SO(2,1) Lie algebra and the Jacobi-matrix method for scattering

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Two apparently distinct instances of quantum-mechanical scattering where the prevailing longrange potential permits application of the Jacobi-matrix method are unified by identifying the underlying SO(2,1) Lie algebra. The resulting three-term recursion is solved in its own right without any reference to the coordinate representation of the scattering wave function but in a manner which brings out the similarity between differential and difference equations. The normalized regular solution of the recursion is obtained, its asymptotic form is analyzed, and it is found to vary sinusoidally. The irregular solution is defined to have the same amplitude as the regular solution in the asymptotic limit and to lead it in phase by $\pi/2$. It is argued that this method is particularly suitable for computing the scattering wave function of the hydrogen atom in a magnetic field.

I. INTRODUCTION

The Jacobi-matrix method for analyzing quantummechanical scattering by expanding the scattering function in a complete set of square-integrable functions was introduced by Heller and Yamani.¹ The initial study of scattering of zero-angular-momentum electrons in the absence of any potential was later extended to arbitrary angular momenta and to allow for a long-range Coulomb potential.² The method turns on the fact that under these conditions there exist complete basis sets of squareintegrable functions in which the Hamiltonian is represented by a symmetric, tridiagonal (Jacobi) matrix. Moreover, this matrix can be diagonalized analytically, i.e., one can obtain analytical, closed-form solutions of the associated three-term recursion relation. Regular and irregular solutions are constructed and form the base pair of solutions for analyzing scattering from a short-range potential $V_s(r)$ whose matrix representation is nonzero only in a finite subspace of the full Hilbert space. Physical potentials are made tractable by truncating their representative matrix and the approximation may be refined systematically by increasing the dimension of the truncated matrix.

Three cases were considered in the original articles: (i) the kinetic-energy operator $T(\mathbf{r})$ was diagonalized in a basis of harmonic oscillator wave functions,³

$$\phi_{\nu lm}(\zeta;\mathbf{r}) = \left[\frac{2\zeta \Gamma(\nu+1)}{\Gamma(\nu+l+\frac{3}{2})}\right]^{1/3} (\zeta r)^{l+1} \exp(-\zeta^2 r^2/2) \\ \times \overline{L}_{\nu}^{l+1/2} (\zeta^2 r^2) Y_{lm}(\hat{\mathbf{r}}) \quad \nu = 0, 1, 2...\infty ; \quad (1.1)$$

(ii) $T(\mathbf{r})$ was also diagonalized in a basis of scaled hydrogenic (or Sturmian) functions,⁴

$$\phi_{\nu lm}(\zeta;\mathbf{r}) = \left[\frac{\Gamma(\nu+1)}{\Gamma(\nu+2l+2)}\right]^{1/2} (2\zeta r)^{l+1} e^{-\zeta r}$$
$$\times \overline{L}_{\nu}^{(2l+1)} (2\zeta r) Y_{lm}(\hat{\mathbf{r}}) \quad \nu = 0, 1, 2...\infty ; \quad (1.2)$$

(iii) the Hamiltonian⁵ $T(\mathbf{r}) + Z/r$ was also diagonalized in the Sturmian basis.

The second instance enumerated here is, of course, just a special case of the third with the charge set to zero. Thus there are two distinct cases, one arising from expansion in a set of harmonic oscillator wave functions and another from expansion in a set of scaled hydrogenic wave functions.

The three-term recursion was solved by converting it to a second-order differential equation and thus relating its regular and irregular solutions to linear combinations of independent solutions of the differential equation. In order to specify the regular solution completely (including its normalization) the authors had to refer to the coordinate representation of the regular solution of the Schrödinger equation. Correspondingly, to specify the irregular solution of the recursion they required knowledge of the regular (at the origin) solution of the Schrödinger equation with an inhomogeneity, which has the same asymptotic behavior as the appropriate irregular solution of the Schrödinger equation.

In this paper I refine the original work of Heller, Yamani, and Fishman in two respects.

First, there is a unity underlying the two seemingly distinct cases considered by Heller, Yamani, and Fishman. One of its expressions is that the bound spectrum of both the harmonic oscillator and the hydrogen atom is generated by an SO(2,1) Lie algebra which is characterized by the commutation relations

$$[T_1, T_2] = -iT_3, \ [T_2, T_3] = iT_1, \ [T_3, T_1] = iT_2.$$
 (1.3)

The basis sets enumerated in Eqs. (1.1) and (1.2) constitute infinite-dimensional, unitary, irreducible representations of different realizations (harmonic oscillator and hydrogenic) of the same SO(2,1) Lie algebra. The functions themselves are eigenfunctions of the compact generator T_3 . Combinations of the noncompact generators,

$$T_{\pm} = T_1 \pm iT_2 \tag{1.4}$$

act as ladder operators in the basis set. In both cases, the

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Hamiltonian $T(\mathbf{r}) + V(r)$ can be written as a linear combination of T_1 and T_3 . The problem of finding the eigenfunctions of the continuous spectrum is thus related to the algebraic problem of diagonalizing a linear combination of the compact and noncompact generators of the algebra in a basis in which the compact generator is diagonal. This has been studied previously in the mathematical physics literature.⁶

A three-term recursion relation for the expansion coefficients of the wave function in the basis functions follows from the commutation relations of the algebra. In both cases it arises from the same generators T_1 and T_3 (although in different linear combinations) and its form is the same. The more general recursion for the Coulomb potential is solved first. The solutions of the other recursion are then obtained by taking appropriate limits.

The second refinement concerns the solution of the recursion. I solve it in its own right without any further reference to the Schrödinger equation or its solutions. The regular and irregular solutions of the recursion are specified in a manner which completely parallels the conventional specification of the corresponding solutions of the Schrödinger equation.

The recursion is of the form

$$f(\nu-1;\eta)a_{\nu-1}(\eta) + g(\nu;\eta)a_{\nu}(\eta) + h(\nu+1;\eta)a_{\nu+1}(\eta) = 0, \quad \nu = 1,2,3,\ldots,\infty, \quad (1.5)$$

where η depends on energy. All quantities may also depend on the angular momentum. The regular solution of the recursion is defined by the initial condition,

$$a_0 \neq 0, \quad h(1;\eta)a_1(\eta) + g(0;\eta) = 0.$$
 (1.6)

It is natural to normalize it so that

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$$\sum_{\nu=0}^{\infty} a_{\nu}^{*}(\eta_{1}) a_{\nu}(\eta_{2}) = \delta(\eta_{1} - \eta_{2})$$
(1.7)

in analogy with the δ -function normalization of the regular solution of the Schrödinger equation. The asymptotic (large- ν) behavior of the solution is analyzed and it is found to vary sinusoidally. Its phase has a logarithmic singularity, much as the asymptotic phase of the wave function $\psi(r)$, and depends correctly on the nuclear charge and the angular momentum.

