Relativistic hydrogen atom revisited

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The hydrogen atom is solved using a simple method. We show that this system has an exact solution that can be written in terms of Laguerre polynomials of noninteger index, instead of the hypergeometric series. This point is important because Laguerre polynomials of integer index appear in the solution of the nonrelativistic hydrogen atom, giving students a more unified point of view for this system. © *2000 American Association of Physics Teachers.*

I. INTRODUCTION

Many of us learned relativistic quantum mechanics in the excellent book *Relativistic Quantum Mechanics*[1] by Bjorken and Drell. In this book the solution to the bound states of the relativistic hydrogen atom appears as a power series, where one cuts the development at a certain power, in order to avoid divergences at infinity. This is an excellent way to illustrate the Frobenius method, but leaves one with the feeling that the solution to this problem is not related to any well-known function and has no exact solution except, perhaps, for an obscure case of the hypergeometric function. Many other books and articles also give the solution either as a series or as a particular case of the hypergeometric function (evaluated at a certain negative integer to avoid the divergences already mentioned).[2–5] Another objection to the usual presentation found in many textbooks is related to invariance under rotations. That is, we know very well that the potential $V(r)=-Ze^2/r$ gives a Hamiltonian invariant under rotations, so angular momentum is a conserved quantity. We thus expect to have a radial Hamiltonian equivalent to the nonrelativistic Schrödinger equation

$$H=-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}-\frac{1}{r}\left(\frac{d}{dr}\right)+\frac{l(l+1)}{2r^2}+V(r). \tag{1}$$

This radial Hamiltonian clearly exists, but it is not often that one sees it.

The purpose of this article is to solve the relativistic hydrogen atom and to show that this problem has an exact solution in terms of Laguerre polynomials, as is also the case in the nonrelativistic problem, giving the student a unified perspective of the quantum hydrogen atom. The Laguerre polynomials are a little bit different than those used in the nonrelativistic case, since these polynomials are labeled by a noninteger index. Nevertheless, they still have a Rodrigues formula, making the ease of handling greater than the series or hypergeometric formulation. We also construct a relativistic radial Hamiltonian equivalent to the nonrelativistic case.

This paper is organized as follows. In Sec. II we introduce the equations of the problem and solve for the angular part of the solutions. In Sec. III we show that the solutions are constructed in terms of Laguerre polynomials of noninteger index. In Sec. IV we find the energy spectrum and use the properties of angular momentum to construct a classification scheme of the eigenstates. We also use the properties of these polynomials to find the normalization constant. In Sec. V we study the nonrelativistic limit to see how we can recover the usual integer Laguerre functions from the ones studied here. In the Appendix we study some properties of Laguerre polynomials of noninteger index. We relate them to the Sonine polynomials and to the hypergeometric function.

II. THE DIRAC HYDROGEN ATOM

Let us begin with the Dirac Hamiltonian of the hydrogen atom

$$H_D=\boldsymbol{\alpha}\cdot\mathbf{p}c+\beta mc^2+V(r), \tag{2}$$

where $V(r)=-Ze^2/4\pi\epsilon_0 r$ is the Coulomb potential, m is the mass of an electron, c is the light velocity, and $\boldsymbol{\alpha}$ and β are the standard Dirac matrices in the Dirac representation[6]

$$\boldsymbol{\alpha}=\begin{pmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{pmatrix},\quad \beta=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{3}$$

Here the 1's and 0's stand, respectively, for 2×2 unit and zero matrices and the $\boldsymbol{\sigma}$ is the standard vector composed of the three Pauli matrices $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$. Since the Hamiltonian (2) is invariant under rotations, we look for simultaneous eigenfunctions of H_D, $|\mathbf{J}|^2$, and J_z, where $\mathbf{J}=\mathbf{L}+\mathbf{S}$ and

$$\mathbf{S}\equiv\frac{1}{2}\boldsymbol{\Sigma}=\frac{\hbar}{2}\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}. \tag{4}$$

