is the same as that obtained by other methods (Appendix B).

By using the factorizations (16) for the operators $\mathbf{C}^{\pm}$ in Eqs. (48) and (49), we can write

$$\mathbf{D}^+ = \hbar^{-2} a \mathbf{U}^+ R^+ Q^+ \,, \tag{107}$$

$$\mathbf{D}^- = \hbar^{-2} a Q^- \mathbf{U}^- R^- \,. \tag{108}$$

The effect of these operators on $|\, nlm \rangle$ is the same as that of

$$\mathbf{D}_{nl}^+ = \hbar^{-2} a \mathbf{U}_l^+ R_l^+ \Delta_n^+ T_n^+ \tag{109}$$

and

$$\mathbf{D}_{nl}^- = \hbar^{-2} a \Delta_n^- T_n^- \mathbf{U}_l^- R_l^- \quad (n\neq 1) \,, \qquad \mathbf{D}_{10}^- = \hbar^{-2} a T_1^- \mathbf{U}_0^- R_0^- \,, \tag{110}$$

where $\mathbf{U}_l^{\pm}$ and $R_l^{\pm}$ are defined in Sec. II, and $\Delta_n^{\pm}$ and $T_n^{\pm}$ are given by Eqs. (76) and (59). The operators $\mathbf{U}_l^{\pm}$, $R_l^{\pm}$, and $T_n^{\pm}$ are linear functions of $\mathbf{p}$ and nonlinear functions of $\mathbf{r}$; in the coordinate representation they are first-order differential operators.

Similarly, by using the factorizations (17) in Eqs. (81) and (82), we can show that the effect of $\tilde{\mathbf{D}}^+$ and $\tilde{\mathbf{D}}^-$, respectively, on $|\, nlm \rangle$ is the same as that of

$$\tilde{\mathbf{D}}_{nl}^+ = i\tfrac{1}{2}\hbar^{-2} a \mathbf{V}_l^+ P_{nl}^+ \Delta_n^+ \tilde{T}_n^+ \tag{111}$$

and

$$\tilde{\mathbf{D}}_{nl}^- = -i\tfrac{1}{2}\hbar^{-2} a \Delta_n^- \tilde{T}_n^- \mathbf{V}_l^- P_{nl}^- \quad (n\neq 1) \,, \qquad \tilde{\mathbf{D}}_{10}^- = -i\tfrac{1}{2}\hbar^{-2} a \tilde{T}_1^- \mathbf{V}_0^- P_{10}^- \,. \tag{112}$$

Here $\mathbf{V}_l^{\pm}$ and $P_{nl}^{\pm}$ are defined in Sec. II, and $\Delta_n^{\pm}$ and $\tilde{T}_n^{\pm}$ are given by Eqs. (76) and (95). The operators $\mathbf{V}_l^{\pm}$, $P_{nl}^{\pm}$, and $\tilde{T}_n^{\pm}$ are linear functions of $\mathbf{r}$ and nonlinear functions of $\mathbf{p}$: In the momentum representation they are first-order differential operators.

$R_l^{\pm}$, $P_{nl}^{\pm}$, $Q_n^{\pm}$, and $\tilde{Q}_n^{\pm}$ factorize operators related to the radial Hamiltonian

$$H_l = (2M)^{-1}[p_r^2 + \hbar^2 l(l+1)r^{-2} - 2\hbar^2 a^{-1} r^{-1}] \tag{113}$$

and the radial Hylleraas operator[13]

$$\Lambda_{nl} = [r_p^2 + \hbar^2 l(l+1)p^{-2}](\mathbf{p}^2 - 2ME)^2 - 2i\hbar\mathbf{p}\cdot\mathbf{r}(\mathbf{p}^2 - 2ME) + 4\hbar^2(\mathbf{p}^2 - 2ME) \,. \tag{114}$$