The irregular solution of the recursion is then specified by the initial condition

$$a_0 \neq 0, \ h(1;\eta)a_1(\eta) + g(0;\eta) \neq 0$$
 (1.8)

and the asymptotic condition that its phase lead the phase of the regular solution by $\pi/2$. It is normalized so that asymptotically its amplitude matches the amplitude of the regular solution.

The rest of this paper is organized as follows. In Sec. II, I summarize the relevant properties of the SO(2,1) Lie algebra and the specific realization of its generators for the harmonic oscillator and the hydrogen atom. The recursion relation is set up for the Coulomb potential and solved in Sec. III. In Sec. IV, the kinetic-energy operator is diagonalized in a harmonic oscillator basis by taking appropriate limits of the results derived in Sec. III. Next,

I argue that this method is ideal for studying the continuous spectrum of the hydrogen atom in a strong magnetic field. Finally, some possible future extensions of this work are indicated.

II. HARMONIC OSCILLATOR AND HYDROGENIC REALIZATIONS OF SO(2,1) LIE ALGEBRA

SO(2,1) Lie algebra,⁷ the algebra of Eq. (1.3) can be equivalently represented by the following commutation relations of the ladder operators T_{\pm} [Eq. (1.4)]:

$$[T_3, T_{\pm}] = \pm T_{\pm}, \ [T_+, T_-] = -2T_3 . \tag{2.1}$$

The eigenvalues of the Casimir invariant,

$$T^{2} = T_{3}^{2} - T_{1}^{2} - T_{2}^{2} = T_{3}^{2} \pm T_{3} - T_{\mp} T_{\pm} , \qquad (2.2)$$

characterize irreducible representations of the algebra, and eigenvalues of T_3 characterize basis functions within a representation. Thus functions

$$\{ |t q\rangle; t > -1, q = t + 1, t + 2, \dots, t + \infty \}$$
(2.3)

so that

$$T^{2} | tq \rangle = t(t+1) | tq \rangle, \quad T_{3} | tq \rangle = q | tq \rangle \qquad (2.4a)$$

constitute an infinite-dimensional, unitary, irreducible representation of the algebra denoted $\mathscr{D}^+(t)$. This is the representation pertinent to the bound spectrum of both the harmonic oscillator and the hydrogen atom and it is also the representation relevant to the present application. The action of the ladder operators T_{\pm} on the members of the set (2.3) is determined by the commutation relations

$$T_{\pm} | t q \rangle = (q \mp t)^{1/2} (q \pm t \pm 1)^{1/2} | t q \pm 1 \rangle . \qquad (2.4b)$$

For the harmonic oscillator $(H = \frac{1}{2}p^2 + \zeta^4 r^2)$, the generators of the algebra are defined by

$$T_3 = \frac{1}{2} (\mathbf{a}^{\dagger} \cdot \mathbf{a} + \frac{3}{2}), \quad T_+ = \frac{1}{2} \mathbf{a}^{\dagger} \cdot \mathbf{a}^{\dagger}, \quad T_- = \frac{1}{2} \mathbf{a} \cdot \mathbf{a} , \quad (2.5)$$

where **a** and \mathbf{a}^{\dagger} are annihilation and creation operators,

$$\mathbf{a} = \frac{1}{\sqrt{2}\xi} (\xi^2 \mathbf{r} + i\mathbf{p}), \quad \mathbf{a}^{\dagger} = \frac{1}{\sqrt{2}\xi} (\xi^2 \mathbf{r} - i\mathbf{p}) . \tag{2.6}$$

Operator T_3 is just the Hamiltonian to within an additive constant and T_{\pm} are the ladder operators familiar from elementary quantum mechanics. It is easily verified that the Casimir invariant $T^2 = \frac{1}{4}(L^2 - \frac{3}{4})$.

The functions in Eq. (1.1) are obviously eigenfunctions of T^2 with eigenvalue t(t+1), $t = \frac{1}{2}l - \frac{1}{4}$. Being harmonic oscillator bound states, these are also eigenfunctions of T_3 with eigenvalue $(\nu + \frac{1}{2}l + \frac{3}{4})$ and the set therefore constitutes a $\mathscr{D}^+(\frac{1}{2}l - \frac{1}{4})$ representation of the Lie algebra.

The application of SO(2,1) Lie algebra to determination of the bound spectrum of hydrogen atom is also well documented. In this case one defines the generators as

$$T_{1} = \frac{1}{2\zeta} r(p^{2} - \zeta^{2}), \quad T_{2} = \mathbf{r} \cdot \mathbf{p} - i, \quad T_{3} = \frac{1}{2\zeta} r(p^{2} + \zeta^{2}) .$$
(2.7)

The Casimir invariant is L^2 . Once again, the functions

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defined in (1.2) are eigenfunctions of T^2 with t = l and it can be shown that they are also eigenfunctions of T_3 with eigenvalue $(\nu + l + 1)$. This set then constitutes a $\mathcal{D}^+(l)$ representation of the algebra.

III. JACOBI MATRIX FOR THE CONTINUOUS SPECTRUM OF THE COULOMB POTENTIAL

A. Obtaining the recursion

In the rest of this paper I will use a special case ($\zeta = 1$) of the SO(2,1) generators defined in the preceding section. The flexibility afforded by parameter ζ will be introduced differently by means of an SO(2,1) tilting transformation,⁸

$$\exp(i\theta T_2)(T_3 - T_1)\exp(-i\theta T_2) = e^{\theta}(T_3 - T_1)$$
, (3.1a)

$$\exp(i\theta T_2)(T_3 + T_1)\exp(-i\theta T_2) = e^{-\theta}(T_3 + T_1)$$
, (3.1b)

in conformity with the usual practice in group-theoretical applications. This amounts to scaling the radial coordinate by e^{θ} and setting this factor equal to ζ amounts to using basis set (1.2).

Consider the Schrödinger equation

$$\left| \frac{1}{2} p^2 - \frac{Z}{r} - E \right| \left| \overline{\psi} \right\rangle = 0 .$$
(3.2)

Multiply the left-hand side by r and rewrite in terms of SO(2,1) generators,

$$\left[\frac{1}{2}(T_3+T_1)-E(T_3-T_1)-Z\right]|\bar{\psi}\rangle = 0.$$
 (3.3)

Next make a tilting transformation and multiply by a suitable constant to obtain

$$(T_{+} + T_{-} + 2\eta_{1}T_{3} - 2\eta_{2}) |\psi\rangle = 0, \qquad (3.4)$$

where

$$\eta_1 = (1 - 2Ee^{2\theta})/(1 + 2Ee^{2\theta})$$
, (3.5a)

$$\eta_2 = 2Ze^{\theta} / (1 + 2Ee^{2\theta})$$
, (3.5b)

and

$$|\psi\rangle = \exp(i\theta T_2) |\bar{\psi}\rangle$$
 (3.5c)

Note that $-1 < \eta_1 < 1$ for $0 < E < \infty$.