To do this, we remark that the spin operator is diagonal in terms of 2×2 Pauli spin matrices; therefore the angular part should be precisely that of the Pauli two-component theory. So, the solutions of the problem can be written in the form

$$\psi(r,\theta,\phi)=\frac{1}{r}\begin{pmatrix}F(r)\mathcal{Y}_{jm}(\theta,\phi)\\ iG(r)\mathcal{Y}'_{jm}(\theta,\phi)\end{pmatrix}, \tag{5}$$

where $\mathcal{Y}_{jm}(\theta,\phi)$ and $\mathcal{Y}'_{jm}(\theta,\phi)$ are two spherical spinors[7] and the i factor is just a matter of convenience. According to the triangle rule of addition of momenta, the orbital angular momentum l is given by $j=l\pm\frac{1}{2}$; consequently the spherical spinors are of the form

$$\mathcal{Y}_{j=l\pm 1/2m}(\theta,\phi)=\frac{1}{\sqrt{2l+1}}\begin{pmatrix}\pm Y_l^{m-1/2}(\theta,\phi)\sqrt{l\pm m+1/2}\\ Y_l^{m+1/2}(\theta,\phi)\sqrt{l\mp m+1/2}\end{pmatrix}. \tag{6}$$

We also remark that parity is a good quantum number in this problem because the Coulomb potential is invariant under reflections. Parity goes as $(-1)^l$, but instead of working directly with parity, we prefer to introduce the quantum number ϵ defined by

$$\epsilon=\begin{cases} 1 & l=j+\frac{1}{2}, \\ -1 & l=j-\frac{1}{2}, \end{cases} \tag{7}$$

thus $l=j+\epsilon/2$ in all cases. Since a parity operation is given by $\psi(r,\theta,\phi)\rightarrow\beta\psi(r,\theta,\phi)$, we have an extra minus sign for the small component. This means that $\mathcal{Y}_{jm}(\theta,\phi)$ and $\mathcal{Y}'_{jm}(\theta,\phi)$ are of opposite parity. This is turn means that when the big component couples with, say, $l=j+1/2$, the small one should couple with the only other option available: $l'=j-1/2$. With this point in mind, we define $l'=j-\epsilon/2$. Accordingly, the spherical spinor $\mathcal{Y}_{jm}(\theta,\phi)$ depends on l whereas the spherical spinor $\mathcal{Y}'_{jm}(\theta,\phi)$, which has an opposite parity, depends on l'. We then put for the wave function

$$\psi(r,\theta,\phi)=\frac{1}{r}\begin{pmatrix} F(r)\mathcal{Y}_{l-\epsilon/2m}(\theta,\phi) \\ iG(r)\mathcal{Y}_{l'+\epsilon/2m}(\theta,\phi) \end{pmatrix}. \tag{8}$$

Writing the solutions in the form (8) completely solves the angular part of the problem. The reader can verify the validity of the solution presented here in many ways. One possibility is to show that the operator $\beta(1+\mathbf{\Sigma}\cdot\mathbf{L})$ commutes with the Hamiltonian H_D. This means that the solutions (8) satisfy the relation

$$\beta(1+\mathbf{\Sigma}\cdot\mathbf{L})\psi(r,\theta,\phi)=\lambda\psi(r,\theta,\phi), \tag{9}$$

or equivalently that $(1+\boldsymbol{\sigma}\cdot\mathbf{L})\mathcal{Y}_{jm}(\theta,\phi)=\pm\lambda\mathcal{Y}_{jm}(\theta,\phi)$. It is not hard to show that $\lambda=-\epsilon(j+1/2)$; with this result, he or she can show that the only (except for a phase) normalized eigenfunctions are precisely the spherical spinors.[8]

III. THE RADIAL PART

Let us now address the radial part of the problem. We are interested in bound states; therefore the quantity $k\equiv(1/\hbar c)\sqrt{m^2c^4-E^2}$ is positive definite. Furthermore, let us define

$$\zeta\equiv\frac{Ze^2}{4\pi\epsilon_0\hbar c}=Z\alpha,\quad \tau_j\equiv\epsilon\left(j+\frac{1}{2}\right),\quad \nu\equiv\sqrt{\frac{mc^2-E}{mc^2+E}}, \tag{10}$$