Here

$$p_r = r^{-1}\mathbf{r}\cdot\mathbf{p} - i\hbar r^{-1} \tag{115}$$

and

$$r_p = p^{-1}\mathbf{p}\cdot\mathbf{r} + i\hbar p^{-1} \tag{116}$$

are, respectively, the canonical conjugates of $r$ and $p$. For $R_l^{\pm}$ and $P_{nl}^{\pm}$ these factorizations are given in Ref. 13. For $Q_n^{\pm} = \Delta_n^{\pm} T_n^{\pm}$ and $\tilde{Q}_n^{\pm} = \Delta_n^{\pm} \tilde{T}_n^{\pm}$ it is straightforward to show that

$$Q_{n\pm 1}^{\mp} Q_n^{\pm} = 2M\mathbf{r}^2(H_{n-(1/2)\pm(1/2)} - E) \tag{117}$$

and

$$\tilde{Q}_{n\pm 1}^{\mp} \tilde{Q}_n^{\pm} = \mathbf{p}^2(\mathbf{p}^2 - 2ME)^{-2}(\Lambda_{n,n-(1/2)\pm(1/2)} - 4\hbar^4 a^{-2}) \,. \tag{118}$$

The connection with the factorization method of Schrödinger[17] and Infeld and Hull[19] is established by taking the appropriate differential forms of the above factorizations.

## V. A SPECTRUM-GENERATING ALGEBRA

The shift operators derived above can be modified so that they form part of a Hermitian basis for a spectrum-generating algebra. The procedure is standard,[20] and involves multiplication by suitable functions of $H$ and $\mathbf{L}^2$.

Define

$$\mathbf{D} = (NS^{-1})^{-1/2}\mathbf{D}^+(NS^{-1})^{1/2} I \,, \tag{119}$$

where $S$ and $N$ are given by Eqs. (9) and (51), and

$$I = \hbar^{-1}\{[N(N+1) - S^2 + \tfrac{1}{4}] \times [1 - (S+\tfrac{1}{2})^2(N+1)^{-2}]\}^{-1/2} \,. \tag{120}$$

The adjoint of D is (Appendix D)

$$\mathbf{D}^\dagger = I(NS^{-1})^{-1/2}\mathbf{D}^-(NS^{-1})^{1/2} \,. \tag{121}$$

From Eqs. (79), (80), and (119)–(121),

$$D_k \,|\, \kappa lm \rangle = \alpha_k^+(l,m)\,|\, \kappa,l+1,m+k \rangle \tag{122}$$

and

$$D_k^\dagger \,|\, \kappa lm \rangle = \alpha_k^-(l,m)\,|\, \kappa,l-1,m+k \rangle \,, \tag{123}$$

where

$$\kappa = n - l \ , \tag{124}$$

and $\alpha_k^{\pm}(l,m)$ are given by Eqs. (12)–(14). From Eqs. (122), (123), (10), and

$$(L_x \pm iL_y)\,|\,\kappa lm\,\rangle = \hbar[(l \mp m)(l \pm m + 1)]^{1/2}\,|\,\kappa,l,m\pm 1\,\rangle \ , \tag{125}$$

it can be shown that $-\frac{1}{2}(\mathbf{D}+\mathbf{D}^{\dagger})$, $\frac{1}{2}i(\mathbf{D}-\mathbf{D}^{\dagger})$, $\mathbf{L}$, and $S$ are a Hermitian basis for the de Sitter algebra SO(3,2).[21]

Also define

$$Q = N^{-1/2}Q^{+}N^{1/2}J \ , \tag{126}$$

where

$$J = \hbar^{-1}(N + S + \tfrac{1}{2})^{-1/2} \ . \tag{127}$$

The adjoint of $Q$ is (Appendix D)

$$Q^{\dagger} = JN^{-1/2}Q^{-}N^{1/2} \ . \tag{128}$$

From Eqs. (74), (124), and (126)–(128)

$$Q\,|\,\kappa lm\,\rangle = \kappa^{1/2}\,|\,\kappa+1,l,m\,\rangle \tag{129}$$

and

$$Q^{\dagger}\,|\,\kappa lm\,\rangle = (\kappa-1)^{1/2}\,|\,\kappa-1,l,m\,\rangle \ . \tag{130}$$