At this stage one may choose the tilting angle so that $\eta_1=0.^9$ However I will not make this choice because it is too restrictive to permit a unified treatment of the two cases. The solution of (3.4) is no more difficult for $\eta_1\neq 0$ than it is for $\eta_1=0$.

Now expand the wave function $|\psi\rangle$ in the basis set

$$\{ |t,q\rangle, q=t+1, t+2, \ldots, t+\infty \},\$$

thus obtaining

$$|\psi\rangle = \sum_{\nu=0}^{\infty} a_{\nu} |t, t+1+\nu\rangle , \qquad (3.6)$$

substitute in (3.4), use Eqs. (2.4b) and (2.4c), and project the result onto the members of the basis set.¹⁰ This gives the following three-term recursion relation for the expansion coefficients:

$$[\nu(\nu+2t+1)]^{1/2}a_{\nu-1}+2[\eta_1(\nu+t+1)-\eta_2]a_{\nu} + [(\nu+1)(\nu+2t+2)]^{1/2}a_{\nu+1}=0, \quad \nu=1,2,3,\ldots,\infty$$
(3.7)

In order to solve this equation rewrite it so that the functions multiplying the expansion coefficients are linear in ν . To this end define

$$a_{\nu} = i^{\nu} \left(\frac{\Gamma(\nu+1)}{\Gamma(\nu+2t+2)} \right)^{1/2} b_{\nu}$$
(3.8)

so that

$$(\nu+2t+1)b_{\nu-1}+2i[\eta_1(\nu+t+1)-\eta_2]b_{\nu} -(\nu+1)b_{\nu+1}=0, \quad \nu=1,2,3... \quad (3.9)$$

B. Solution of the recursion by the method of Laplace

The recursion (3.9) may be solved by the method of Laplace,¹¹ assuming a solution of the form

$$b_{\nu} = \int_{C} dz \, z^{\nu+t} f(z) \,, \tag{3.10}$$

where the contour C is to be specified later. Insertion of this form in (3.9) gives two conditions which must be satisfied. The first is a first-order differential equation for f(z) which can be solved immediately to give

$$f(z) = z^{t+1}(z-z_1)^{-t-1+i\gamma}(z-z_2)^{-t-1-i\gamma}$$
, (3.11a)

where

$$z_1 = (1 - \eta_1^2)^{1/2} + i\eta_1 \equiv \exp[i(\phi - \pi/2)], \qquad (3.11b)$$

$$z_2 = -(1 - \eta_1^2)^{1/2} + i\eta_1 \equiv \exp[-i(\phi + \pi/2)], \quad (3.11c)$$

and

$$\gamma = \eta_2 / (1 - \eta_1^2)^{1/2} = Z/k$$
 (3.11d)

(Note that $0 < \phi < \pi$ for $-1 < \eta_1 < 1$.) The second condition restricts the contour; if C were to go from t=0 to t=1 just under the branch cut, circle infinitesimally around t=1, return to t=0 just above the cut, and close, this condition is also met. The right-hand side of (3.10) is then just the integral representation of the hypergeometric function.¹²⁻¹⁴ By judicious use of the identities

$$\Gamma(z)\Gamma(1-z) = \pi/\sin(\pi z) \tag{3.12a}$$

and

$$\frac{\Gamma(-z+n)}{\Gamma(-z)} = (-1)^n \frac{\Gamma(z+1)}{\Gamma(z-n+1)}$$
(3.12b)

it can be brought to the form

$$b_{\nu}^{I}(\gamma) = \exp[i\nu(\phi - \pi/2)]\exp[i2(t+1)\phi] \\ \times \frac{\Gamma(\nu + 2t + 2)}{\Gamma(\nu + t + 2 + i\gamma)\Gamma(t+1 - i\gamma)} {}_{2}F_{1}(t+1 + i\gamma, \nu + 2t + 2; \nu + t + 2 + i\gamma; e^{i2\phi}).$$
(3.13a)

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The recursion (3.9) being a second-order difference equation possesses another linearly independent solution. It is obtained from $b_{\nu}^{I}(\gamma)$ by simultaneously interchanging $Z_1 \rightleftharpoons Z_2$ (i.e., replacing $\phi \rightarrow -\phi$) and replacing $\gamma \rightarrow -\gamma$ (this leaves combinations $\eta_1 = -\cos\phi$ and $\eta_2 = \gamma \sin\phi$ unchanged):

$$b_{\nu}^{\Pi}(\gamma) = \exp[-i\nu(\phi + \pi/2)]\exp[-i2(t+1)\phi] \\ \times \frac{\Gamma(\nu+2t+2)}{\Gamma(\nu+t+2-i\gamma)\Gamma(t+1+i\gamma)} {}_{2}F_{1}(t+1-i\gamma,\nu+2t+2;\nu+t+2-i\gamma;e^{-2i\phi}).$$
(3.13b)

The asymptotic forms of these functions may be obtained by first making a suitable linear transformation of the hypergeometric function and then applying standard formulas for the asymptotic forms of the hypergeometric function and ratios of Γ functions. Then, to leading order in $(\nu + t + 1)$, I find

$$b_{\nu}^{I}(\gamma) \sim \frac{e^{\gamma(\phi - \pi/2)}}{(2\sin\phi)^{t+1} |\Gamma(t+1-i\gamma)|} (\nu+t+1)^{t} \exp\{-i\gamma \ln[2(\nu+t+1)\sin\phi]\} \times \exp[i\arg\Gamma(t+1+i\gamma)] \exp[i(\nu+t+1)(\phi - \pi/2)] \exp[i\pi(t+1)]$$
(3.14a)

and correspondingly,

$$b_{\nu}^{II}(\gamma) \sim \frac{e^{\gamma(\phi - \pi/2)}}{(2\sin\phi)^{t+1} |\Gamma(t+1+i\gamma)|} (\nu+t+1)^{t} \exp\{i\gamma \ln[2(\nu+t+1)\sin\phi]\} \times \exp[-i\arg\Gamma(t+1+i\gamma)] \exp[-i(\nu+t+1)(\phi+\pi/2)].$$
(3.14b)

C. Regular solution of the recursion

The unnormalized regular solution of the recursion (3.9) is defined by the initial condition

$$\overline{s}_0(\gamma) \neq 0, \ \overline{s}_1(\gamma) - i 2[\eta_1(t+1) - \eta_2] \overline{s}_0(\gamma) = 0.$$
 (3.15)

In order to obtain this from a linear combination of $b_{\nu}^{I}(\gamma)$ and $b_{\nu}^{II}(\gamma)$, note that

$$b_{-1}^{II}(\gamma) = \exp[-i\pi(2t+1)]b_{-1}^{I}(\gamma)$$
.