where $\alpha=1/137$ is structure fine constant. To construct the radial Hamiltonian, we use first the relation $(\boldsymbol{\alpha}\cdot\mathbf{r})(\boldsymbol{\alpha}\cdot\mathbf{p})=(1/\hbar^2)(\mathbf{\Sigma}\cdot\mathbf{r})(\mathbf{\Sigma}\cdot\mathbf{p})=\mathbf{r}\cdot\mathbf{p}+(i/\hbar)\mathbf{\Sigma}\cdot\mathbf{L}$. We then use that $\mathbf{J}^2=[\mathbf{L}+(1/2)\mathbf{\Sigma}]^2=\mathbf{L}^2+\mathbf{\Sigma}\cdot\mathbf{L}+(3/4)\hbar^2$. So we now need an expression for $\mathbf{L}^2$ to obtain $\mathbf{L}\cdot\mathbf{\Sigma}$. The point here is that $\mathbf{L}^2$ is not a good quantum number, since only the total angular momentum commutes with the Hamiltonian. From the general form of $\psi(r,\theta,\phi)$ [Eq. (8)] we see that when $\mathbf{L}^2$ is applied to a solution, the big component behaves with the orbital quantum number $l=j+\epsilon/2$, whereas for the small one the orbital quantum number is $l'=j-\epsilon/2$. We then have

$$l(l+1)=j(j+1)+\epsilon(j+\tfrac{1}{2})+\tfrac{1}{4} \tag{11a}$$

for the big component, and

$$l'(l'+1)=j(j+1)-\epsilon(j+\tfrac{1}{2})+\tfrac{1}{4} \tag{11b}$$

for the small one. Thus the action of $\mathbf{L}^2$ over one solution of the form given by (8) is always

$$\mathbf{L}^2=\hbar^2[j(j+1)+\beta\epsilon(j+\tfrac{1}{2})+\tfrac{1}{4}], \tag{12}$$

where β is given in Eq. (3). From this result we can deduce the term $\mathbf{L}\cdot\mathbf{\Sigma}$ and substitute it into $(\boldsymbol{\alpha}\cdot\mathbf{p})$. We finally obtain

$$(\boldsymbol{\alpha}\cdot\mathbf{p})=\alpha_r\left[p_r-i\hbar\beta\frac{\epsilon}{r}\left(j+\frac{1}{2}\right)\right], \tag{13}$$

where

$$\alpha_r\equiv\frac{1}{r}\boldsymbol{\alpha}\cdot\mathbf{r},$$
$$p_r\equiv\frac{(-i\hbar)}{r}\frac{d}{dr}r=-\frac{i\hbar}{r}\left(1+r\frac{d}{dr}\right). \tag{14}$$

We are then ready to write the relativistic radial Hamiltonian [equivalent to Eq. (1) of the nonrelativistic case]. The result is very simple,

$$H_D=\alpha_r\left[p_r-i\hbar\beta\frac{\epsilon}{r}\left(j+\frac{1}{2}\right)\right]+\beta mc^2+V(r). \tag{15}$$

We see that in the relativistic case the equivalent term for the centrifugal force term $l(l+1)/r^2$ is now $-i\hbar\alpha_r\beta\epsilon(j+1/2)/r$. The important point here is that this result is valid for any central potential $V(r)$.

Now we are ready to study the radial part of our problem. The first things we need to consider are the terms $\boldsymbol{\sigma}\cdot r$ that come in the α_r term. Since the $\boldsymbol{\alpha}$ matrix is nondiagonal [Eq. (3)], the equation for the big component has a mixed term of the form $(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l'+\epsilon/2m}$ and exactly the opposite for the small one, where we must deal with $(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l-\epsilon/2m}$. Of course we know that both terms should be canceled out, so we suspect that we have a proportionality relation of the form $(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l\pm\epsilon/2m}\sim\mathcal{Y}_{l\mp\epsilon/2m}$. We can show that this is exactly the case using the following argument. First notice that if we perform a reflection through the origin, the term, say $(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l+\epsilon/2m}$, goes as $(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l+\epsilon/2m}\rightarrow-(-1)^l(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l+\epsilon/2m}$; because of the extra change of sign produced by $(\boldsymbol{\sigma}\cdot r)$. But this is precisely the behavior of the only other spherical spinor available, $\mathcal{Y}_{l-\epsilon/2m}$, so both terms should be proportional. Let us call the constant of proportionality a. From the well-known relation $Y_l^m(0,\phi)=[(2l+1)/4\pi]^{1/2}]\delta_{m0}$ we find[9,10]

$$(\boldsymbol{\sigma}\cdot r)\mathcal{Y}_{l\pm\epsilon/2m}(\theta,\phi)|_{\theta=0}=-\mathcal{Y}_{l\mp\epsilon/2m}(\theta,\phi)|_{\theta=0}. \tag{16}$$

So we conclude that $a=-1$.