Let

$$K_1 = \tfrac{1}{4}(QQ + Q^{\dagger}Q^{\dagger}) \ , \tag{131}$$

$$K_2 = -\tfrac{1}{4}i(QQ - Q^{\dagger}Q^{\dagger}) \ , \tag{132}$$

$$K_3 = \tfrac{1}{2}(QQ^{\dagger} + \tfrac{1}{2}) \ . \tag{133}$$

Then from Eqs. (129)–(133),

$$[K_1,K_2] = -iK_3 \ , \tag{134}$$

$$[K_2,K_3] = iK_1 \ , \tag{135}$$

$$[K_3,K_1] = iK_2 \ . \tag{136}$$

Thus $K_i$ are a Hermitian basis for the algebra SO(2,1). From Eqs. (10), (122), (123), (125), and (129)–(133), $K_i$ commute with $\mathbf{D}$, $\mathbf{D}^{\dagger}$, $\mathbf{L}$, and $S$. Thus the spectrum-generating algebra is SO(2,1)⊕SO(3,2).

Similar results can be obtained using the operators $\tilde{\mathbf{D}}^{\pm}$ and $\tilde{Q}^{\pm}$ derived in Sec. IV. Define

$$\tilde{\mathbf{D}} = (NS)^{1/2}\tilde{\mathbf{D}}^{+}(NS)^{-1/2}I \tag{137}$$

and

$$\tilde{Q} = N^{1/2}\tilde{Q}^{+}N^{-1/2}J \ . \tag{138}$$

Then

$$\tilde{\mathbf{D}}^{\dagger} = I(NS)^{1/2}\tilde{\mathbf{D}}^{-}(NS)^{-1/2} \tag{139}$$

and

$$\tilde{Q}^{\dagger} = JN^{1/2}\tilde{Q}^{-}N^{-1/2} \ . \tag{140}$$

From Eqs. (102), (103), (137), (139), $\tilde{\mathbf{D}}$ and $\tilde{\mathbf{D}}^{\dagger}$ satisfy Eqs. (122) and (123). From Eqs. (101), (138), (140), $\tilde{Q}$ and $\tilde{Q}^{\dagger}$ satisfy Eqs. (129) and (130). Thus we are led to the same spectrum-generating algebra as above.

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## APPENDIX A

We present a discussion for the oscillator which parallels that for the Coulomb problem in Secs. II–IV. This derivation is the inverse of that given by Bracken and Leemon.[7] They used boson operators and the dimension operator to obtain basis operators for a spectrum-generating algebra, and showed that in the classical limit their operators have a simple interpretation.

For the classical oscillator one can readily write down two complex vectors which are orthogonal to $\mathbf{L}$, which have moduli of constant, equal magnitude, and which rotate with angular velocity $\boldsymbol{\omega} = \omega\hat{\mathbf{L}}$,

$$\mathbf{F}_c(\omega) = (-M\omega\mathbf{r}\times\mathbf{L} + \mathbf{p}L)e^{i\delta} \tag{A1}$$

and

$$\mathbf{G}_c(\omega) = \mathbf{F}_c(\omega)\times\hat{\mathbf{L}} = (\mathbf{p}\times\mathbf{L} + M\omega\mathbf{r}L)e^{i\delta} \ , \tag{A2}$$

where $\delta$ is a real function of $\mathbf{r}$ and $\mathbf{p}$. [Note that because the Laplace-Runge-Lenz vector $\mathbf{A}_c$ for the oscillator does not generalize to a quantum-mechanical operator,[22] it is not useful to express $\mathbf{F}_c$ and $\mathbf{G}_c$ in terms of $\mathbf{A}_c$ and $\mathbf{A}_c\times\hat{\mathbf{L}}$, as we did for the Coulomb potential in Eqs. (25) and (26).] Let $\mathbf{X}(\omega)$ denote the modulus

$$\mathbf{X}(\omega) = e^{-i\delta}\mathbf{F}_c \quad \text{or} \ e^{-i\delta}\mathbf{G}_c \ . \tag{A3}$$

It can be verified that

$$\dot{\mathbf{X}}(\omega) = \boldsymbol{\omega}\times\mathbf{X}(\omega) \tag{A4}$$

and

$$\mathbf{X}^2(\omega) = 2M(H + \omega L)\mathbf{L}^2 \ , \tag{A5}$$

where $H = (2M)^{-1}\mathbf{p}^2 + \frac{1}{2}M\omega^2\mathbf{r}^2$.