Therefore,

$$\overline{s}_{\nu}(\gamma) = \exp[-i\pi(t+1)]b_{\nu}^{1}(\gamma) + \exp[i\pi(t+1)]b_{\nu}^{1}(\gamma)$$
(3.16)

is a satisfactory linear combination. It is brought to a finite polynomial form by a linear transformation of the hypergeometric function and application of the identity (3.12b)

$$\overline{s}_{\nu}(\gamma) = e^{\gamma(2\phi - \pi)} \exp[i\nu(\phi - \pi/2)] \frac{\Gamma(\nu + t + 1 - i\gamma)}{\Gamma(\nu + 1)\Gamma(t + 1 - i\gamma)} \times {}_{2}F_{1}(t + 1 + i\gamma, -\nu; -\nu - t + i\gamma; e^{-i2\phi}).$$

In order to write it as $\exp[\gamma(2\phi - \pi)]$ times a polynomial in γ , make another linear transformation of the hypergeometric function and then apply the inversion formula for finite hypergeometric series.¹⁵ This gives

$$\bar{s}_{\nu}(\gamma) = e^{\gamma(2\phi - \pi)} \exp[i\nu(\phi - \pi/2)] \frac{\Gamma(\nu + 2t + 2)}{\Gamma(\nu + 1)\Gamma(2t + 2)} \\ \times {}_{2}F_{1}(-\nu, t + 1 + i\gamma; 2t + 2; 1 - e^{-i2\phi}) .$$

Referring to the Appendix, this can be written in terms of normalized Pollaczek polynomials:

$$\overline{s}_{\nu}(\gamma) = e^{\gamma(2\phi - \pi)} e^{-i\nu\pi/2} \\ \times \left[\frac{\Gamma(\nu + 2t + 2)}{\Gamma(\nu + 1)\Gamma(2t + 2)} \right]^{1/2} P_{\nu}^{t+1}(\phi) . \quad (3.17)$$

The corresponding solution $\mathcal{S}_{\nu}(\gamma)$ of the recursion (3.7) is obtained by multiplying (3.17) by the factor in (3.8), and it is normalized in the sense of a δ function:

$$\sum_{\nu=0}^{\infty} \mathscr{S}_{\nu}^{*}(\gamma) \mathscr{S}_{\nu}(\gamma') = \delta(\gamma - \gamma') . \qquad (3.18)$$

In comparison with the completeness relation for Pollaczek polynomials,

$$\mathscr{S}_{v}(\gamma) = [W_{P}^{t+1}(\gamma;\phi)]^{1/2} P_{v}^{t+1}(\gamma;\phi) , \qquad (3.19)$$

where $W_P^{t+1}(\gamma;\phi)$ is the weight for the Pollaczek polynomials. The asymptotic form of $\mathscr{S}_{\nu}(\gamma)$ is obtained from the asymptotic forms of $b_{\nu}^{I}(\gamma)$ and $b_{\nu}^{II}(\gamma)$ [(3.14a)-(3.16)]:

$$\mathscr{S}_{\mathbf{v}}(\gamma) \underset{\mathbf{v} \to \infty}{\sim} \left[\frac{2}{\pi} \right]^{1/2} \frac{(-1)^{\mathbf{v}}}{\sqrt{\mathbf{v} + t + 1}} \\ \times \sin\{(\mathbf{v} + t + 1)(\pi - \phi) \\ + \gamma \ln[2(\mathbf{v} + t + 1)\sin(\pi - \phi)] \\ - \arg\Gamma(t + 1 + i\gamma) - \pi t/2 \}.$$
(3.20)

In going from the coordinate representation (Schrödinger equation) to the "discrete representation" (3.8), we have replaced the continuous coordinate r by the "discrete coordinate" $(\nu+t+1)$. Asymptotically, the phase of the wave function $\mathcal{S}_{\nu}(\gamma)$ in the "discrete representation" has a logarithmic singularity, the characteristic Coulomb shift $\arg\Gamma(t+1+i\gamma)$, and the angular<u>34</u>

momentum dependent shift $\pi t/2$. (For the Coulomb Hamiltonian, t=1, from Sec. II). Note the *exact* correspondence with the asymptotic behavior of the coordinate space wave function $\psi(r)$.

D. Irregular solution of the recursion

The normalized irregular solution of the recursion (3.7) is specified by the initial condition

. ...

 $\mathscr{C}_0(\gamma) \neq 0,$

$$\sqrt{(2t+2)}\mathscr{C}_{1}(\gamma) + 2[\eta_{1}(t+1) - \eta_{2}]\mathscr{C}_{0}(\gamma) \neq 0 \quad (3.21)$$

and the condition that asymptotically, its amplitude matches the amplitude of $\mathscr{S}_{\nu}(\gamma)$ and its phase leads the phase of $\mathscr{S}_{\nu}(\gamma)$ by $\pi/2$, i.e.,

$$\mathscr{C}_{\nu}(\gamma) \underset{\nu \to \infty}{\sim} \left[\frac{2}{\pi} \right]^{1/2} \frac{(-1)^{\nu}}{\sqrt{\nu + t + 1}} \cos\{(\nu + t + 1)(\pi - \phi) + \gamma \ln[2(\nu + t + 1)\sin(\pi - \phi)] - \arg\Gamma(t + 1 + i\gamma) - \pi t/2\} .$$
(3.22)

This is assured if we choose the following linear combination of $b_{\nu}^{I}(\gamma)$ and $b_{\nu}^{II}(\gamma)$:

$$\mathscr{C}_{\nu}(\gamma) = e^{i\pi\nu/2} \left[\frac{\Gamma(\nu+1)}{\Gamma(\nu+2t+2)} \right]^{1/2} N(\gamma)i\{-\exp[-i\pi(t+1)]b_{\nu}^{\mathrm{I}}(\gamma) + \exp[i\pi(t+1)]b_{\nu}^{\mathrm{II}}(\gamma)\}$$

Once again, by a suitable linear transformation of the hypergeometric function, it can be reduced to the form given by Yamani and Fishman:

$$\mathscr{C}_{\nu}(\gamma) + i \mathscr{S}_{\nu}(\gamma) = -\left[\frac{2}{\pi}\right]^{1/2} \frac{e^{-\gamma(\phi - \pi/2)}}{(2\sin\phi)^{t}} e^{-i(\nu+1)\phi} \exp[-i\arg\Gamma(t+1+i\gamma)] \\ \times \frac{[\Gamma(\nu+1)\Gamma(\nu+2t+2)]^{1/2}}{\Gamma(\nu+t+2-i\gamma)} {}_{2}F_{1}(\nu+1, -t-i\gamma;\nu+t+2-i\gamma;e^{-i2\phi}).$$
(3.23)

Accounting for the fact that the basis functions used by Yamani and Fishman were not normalized, my expressions for $\mathscr{S}_{\nu}(\gamma)$ and $\mathscr{C}_{\nu}(\gamma)$ agree with theirs except for the numerical prefactor of $\sqrt{2/\pi}$.