Now we can write the differential equations for the radial part of the problem in terms of the dimensionless variable $\rho=kr$ as

$$\left(-\frac{d}{d\rho}+\frac{\tau_j}{\rho}\right)G(\rho)=\left(-\nu+\frac{\zeta}{\rho}\right)F(\rho) \tag{17a}$$

and

$$\left(\frac{d}{d\rho}+\frac{\tau_j}{\rho}\right)F(\rho)=\left(\nu^{-1}+\frac{\zeta}{\rho}\right)G(\rho), \tag{17b}$$

where we use the Coulomb potential $V(r)=-Ze^2/4\pi\epsilon_0 r$.

We now redefine the radial functions $F(\rho)$ and $G(\rho)$ in Eqs. (17a) and (17b) to the form

$$F(\rho)=\sqrt{mc^2+E}[\psi_+(\rho)-\psi_-(\rho)], \tag{18}$$

$$G(\rho)=\sqrt{mc^2-E}[\psi_+(\rho)+\psi_-(\rho)]. \tag{19}$$

In terms of the new functions $\psi_+(\rho)$ and $\psi_-(\rho)$, we thus arrive at the following set of equations for our problem:

$$\left[\rho\frac{d}{d\rho}-\rho+\frac{\zeta E}{\sqrt{m^2c^4-E^2}}\right]\psi_-(\rho)=\left(\frac{\zeta m}{\sqrt{m^2c^4-E^2}}+\tau_j\right)\psi_+(\rho) \tag{20}$$

and

$$\left[-\rho\frac{d}{d\rho}-\rho+\frac{\zeta e}{\sqrt{m^2c^4-E^2}}\right]\psi_+(\rho)=\left(\frac{\zeta m}{\sqrt{m^2c^4-E^2}}-\tau_j\right)\psi_-(\rho). \tag{21}$$

This first-order system can be uncoupled multiplying by the left the first equation [Eq. (20)] times the operators that appear between square brackets in the second equation and, vice versa, by multiplying the second equation [Eq. (21)] times the operators that appear (between square brackets) in the first one. This procedure gives us the second-order system

$$\left[-\rho^2\frac{d^2}{d\rho^2}-\rho\frac{d}{d\rho}-2(\mu-1)\rho+\rho^2+(\tau_j^2-\zeta^2)\right]\psi_-(\rho)=0 \tag{22}$$

and

$$\left[-\rho^2\frac{d^2}{d\rho^2}-\rho\frac{d}{d\rho}-2\mu\rho+\rho^2+(\tau_j^2-\zeta^2)\right]\psi_+(\rho)=0, \tag{23}$$

where we have defined

$$\mu\equiv\frac{\zeta E}{\sqrt{m^2-E^2}}+\frac{1}{2}. \tag{24}$$

Let us now study $\psi_+(\rho)$. To that end, we first define the function $v(\rho)$ according to $\psi_+(\rho)\equiv\rho^s\exp(-\rho)v(\rho)$. After that, we put $\mathcal{L}(\rho)\equiv v(\rho/2)$ to finally get

$$\rho\frac{d^2\mathcal{L}(\rho)}{d\rho^2}+[(2s+1)-\rho]\frac{d\mathcal{L}(\rho)}{d\rho}+\left[\frac{(s^2+\zeta^2-\tau_j^2)}{\rho}+(\mu-s-1/2)\right]\mathcal{L}(\rho)=0. \tag{25}$$

We now impose the condition that the solution must be well behaved at the origin. This in turn implies that the term $1/\rho$ should vanish:

$$s^2+\zeta^2-\tau_j^2=0, \tag{26a}$$

where we choose the positive root to avoid the divergence already mentioned,

$$s=+\sqrt{\tau_j^2-\zeta^2}. \tag{26b}$$

This condition is precisely the same one obtained in the power series method, when one asks for a regular behavior at the origin.