From the vectors

$$\mathbf{D}_c(\omega) = \mathbf{F}_c(\omega) + i\mathbf{G}_c(\omega) \tag{A6}$$

and $\mathbf{D}_c^{*}(\omega)$, we construct the operators

$$\mathbf{D}^{\pm}(\omega) = [-M\omega\mathbf{r}\times\mathbf{L} + \mathbf{p}K \pm i(\mathbf{p}\times\mathbf{L} + M\omega\mathbf{r}K)]\Delta^{\pm} \ . \tag{A7}$$

Here $K$ is a function of $\mathbf{L}^2$ such that as $\hbar\to 0$,

$$K \to (\mathbf{L}^2)^{1/2} \ . \tag{A8}$$

$\Delta^{\pm}$ correspond to the phase factors $\exp(\pm i\delta)$; apart from any dependence on $\mathbf{r}$ and $\mathbf{p}$, $\Delta^{\pm}$ may also depend on constants of the motion. $\mathbf{D}^{\pm}$ will be vector operators if $\Delta^{\pm}$ are scalars. Thus we assume

$$[L_i,\Delta^{\pm}] = 0 \ . \tag{A9}$$

In (A7) we have adopted a convenient ordering of operators, with functions of constants of the motion placed to the right. From (A7) and the commutation relations for **r** and **p**,

$$[L_i, D_j^{\pm}(\omega)] = i\hbar\varepsilon_{ijk}D_k^{\pm}(\omega) \;, \tag{A10}$$

$$[\mathbf{L}^2, \mathbf{D}^{\pm}(\omega)] = \pm 2\hbar\mathbf{D}^{\pm}(\omega)K - 2i\hbar(M\omega\mathbf{r} \mp i\mathbf{p})(K^2 \mp \hbar K - \mathbf{L}^2)\Delta^{\pm} \;, \tag{A11}$$

$$[H, \mathbf{D}^{\pm}(\omega)] = \pm\hbar\omega\mathbf{D}^{\pm}(\omega) + [-M\omega\mathbf{r}\times\mathbf{L} + \mathbf{p}K \pm i(\mathbf{p}\times\mathbf{L} + M\omega\mathbf{r}K)][H, \Delta^{\pm}] \;. \tag{A12}$$

From (A10) and (A11) $\mathbf{D}^{\pm}$ will be shift operators for angular momentum if

$$K^2 \mp \hbar K - \mathbf{L}^2 = 0 \;. \tag{A13}$$

The roots of (A13) which have the classical limit (A8) are

$$K^{\pm} = \hbar(S \pm \tfrac{1}{2}) \;, \tag{A14}$$

where $S$ is given by Eq. (9). From (A12), $\mathbf{D}^{\pm}$ will be shift operators for energy if $[H, \Delta^{\pm}] = 0$. Therefore we take

$$\Delta^{\pm} = 1 \;. \tag{A15}$$

Thus with $K = \hbar(S \pm \frac{1}{2})$ and $\Delta^{\pm} = 1$ in (A7), the operators $\mathbf{D}^{\pm}$ provide the shift operations

$$D_k^{\pm}(\omega)\,|\,Elm\,\rangle = \alpha_k^{\pm}(\omega)\,|\,E \pm \hbar\omega, l \pm 1, m + k\,\rangle \;, \tag{A16}$$

where $k = \pm 1$ or 0, $D_{\pm 1} = D_x \pm iD_y$, and $D_0 = D_z$. $\mathbf{D}^{\pm}(\omega)$ are quantum-mechanical analogs of the classical vectors

$$\mathbf{D}_c^{\pm}(\omega) = (1 \mp i\hat{\mathbf{L}}\times)\mathbf{F}_c(\omega) \;. \tag{A17}$$