The Wronskian of these two solutions,

$$W[\mathscr{S}(\gamma),\mathscr{C}(\gamma)] = b_{\nu+1}[\mathscr{S}_{\nu+1}(\gamma)\mathscr{C}_{\nu}(\gamma) - \mathscr{S}_{\nu}(\gamma)\mathscr{C}_{\nu+1}(\gamma)],$$

where $b_{\nu+1}$ is the coefficient multiplying $P_{\nu+1}$ in the symmetric recurrence (A3c), can be shown to be $1/\pi$.

IV. JACOBI MATRIX FOR KINETIC ENERGY FROM HARMONIC OSCILLATOR ALGEBRA

A. The recursion

Once again I will use the special case ($\zeta = 1$) of the SO(2,1) generators defined in Sec. II. An SO(2,1) tilt by angle 2θ now corresponds to scaling the radial coordinate by e^{θ} —choosing this angle so that this factor is ζ , amounts to using the basis set in (1.1).

The kinetic-energy operator can be written in terms of SO(2,1) generators from Eqs. (2.5) and (2.6). The Schrödinger equation may be rewritten as

$$\left[T_{+} + T_{-} - 2T_{3} + \frac{2E}{e^{2\theta}}\right] |\psi\rangle = 0.$$
 (4.1)

In comparison with Eq. (3.4), one obtains

$$\eta_1 = -1 \tag{4.2a}$$

 $\eta_2 = -E/e^{2\theta} . \tag{4.2b}$

We must set η_2 accordingly, and take the limit $\eta_1 \rightarrow -1$ in the results of Sec. III.

B. Regular and irregular solutions

In the limit $\eta_1 \rightarrow -1$, the Pollaczek polynomial in Eq. (3.22) goes to normalized Laguerre polynomial, $L_v^{2t+1}(-2\eta_2)$ (see Appendix). δ -function normalization of the regular solution is assured if

$$\mathscr{S}_{\nu}^{\rm HO}(\eta^2) = [W_L^{l+1/2}(\eta^2)]^{1/2} L_{\nu}^{l+1/2}(\eta^2) , \qquad (4.3)$$

where I have defined

$$\eta^2 = -2\eta_2 = 2E/e^{2\theta}$$

to conform with the notation of Yamani and Fishman and set $t = \frac{1}{2}l - \frac{1}{4}$ corresponding to the harmonic oscillator (HO) case. This result is obtained by taking the following limit of the hydrogenic regular solution:

$$\mathscr{S}_{\nu}^{\mathrm{HO}}(\eta^2) = \lim_{\eta_1 \to -1} \frac{1}{\sqrt{2 \sin \phi}} \mathscr{S}_{\nu}(\gamma)$$

Correspondingly, the irregular solution of the recursion is obtained from

$$\mathscr{C}_{\nu}^{\mathrm{HO}}(\eta^{2}) + i \mathscr{S}_{\nu}^{\mathrm{HO}}(\eta^{2}) = \lim_{\eta_{1} \to -1} \frac{1}{\sqrt{2 \sin \phi}} \times [\mathscr{C}_{\nu}(\gamma) + i \mathscr{S}_{\nu}(\gamma)].$$

This limit is taken by first making a linear transformation of the hypergeometric function in Eq. (3.23) [Eq. (15.3.6)

of Ref. 14]. One then notes that as $\eta_1 \rightarrow -1$, $\phi \rightarrow 0$, and the following limits exist:

$$\lim_{\eta_1 \to -1} {}_{2}F_1(\nu+1, -t - i\gamma; -2t; 1 - e^{-i2\phi})$$

= $e^{-\eta^2} {}_{1}F_1(-\nu - 2t - 1; -2t; \eta^2)$,
$$\lim_{\eta_1 \to -1} {}_{2}F_1(t + 1 - i\gamma, \nu + 2t + 2; 2t + 2; 1 - e^{-i2\phi})$$

= $e^{-\eta^2} {}_{1}F_1(-\nu; 2t + 2; \eta^2)$,

and

$$\lim_{\eta_1 \to -1} \frac{\Gamma(t+1-i\gamma)}{\Gamma(-t-i\gamma)} (1-e^{-i2\phi})^{2t+1} = e^{i\pi(2t+1)}(\eta^2)^{2t+1} .$$

Finally, setting $t = \frac{1}{2}l - \frac{1}{4}$ for the harmonic oscillator case,

$$\mathscr{C}_{\mathbf{v}}^{\mathrm{HO}}(\eta^{2}) = -\frac{1}{\pi} e^{-\eta^{2}/2} \eta^{-l-1/2} \left[\frac{\Gamma(\nu+1)}{\Gamma(\nu+l+\frac{3}{2})} \right]^{1/2} \Gamma(l+\frac{1}{2}) \\ \times {}_{1}F_{1}(-\nu-l-\frac{1}{2};-l+\frac{1}{2};\eta^{2}) .$$
(4.4)

The asymptotic forms of $\mathscr{S}_{\nu}^{\rm HO}(\eta^2)$ and $\mathscr{C}_{\nu}^{\rm HO}(\eta^2)$ are derived from known asymptotic forms of ratios of γ functions [Eq. (6.1.46) of Ref. 14] and the asymptotic form of the confluent hypergeometric function;¹⁶

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$$\mathcal{S}_{\nu}^{\text{HO}}(\eta^{2})_{\nu \to \infty} \left[\frac{2}{\pi} \right]^{1/2} [4\eta^{2}(\nu + \frac{1}{2}l + \frac{3}{4})]^{-1/4} \\ \times \sin \left\{ \left[4\eta^{2} \left[\nu + \frac{l}{2} + \frac{3}{4} \right] \right]^{1/2} - \pi l/2 \right\}$$
(4.5a)

and

$$\mathscr{C}_{\nu}^{\text{HO}}(\eta^{2})_{\nu \to \infty} - \left[\frac{2}{\pi}\right]^{1/2} \left[4\eta^{2}\left[\nu + \frac{l}{2} + \frac{3}{4}\right]\right]^{-1/4} \times \cos\left\{\left[4\eta^{2}\left[\nu + \frac{l}{2} + \frac{3}{4}\right]\right]^{1/2} - \pi l/2\right\}.$$
(4.5b)

Note that the phase of the irregular solution now lags the phase of the regular solution by $\pi/2$ in contrast to the phase relation before the limit is taken. This somewhat surprising change arises from the change in sign of the coefficients b_{ν} in going from the symmetric recurrence for Pollaczek polynomials to that for Laguerre polynomials. As a consequence the Wronskian

$$W[\mathscr{S}^{\mathrm{HO}}(\eta^2), \mathscr{C}^{\mathrm{HO}}(\eta^2)] = -1/\pi$$

now has a different sign.