We also look for vanishing solutions at infinity. From Eq. (25) we see that in this limit the terms proportional to ρ dominate, so for very large ρ we have $\rho d^2\mathcal{L}(\rho)/d\rho^2-\rho d\mathcal{L}(\rho)/d\rho\approx 0$. The solution to this equation is clearly an exponential plus a constant, unimportant for the point at hand. We then obtain that for very large ρ, $v(\rho)\approx e^{2\rho}$; or equivalently that $\psi_+(\rho)\approx\rho^s e^{\rho}$. This solution diverges at infinity unless we ask for the series to be a polynomial. If we choose

$$\mu-s-1/2=n, \tag{27}$$

where n is an integer, then the resultant equation can be regarded as a generalization to the noninteger index s of the usual associated Laguerre differential equation.[11] From Eq. (27) we can deduce the energy spectrum, without explicitly solving the differential equation (25), but we shall discuss this point in Sec. IV.[12] As shown in the Appendix, the solutions to this differential equation are polynomials of order n. The equation corresponding to $\psi_-(\rho)$ can be obtained in analogous fashion. The complete solution can then be written as

$$\begin{aligned}\psi_-(\rho)&=a\rho^s\exp(-\rho)\mathcal{L}_{n-1}^{2s}(2\rho),\\ \psi_+(\rho)&=b\rho^s\exp(-\rho)\mathcal{L}_n^{2s}(2\rho),\end{aligned} \tag{28}$$

where a and b are, at present, unknown constants.

The Laguerre polynomials $\mathcal{L}_n^{\alpha}(\rho)$ of noninteger index are related to both the hypergeometric ${}_1F_1(-n,\alpha+1;\rho)$ and the Sonine polynomials[13] $T_{\alpha}^{(n)}(\rho)$ through the relation

$$\begin{aligned}\mathcal{L}_n^{\alpha}(\rho)&=\frac{\Gamma(\alpha+n+1)}{n!\Gamma(\alpha+1)}\,{}_1F_1(-n,\alpha+1;\rho)\\ &=(-1)^n\Gamma(\alpha+n+1)T_{\alpha}^{(n)}(\rho).\end{aligned} \tag{29}$$

As we shall see in the Appendix, these polynomials are very similar to the usual integer index Laguerre polynomials. In the Appendix we also study some of their more important properties.

IV. THE ENERGY SPECTRUM

The energy spectrum is easily obtained from the solutions we found here. We substitute Eq. (28) into the original radial differential equations [Eqs. (17a) and (17b)] and substitute the recurrence relations (A2) from the Appendix to obtain the following conditions:

$$\begin{aligned}a(\tau_j+s-\zeta\nu^{-1}+n)+b(n+2s)&=0,\\ b(\tau_j-s+\zeta\nu^{-1}-n)-an&=0.\end{aligned} \tag{30}$$

Solving these last two equations gives us a relationship between n and ν. From Eq. (10) we see that we can then solve for the energy E and obtain the energy spectrum; the result is given by

$$E=mc^2\left[1+\frac{\zeta^2}{(\mu-1/2)^2}\right]^{-1/2}. \tag{31a}$$

We can write our result in a more familiar form if we define the principal quantum number as $N\equiv j+1/2+n$, and ϵ_j as

$$\epsilon_j\equiv N-s-n=j+\tfrac{1}{2}-s, \tag{31b}$$

then $\mu-1/2=s+n=N-\epsilon_j$, which gives precisely the well-known energy spectrum.[14–16] This result is exactly the same as the one obtained from Eq. (27), so we are now very confident of the validity of (30).

To proceed, we shall take $b=-a(\tau_j+s+n-\zeta\nu^{-1})/(n+2s)$, and write the result in a symmetrized form:

Table I. We can classify the eigenstates of the relativistic hydrogen atom for each value of the principal quantum number N, according to the way the orbital angular momentum couples with the spin. If $\epsilon=+1$ then $j=l-1/2$. Otherwise $\epsilon=-1$ and $l=j-1/2$. Note that for each N the state with the highest angular momentum exists only for $\epsilon=-1$.

States		$Nl_j(\epsilon)$		
N	j	$l=0$	$l=1$	$l=2$
1	1/2	$1S_{1/2}$ $(\epsilon=-1)$		
2	1/2	$2S_{1/2}$ $(\epsilon=-1)$	$2P_{1/2}$ $(\epsilon=1)$	
	3/2		$2P_{3/2}$ $(\epsilon=-1)$	
3	1/2	$3S_{1/2}$ $(\epsilon=-1)$	$3P_{1/2}$ $(\epsilon=1)$	
	3/2		$3P_{3/2}$ $(\epsilon=-1)$	$3d_{3/2}$ $(\epsilon=1)$
	5/2			$3d_{5/2}$ $(\epsilon=-1)$