The shift operators $\lambda$ and $\nu$ derived in Ref. 7 are related to $\mathbf{D}^{\pm}$:

$$\lambda = i(4M\hbar^3\omega)^{-1/2}\mathbf{D}^{-}(\omega)(N + S + \tfrac{1}{2})^{-1/2}S^{-1/2} \;, \tag{A18}$$

$$\nu = -(2\sqrt{2}M\hbar^3\omega)^{-1}[\mathbf{D}^{+}(-\omega)\cdot\mathbf{D}^{-}(\omega) + \mathbf{D}^{-}(\omega)\cdot\mathbf{D}^{+}(-\omega)](N + S + \tfrac{1}{2})^{-1/2} \;, \tag{A19}$$

where $N = (\hbar\omega)^{-1}H - \frac{3}{2}$. Thus, as in Ref. 7, a Hermitian basis for a spectrum-generating algebra can be obtained from the vector operators $\mathbf{D}^{\pm}(\omega)$ and $\mathbf{D}^{\pm}(-\omega)$.

## APPENDIX B

We choose basis eigenkets such that[23]

$$\langle E, l+1 \| \mathbf{A} \| E, l \rangle = -[(2l+1)/(2l+3)]^{1/2} \times \langle E, l \| \mathbf{A} \| E, l+1 \rangle \;. \tag{B1}$$

This choice is the same as that in Ref. 12 (p. 344), but differs from that in Ref. 1 and Ref. 23 (p. 145).

These eigenkets appear in the coordinate representation as

$$\psi_{nlm}(\mathbf{r}) = (-1)^{n-l-1}\frac{2}{n^2}\left[\frac{(n-l-1)!}{a^3(n+l)!}\right]^{1/2}\left[\frac{2r}{na}\right]^l \times e^{-r/(na)}L_{n-l-1}^{2l+1}\left[\frac{2r}{na}\right]Y_{lm}(\theta,\phi) \;, \tag{B2}$$

and in the momentum representation as

$$\phi_{nlm}(\mathbf{p}) = (-1)^n i^l\left[\left[\frac{a}{\hbar}\right]^3\frac{n^4(n-l-1)!}{(n+l)!}\right]^{1/2} \times (1-z)^2(1-z^2)^{l/2}T_{n-l-1}^{l+1/2}(z)Y_{lm}(\theta,\phi) \;, \tag{B3}$$

where

$$z = (n^2\mathbf{p}^2 - \hbar^2 a^{-2})(n^2\mathbf{p}^2 + \hbar^2 a^{-2})^{-1} \;. \tag{B4}$$

Here $Y_{lm}$ is a spherical harmonic and $L_{n-l-1}^{2l+1}$ is an associated Laguerre polynomial, defined as in Ref. 12 (pp. 69 and 345, respectively); $T_{n-l-1}^{l+(1/2)}$ is a Gegenbauer polynomial, defined as in Ref. 24 (p. 782). In (B2) a factor $(-1)^{n-1}$ has been included following Biedenharn and Louck.[12] $\phi_{nlm}$ is the Fourier transform of $\psi_{nlm}$.[25] With the aid of the factorizations (16)–(21), it is straightforward to verify that (B2) and (B3) satisfy Eqs. (11)–(15). The radial parts of the momentum-space wave functions (B3) are also solutions to the linear equations (104)–(106).