V. APPLICATION TO PHOTOIONIZATION OF HYDROGEN ATOM IN A MAGNETIC FIELD

Consider a hydrogen atom placed in a uniform magnetic field, $\mathbf{B} = B\hat{\mathbf{z}}$ and choose the symmetric gauge so that the vector potential $\mathbf{A} = -\frac{1}{2}\mathbf{r} \times \mathbf{B}$. In this gauge, the Schrödinger equation may be written as

$$\left|\frac{\frac{1}{2}p^2 - \frac{Z}{r} + \beta L_z + \frac{1}{2}\beta^2 r^2 \sin^2\theta - E\right|\psi(\mathbf{r}) = 0 \qquad (5.1)$$

with $\beta = \frac{1}{2}\omega = eB/2mc$ and ω is the cyclotron frequency.

Since L_z is a constant of motion, the βL_z term in the Hamiltonian may be absorbed in the energy E and then ignored. Near ionization threshold, the quadratic Zeeman term, $\frac{1}{2}\beta^2 r^2 \sin^2\theta$, is comparable in importance to the Coulomb potential even for weak laboratory strength fields because the electron makes large excursions away from the nucleus. The competition between electrostatic and magnetic effects leads to characteristic regular structures in the photoabsorption spectrum which continue smoothly across the ionization threshold.¹⁷

A quantitative analysis of the wave function in this regime is difficult because a large number of angular momenta and principal quantum numbers are mixed by the quadratic Zeeman term. (Since parity is a good quantum number, one need consider only odd or even angular momenta.) However, the matrix element of $\frac{1}{2}\beta^2 r^2 \sin^2\theta$ between Sturmian basis functions is nonzero only if $|\Delta n| \leq 3$ and $\Delta l = 0, \pm 2$. The matrix element of the Coulomb Hamiltonian and the overlap matrix are of course nonzero only if $\Delta l = 0, |\Delta n| \leq 1$. Therefore, with suitable ordering of the basis set into blocks labeled by increasing angular-momentum quantum number $(l = l_0, l_0 + 2, l_0 + 4, ...)$ and within each block by increasing principal quantum number, the Schrödinger equation (5.1) reduces to a generalized matrix eigenvalue problem

$$[\underline{H} - \underline{E}\underline{S}]\psi = 0,$$

with banded matrices \underline{H} and \underline{S} . This feature permits use of a large basis set while keeping storage requirement within reasonable limits and was crucial to a successful calculation of the bound spectrum.¹⁸

The Jacobi-matrix method provides a natural extension of this work to the continuous part of the spectrum. In the spirit of Heller, Yamani, and Fishman, one now approximates the quadratic Zeeman term by truncating its (infinite-dimensional) matrix representation to a matrix of finite, albeit large, dimension. This amounts to replacing the infinitely thick barrier for electron motion perpendicular to the magnetic field by a barrier of finite but large thickness. For a sufficiently large representative matrix of $\frac{1}{2}\beta^2 r^2 \sin^2\theta$, the barrier is thick enough so that there is little loss of flux in the ρ direction and the exact continuum wave function can be approximated sufficiently well.

The wave function itself may be obtained by multichannel generalization of the Jacobi-matrix method, the number of channels being the same as the number of angular momenta retained in the matrix representation of the quadratic Zeeman term. The numerical problem reduces to solving a matrix equation of the form

$\underline{H} \underline{a} = \underline{b}$,

where \underline{H} is a banded matrix, the driving matrix \underline{b} is known, and \underline{a} determines the wave function. Once again, because of the banded nature of \underline{H} , one can include a large

number of basis functions in a practical calculation. I see no difficulty in considering magnetic fields of laboratory strength (~ 4.7 T), a range which so far has been inaccessible to numerical calculation.

VI. POSSIBLE FUTURE EXTENSIONS

In this paper I have restricted my attention to just two potentials which admit an SO(2,1) spectrum generating algebra, corresponding to the cases considered by Heller, Yamani, and Fishman. A simple extension is to add a potential, $-b/2r^2$, to the Coulomb potential. The resulting problem still admits an SO(2,1) spectrum generating algebra.¹⁹ As long as $b \le l(l+1) + \frac{1}{4}$, one simply has to set t in Sec. III so that t(t+1)=l(l+1)-b. [For $b > l(l+1) + \frac{1}{4}$, well-known problems due to the singularity at r=0 arise.]²⁰ The zero-angular-momentum states of a Morse oscillator also fall within this framework but the parameter η_2 in (3.4) is now imaginary. A somewhat exotic potential which arises in nuclear physics²¹ and whose bound spectrum also seems to be generated by an SO(2,1) algebra should be amenable to similar analysis. I am presently investigating both these problems.

An interesting question is whether one can get a solvable Jacobi matrix for the $-\alpha/r^4$ potential, the remaining exactly solvable potential of quantum mechanics²² which has no known connection with SO(2,1) Lie algebra. This particular extension, if possible, would allow one to include the polarization of an electrically neutral target by charged particles within the Jacobi-matrix formalism.

It is also possible to formulate quantum defect theory in terms of transformations between alternative pairs of solutions of the recursion. This development will exactly parallel the conventional formulation in terms of transformations between alternative pairs of solutions of the Schrödinger equation.²³ It is unclear if this exercise would give anything new but there may very well be some differences due to the fact that the coordinate space wave function reconstructed from the irregular solution of the recursion is not the irregular solution of the Schrödinger equation but the regular solution of an inhomogeneous differential equation.

Finally, relatively little has been done to develop the Jacobi-matrix method as a practical tool for numerical calculation of scattering of electrons from neutral atoms, molecules and ions.²⁴ Considering that it is potentially as powerful as the enormously successful *R*-matrix method,²⁵ much remains to be done.

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APPENDIX: NORMALIZED POLLACZEK AND LAGUERRE POLYNOMIALS

The unnormalized Pollaczek polynomials²⁶

$$\overline{P}_{\nu}^{\lambda}(x;\phi) = e^{i\nu\phi} \frac{\Gamma(2\lambda+\nu)}{\Gamma(2\lambda)\Gamma(\nu+1)} {}_{2}F_{1}(-\nu,\lambda+ix;2\lambda;1-e^{-i2\phi}) \quad (\lambda > 0, \quad 0 < \phi < \pi) , \qquad (A1)$$

are orthogonal over the interval $-\infty < x < \infty$ with weight

$$\overline{W}_{P}^{\lambda}(x;\phi) = \frac{(2\sin\phi)^{2\lambda-1}}{\pi} \exp\left[-(\pi-2\phi)x\right] |\Gamma(\lambda+ix)|^{2}.$$
(A2)

Alternatively, the polynomials may be defined by the initial condition

$$\overline{P}_{-1}^{\lambda} = 0, \ \overline{P}_{0}^{\lambda} = 1 \tag{A3a}$$

and the recurrence

$$(\nu+1)\bar{P}_{\nu+1}^{\lambda}(x;\phi) - 2[(\nu+\lambda)\cos\phi + x\sin\phi]\bar{P}_{\nu}^{\lambda}(x;\phi) + (\nu-1+2\lambda)\bar{P}_{\nu-1}^{\lambda}(x;\phi) = 0, \quad \nu=0,1,2,\dots.$$
(A3b)

Since this recurrence is not symmetric, i.e., it is not of the form

$$b_{\nu+1}P_{\nu+1}(x) + a_{\nu}P_{\nu}(x) + b_{\nu}P_{\nu-1}(x) = xP_{\nu}(x) , \qquad (A3c)$$

so that the associated Jacobi matrix is not symmetric, the polynomials are not normalized.²⁷ However, let us define

$$P_{\nu}^{\lambda}(x;\phi) = \left[\frac{\Gamma(\nu+1)\Gamma(2\lambda)}{\Gamma(\nu+2\lambda)}\right]^{1/2} \bar{P}_{\nu}^{\lambda}(x;\phi) , \qquad (A4)$$

so that

$$P_{-1}^{\lambda}(x;\phi) = 0, \ P_{0}^{\lambda}(x;\phi) = 1$$
 (A5a)

Then the recurrence relation

$$\frac{(\nu+1)^{1/2}(\nu+2\lambda)^{1/2}}{2\sin\phi}P_{\nu+1}^{\lambda}(x;\phi) - (\nu+\lambda)\cot\phi P_{\nu}^{\lambda}(x;\phi) + \frac{[\nu(\nu+2\lambda-1)]^{1/2}}{2\sin\phi}P_{\nu-1}^{\lambda}(x;\phi) = xP_{\nu}^{\lambda}(x;\phi), \quad \nu=0,1,2,\ldots,$$
(A5b)

$$\int_{-\infty}^{\infty} dx \ W_P^{\lambda}(x;\phi) [P_{\nu_1}^{\lambda}(x;\phi)]^* P_{\nu_2}^{\lambda}(x;\phi) = \delta_{\nu,\nu_2}, \qquad (A6a)$$

with weight

$$W_P^{\lambda}(x;\phi) = \overline{W}_P^{\lambda}(x;\phi) \bigg/ \int_{-\infty}^{\infty} dx \ \overline{W}_P^{\lambda}(x;\phi) \ . \tag{A6b}$$

The integral in the denominator is evaluated by noting that it is analytic in the angle $\alpha = \pi - 2\phi$. This is proved by showing that for complex α , real and imaginary parts of the integral satisfy the Cauchy-Riemann conditions. The integral is then evaluated for imaginary values of α , either by contour integration using known residues of Γ functions at their poles, or by introducing integral representations of Γ functions and changing the order of integration. When continued analytically to real values of α , the result is $\Gamma(2\lambda)/\sin\phi$. Then from Eqs. (A2) and (A6b), one finds

$$W_P^{\lambda}(x;\phi) = \frac{(2\sin\phi)^{2\lambda}}{2\pi\Gamma(2\lambda)} \exp[-(\pi-2\phi)x] |\Gamma(\lambda+ix)|^2.$$

Completeness of the polynomials is expressed by the following relations:

$$W_P^{\lambda}(x;\phi) \sum_{\nu=0}^{\infty} \left[P_{\nu}^{\lambda}(x;\phi) \right]^* P_{\nu}^{\lambda}(x';\phi) = \delta(x-x') . \quad (A7)$$

Similarly, the unnormalized Laguerre polynomials

$$\overline{L}_{\nu}^{\alpha}(x) = \frac{\Gamma(\nu+\alpha+1)}{\Gamma(\nu+1)\Gamma(\alpha+1)} {}_{1}F_{1}(-\nu;\alpha+1;x)$$
(A8)

are orthogonal over the interval $0 \le x \le \infty$ with (unnormalized) weight

$$\overline{W}_{L}^{\alpha}(x) = e^{-x} x^{\alpha} . \tag{A9}$$

They may also be defined by the initial condition

$$\bar{L}_{-1}^{\alpha}(x) = 0, \ \bar{L}_{0}^{\alpha}(x) = 1,$$
 (A10a)

and the recurrence relation

$$-(\nu+1)\overline{L}_{\nu+1}^{\alpha}(x) + (2\nu+\alpha+1)\overline{L}_{\nu}^{\alpha}(x)$$
$$-(\nu+\alpha)\overline{L}_{\nu-1}^{\alpha}(x) = x\overline{L}_{\nu}^{\alpha}(x) . \quad (A10b)$$

¹E. J. Heller and H. A. Yamani, Phys. Rev. A 9, 1201 (1974).

- ²H. A. Yamani and L. Fishman, J. Math. Phys. 16, 410 (1975).
- ³In fact, Heller, Yamani, and Fishman used unnormalized basis functions whereas I prefer to normalize them. The overbar denotes unnormalized polynomial $\overline{P}_{\nu}^{\alpha}(x)$ which are orthogonal over the interval $a \le x \le b$ with an unnormalized weight $\overline{W}^{\alpha}(x)$. The corresponding normalized weight is denoted by $W^{\alpha}(x) = \overline{W}^{\alpha}(x) / \int_{a}^{b} dx \overline{W}^{\alpha}(x)$ and the corresponding normalized polynomials by $P_{\nu}^{\alpha}(x)$.
- ⁴These are orthonormal when the inner product is defined by $\langle v_1 | v_2 \rangle = \int_0^\infty d(\zeta r) \phi_{v_1}^*(\zeta r) (1/\zeta r) \phi_{v_2}(\zeta r).$
- ⁵Both repulsive and attractive Coulomb potentials are permitted.
- ⁶G. Lindblad and B. Nagel, Ann. Inst. Henri Poincaré 13A, 27 (1970).