## APPENDIX C

In the calculations below we require the expectation values

$$\langle r \rangle = \tfrac{1}{2}a[3n^2 - l(l+1)] \;, \tag{C1}$$

$$\langle r^2 \rangle = \tfrac{1}{2}a^2n^2[5n^2 - 3l(l+1) + 1] \;, \tag{C2}$$

$$\langle \mathbf{r}\cdot\mathbf{p} \rangle = \tfrac{3}{2}i\hbar \;, \tag{C3}$$

$$\langle r\mathbf{r}\cdot\mathbf{p} \rangle = i\hbar a[3n^2 - l(l+1)] \;. \tag{C4}$$

(These results can be proved using the hypervirial theorem.[26])

We wish to evaluate the coefficients $\gamma^{\pm}$ in Eq. (74). From Eqs. (74) and (68),

$$|\,\gamma^{\pm}\,|^2 = \langle (T_n^{\pm})^{\dagger}(\Delta_n^{\pm})^{\dagger}\Delta_n^{\pm}T_n^{\pm} \rangle = \langle (T_n^{\pm})^{\dagger}T_n^{\pm} \rangle \tag{C5}$$

if $\Delta_n^{\pm}$ are unitary. Multiplying out the product in (C5) and using the identity

$$\mathbf{L}^2 = \mathbf{r}^2\mathbf{p}^2 - (\mathbf{r}\cdot\mathbf{p})^2 + i\hbar\mathbf{r}\cdot\mathbf{p} \;, \tag{C6}$$

we find

$$|\,\gamma^{\pm}\,|^2 = \langle \pm 2\hbar^2(an)^{-1}r - \hbar^2 l(l+1) - 2i\hbar\mathbf{r}\cdot\mathbf{p} + \hbar^2(n \pm 1)(n \mp 2) \rangle \;. \tag{C7}$$

From (C7), (C1), and (C3) we obtain Eq. (75). [The choice of phase factor in Eq. (75) is consistent with that made in Appendix B.] Equation (C7) is valid also for $n=1$, and is consistent with Eq. (71).

To evaluate the coefficients $\tilde{\gamma}^{\pm}$ in Eqs. (96) and (101), we start with

$$|\tilde{\gamma}^{\pm}|^2=\langle(\tilde{T}_n^{\pm})^{\dagger}\tilde{T}_n^{\pm}\rangle , \quad \text{(C8)}$$

where $\tilde{T}_n^{\pm}$ are given by Eq. (95). Multiplying out the product in (C8) and using (C6), we find

$$|\tilde{\gamma}^{\pm}|^2=\langle \mathbf{r}^2\mathbf{p}^2-\hbar^2 l(l+1)+\hbar^2 n(n\mp 3)-2i\hbar\mathbf{r}\cdot\mathbf{p} -2\frac{\hbar^4}{a^2}\frac{n\mp1}{n^2}(2n\mp5)(\mathbf{p}^2-2ME)^{-1} +4\frac{\hbar^6}{a^4}\frac{n\mp1}{n^4}(n\mp2)(\mathbf{p}^2-2ME)^{-2}\rangle . \quad \text{(C9)}$$

To calculate the expectation values of $(\mathbf{p}^2-2ME)^{-1}$ and $(\mathbf{p}^2-2ME)^{-2}$ in (C9), we use Hylleraas's equation (84). Let $\Omega$ be some operator. Multiplication of Eq. (84) with $(\mathbf{p}^2-2ME)^{-1}\Omega$ yields

$$(\mathbf{p}^2-2ME)^{-1}\Omega\,|nlm\rangle=\tfrac{1}{4}\hbar^{-4}a^2(\mathbf{p}^2-2ME)^{-1}\Omega[\mathbf{r}^2(\mathbf{p}^2-2ME)^2-2i\hbar\mathbf{p}\cdot\mathbf{r}(\mathbf{p}^2-2ME)+4\hbar^2(\mathbf{p}^2-2ME)]\,|nlm\rangle . \quad \text{(C10)}$$