The normalized Laguerre polynomials are defined by

$$L_{\nu}^{\alpha}(x) = \left(\frac{\Gamma(\nu+1)\Gamma(\alpha+1)}{\Gamma(\nu+\alpha+1)}\right)^{1/2} \overline{L}_{\nu}^{\alpha}(x) , \qquad (A11)$$

so that

$$L_{-1}^{\alpha}(x) = 0, \ L_{0}^{\alpha}(x) = 1,$$
 (A12a)

with symmetric recurrence

$$-[(\nu+1)(\nu+\alpha+1)]^{1/2}L^{\alpha}_{\nu+1}(x) + (2\nu+\alpha+1)L^{\alpha}_{\nu}(x) -[\nu(\nu+\alpha)]^{1/2}L^{\alpha}_{\nu-1}(x) = xL^{\alpha}_{\nu}(x) . \quad (A12b)$$

These polynomials are then orthonormal with normalized weight

$$W_L^{\alpha}(x) = e^{-x} x^{\alpha} / \Gamma(\alpha + 1) .$$
(A13)

The limiting case of Pollaczek polynomials

$$\lim_{\epsilon \to \infty} P_{\nu}^{\lambda}(x/\epsilon;\epsilon\phi) = L_{\nu}^{2\lambda-1}(-2\phi x) , \qquad (A14)$$

which is derived from the limiting form of the hypergeometric function in (A1), is used in Sec. IV. The corresponding limit of the normalization integral

$$I_{\nu_{1}\nu_{2}}(\epsilon) = \delta_{\nu_{1}\nu_{2}} = \int_{-\infty}^{\infty} d(x/\epsilon) W_{p}^{\lambda}(x/\epsilon;\epsilon\phi) \\ \times [P_{\nu_{1}}^{\lambda}(x/\epsilon;\epsilon\phi)]^{*} P_{\nu_{2}}^{\lambda}(x/\epsilon;\epsilon\phi)$$
(A15)

is taken by demonstrating that

$$\lim_{\epsilon \to 0} \frac{1}{2\phi\epsilon} W_P^{\lambda}(x/\epsilon;\epsilon\phi) = \begin{cases} 0 \text{ for } x > 0 \\ \\ W_L^{2\lambda-1}(-2\phi x) \text{ for } x \le 0 \end{cases}$$
(A16)

This result follows from Eq. (6.1.45) of Ref. 14. The relation

$$\lim_{\epsilon \to 0} I_{\nu_1 \nu_2}(\epsilon) = \int_0^\infty d(2\phi x) W_L^{2\lambda - 1}(2\phi x) \\ \times [L_{\nu_1}^{2\lambda - 1}(2\phi x)]^* L_{\nu_2}^{2\lambda - 1}(2\phi x) , \quad (A17)$$

is just the normalization integral for Laguerre polynomials. Similarly, the limiting form of (A7) gives the completeness relation for Laguerre polynomials.

(A6c)

⁷An elementary application of SO(2,1) Lie algebra to the harmonic oscillator in the form of algebraic determination of its bound spectrum is standard material in quantum mechanics. B. G. Wybourne, *Classical Groups for Physicists* (Wiley-Interscience, New York, 1974) contains two comprehensive chapters on the group theory of the harmonic oscillator and the hydrogen atom as well as a general introduction to Lie groups. A very clear summary of noncompact Lie algebras for the hydrogen atom is given by B. G. Adams, J. Čížek, and J. Paldus, Int. J. Quant. Chem. 21, 153 (1982).

⁸Although the basis sets (1.1) and (1.2) are complete, in any practical calculation they must be truncated. The freedom to vary ζ so that a basis set with the fewest possible functions is effectively complete in the part of Hilbert space of interest is then of crucial importance.

- ⁹The bound spectrum is generated by choosing θ so that $(1/\eta_1)=0$. Also see Ref. 7.
- ¹⁰This set is orthonormal with a suitably defined inner product.
- ¹¹C. Jordan, Calculus of Finite Differences (Chelsea, New York, 1950).
- ¹²Hereafter I display the dependence of the solutions of the recursion on γ which is the significant parameter.
- ¹³A. Erdelyi, High Transcendental Functions (McGraw-Hill, New York, 1953), Vol. 1, p. 60, Eq. 13.
- ¹⁴M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (National Bureau of Standards, Washington, D.C., 1964).
- ¹⁵The proof of this formula is outlined correctly by L. J. Slater, in Generalized Hypergeometric Series (Cambridge University Press, Cambridge, England, 1966), p. 48, but the result given there is incorrect. The correct result for Gauss's hypergeometric series should read as

$${}_{2}F_{1}(-m,b;c;z) = (b)_{m}(-z)^{m}/(c)_{m} {}_{2}F_{1}(-m,1-c-m;1-b-m;1/z) ,$$

where

 $(a)_{b} = \Gamma(a+p)/\Gamma(a)$, etc.

.

- ¹⁶The asymptotic form given in Eq. (12) of Sec. 6.13.2 of Ref. 13 seems to be incorrect. The correct result is given in Eq. 13.5.14 of Ref. 14.
- ¹⁷These "quasi-Landau resonances" with spacing $\frac{3}{2}\omega$ were the first observed by W. R. S. Garton and F. S. Tomkins, J. Astrophys. 158, 839 (1969). A semiclassical interpretation was given by A. R. Edmonds, J. Phys. (Paris) Collog. 31, C4-71 (1970) and A. F. Starace, J. Phys. B 6, 585 (1973). A. R. P. Rau, Phys. Rev. A 16, 613 (1977), has emphasized the equal

role of Coulomb and magnetic fields near the ionization threshold.

- ¹⁸A. R. Edmonds, J. Phys. B 6, 1603 (1973), was the first to use a Sturmian basis set in considering the quadratic Zeeman effect for bound states of the hydrogen atom. However, this expansion was properly exploited only after the software for solving a generalized matrix eigenvalue problem with banded matrices became available [C. W. Clark and K. T. Taylor, J. Phys. B 15, 1175 (1982)].
- ¹⁹R. Aldrovandi and P. L. Ferreira, Lett. Nuovo Cimento 1, 317 (1969).
- ²⁰P. M. Morse and H. Feshbach, Methods of Theoretical Physics (McGraw-Hill, New York, 1953).
- ²¹J. N. Ginnocchio, Ann. Phys. (N.Y.) 152, 203 (1984); 159, 467 (1985).
- ²²In this case the Schrödinger equation is solved by transforming it to the Mathieu equation. See, E. Vogt and G. H. Wannier, Phys. Rev. 95, 1190 (1954).
- ²³M. J. Seaton, Rep. Prog. Phys. 46, 167 (1983); C. H. Greene, A. R. P. Rau, and U. Fano, Phys. Rev. A 26, 2441 (1982).
- ²⁴The application of Jacobi matrix and related methods to problems in atomic and molecular physics has been reviewed by W. P. Reinhardt, Comput. Phys. Commun. 17, 1 (1979).
- ²⁵There is a close connection between the two methods which was recognized at the outset by Heller and Yamani (Ref. 1).
- ²⁶A. Erdelyi, Higher Transcendental Function (McGraw-Hill, New York, 1953), Vol. 2, p. 221; G. Szegö, Orthogonal Polynomials, 4th ed. (American Mathematical Society, New York, 1975), p. 393.
- ²⁷Starting from a set of orthogonal polynomials, Szegö (Ref. 26) derives the recurrence (Theorem 3.2.1) which is easily put in a manifestly symmetric form. The converse is also true.