(i) With $\Omega=1$ in (C10) and using the commutators

$$[\mathbf{r}^2,(\mathbf{p}^2-2ME)^2]=8i\hbar(\mathbf{p}^2-2ME)\mathbf{p}\cdot\mathbf{r} -20\hbar^2(\mathbf{p}^2-2ME)-16\hbar^2 ME \quad \text{(C11)}$$

and

$$[\mathbf{p}\cdot\mathbf{r},\mathbf{p}^2-2ME]=2i\hbar\mathbf{p}^2 , \quad \text{(C12)}$$

we find

$$(1-n^{-2})(\mathbf{p}^2-2ME)^{-1}\,|nlm\rangle =\tfrac{1}{4}\hbar^{-4}a^2[(\mathbf{p}^2-2ME)\mathbf{r}^2+6i\hbar\mathbf{r}\cdot\mathbf{p}+6\hbar^2]\,|nlm\rangle . \quad \text{(C13)}$$

From (C13), (1), (C1), and (C3),

$$(1-n^{-2})\langle(\mathbf{p}^2-2ME)^{-1}\rangle=\tfrac{1}{4}\hbar^{-2}a^2[3n^2-l(l+1)-3] . \quad \text{(C14)}$$

(ii) Similarly, by taking $\Omega=\mathbf{p}\cdot\mathbf{r}$ and $\Omega=(\mathbf{p}^2-2ME)^{-1}$ in (C10), and using (C1)–(C4),

$$(1-n^{-2})\langle(\mathbf{p}^2-2ME)^{-2}\rangle =\tfrac{1}{8}\hbar^{-4}a^4n^2[5n^2-3l(l+1)-5] . \quad \text{(C15)}$$

Substituting Eqs. (1), (C1)–(C3), (C14), and (C15) in (C9), we obtain the first of Eqs. (98). [The choice of phase factor in Eqs. (98) is consistent with that made in Appendix B.]

Next we prove Eq. (97). It is straightforward to show that[13]

$$P^{+}\,|100\rangle=0 , \quad \text{(C16)}$$

where $P^{+}$ is given by Eq. (21). From Eqs. (C16) and (21)

$$[-i\hbar^{-1}(\mathbf{p}\cdot\mathbf{r})(\mathbf{p}^2-2ME)+2\mathbf{p}^2]\,|100\rangle=0 . \quad \text{(C17)}$$

Multiplying (C17) on the left with $(\mathbf{p}^2-2ME)^{-1}$ and using (C12) yields

$$[i\mathbf{r}\cdot\mathbf{p}+4\hbar^3a^{-2}(\mathbf{p}^2-2ME)^{-1}-\hbar]\,|100\rangle=0 , \quad \text{(C18)}$$

which is Eq. (97). From (C13), with $n=1$, and (C18),

$$(\mathbf{p}^2-2ME)^{-1}\,|100\rangle =(24\hbar^4)^{-1}a^2[\mathbf{p}^2\mathbf{r}^2+\hbar^2a^{-2}\mathbf{r}^2+12\hbar^2]\,|100\rangle , \quad \text{(C19)}$$

which is used to eliminate $(\mathbf{p}^2-2ME)^{-1}$ from Eq. (97).

## APPENDIX D

We verify that (121) is the adjoint of (119). From Eqs. (121) and (79)

$$\langle n'l'm'|\,D_z\,|nlm\rangle=[(l-m+1)(l+m+1)]^{1/2} \times\delta_{n',n+1}\delta_{l',l+1}\delta_{m'm} . \quad \text{(D1)}$$

From (123) and (80)

$$\langle nlm\,|\,D_z^{\dagger}\,|n'l'm'\rangle=[(l'-m')(l'+m')]^{1/2} \times\delta_{n,n'-1}\delta_{l,l'-1}\delta_{m'm} . \quad \text{(D2)}$$

Take the complex conjugate of (D2):

$$\langle nlm\,|\,D_z^{\dagger}\,|n'l'm'\rangle^{*}=[(l+1-m)(l+1+m)]^{1/2} \times\delta_{n',n+1}\delta_{l',l+1}\delta_{m'm} =\langle n'l'm'|\,D_z\,|nlm\rangle , \quad \text{(D3)}$$

using (D1). Similarly for the other components of $\mathbf{D}$ and $\mathbf{D}^{\dagger}$, and for Eqs. (137)–(140).


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