$$F(\rho)=\sqrt{mc^2+E}C\rho^s e^{-\rho}[A_n\mathcal{L}_n^{2s}(2\rho)+B_n\mathcal{L}_{n-1}^{2s}(2\rho)],$$
$$G(\rho)=-\sqrt{mc^2-E}C\rho^s e^{-\rho}[A_n\mathcal{L}_n^{2s}(2\rho)-B_n\mathcal{L}_{n-1}^{2s}(2\rho)], \tag{32a}$$

where A_n and B_n are given by

$$A_n=(\tau_j+s+n-\zeta\nu^{-1})^{1/2},$$
$$B_n=(n+2s)(\tau_j+s+n-\zeta\nu^{-1})^{-1/2} \tag{32b}$$

and C is a normalization constant. It can be obtained from

$$\int_0^\infty e^{-x}x^\alpha\mathcal{L}_n^\alpha(x)\mathcal{L}_m^\alpha(x)dx=\delta_{mn}\frac{\Gamma(n+\alpha+1)}{n!}. \tag{33}$$

In the Appendix we give a simple proof of this result. We again need to use relations (30) in order to obtain $(\tau_j+s+n-\zeta\nu^{-1})^{-1}=(n+s-\tau_j-\zeta\nu^{-1})/n(n+2s)$. We also will need $(n+s)=\zeta E/\sqrt{m^2c^4-E^2}$, which is obtained from the expression for the energy [Eq. (31a)]. Elementary algebra gives the result

$$|C|=\frac{\hbar 2^{s-1}}{Z\alpha c^2}\sqrt{\frac{n!k}{2m^3}}[\Gamma(n+2s+1)]^{-1/2}. \tag{34}$$

Although Eq. (32) was discovered a long time ago by L. Davies,[17] it has remained largely unknown.[18] Nevertheless, its importance should not be neglected. In fact, it is possible to obtain complex results in an easy way with the results found here. For instance, it has recently been employed to calculate arbitrary matrix elements of powers of $\langle r^q\rangle$, and recurrence relations for arbitrary nondiagonal, radial hydrogenic relativistic matrix elements, including a relativistic version of the Pasternack–Sternheimer rule.[19]

Another point worthy of mention concerns the classification of the states of this system. We recall that according to our definition, the principal quantum number is given by $N=j+1/2+n$, where n is the degree of the Laguerre polynomial associated with this state. For the ground state $N=1$, we have only $j=1/2$ and $n=0$. Since $l=j+\epsilon/2$, we have two choices, $l=0$ for $\epsilon=-1$ and $l=1$ for $\epsilon=1$. This last result is not possible, since l cannot be greater than j, so this state does not exist. In the traditional spectroscopic notation Nl_j, we have only one state $1S_{1/2}(\epsilon=-1)$. For the next energy level, we have $n=2$, and $j=1/2$, 3/2; but again the state $j=3/2$ and $\epsilon=1$ does not exist. We then have only three states: $2S_{1/2}(\epsilon=-1)$, $2P_{1/2}(\epsilon=1)$, and $2P_{3/2}(\epsilon=-1)$. Continuing in this way, we obtain Table I.

V. THE NONRELATIVISTIC LIMIT

It is interesting to study how we recover from our results the usual Laguerre polynomials that appear in the nonrelativistic hydrogen atom. First we recall that the nonrelativistic limit for the energy is obtained from the series development of E, retaining only the first two terms,

$$E=mc^2\left[1+\frac{\zeta^2}{(N-\epsilon_j)^2}\right]^{-1/2}\approx mc^2\left[1-\frac{\zeta^2}{2N^2}\right]. \tag{35}$$

So, in this limit we have $\epsilon_j=j+1/2-s\approx 0$, because $s=\sqrt{\tau_j^2-\zeta^2}\approx j+1/2$. That is, in this limit s becomes an integer and the Laguerre polynomials in Eq. (32a) are now the same as those employed in the nonrelativistic case. Since $\zeta=Z\alpha$ this means that the effects of the fine structure constant are negligible, as they should be. For other energy-dependent quantities we follow the same recipe. For instance for ν and k, we easily find that in the nonrelativistic limit

$$\nu=\sqrt{\frac{mc^2-E}{mc^2+E}}\approx\frac{\zeta}{2N},$$
$$k=(1/\hbar c)\sqrt{m^2c^4-E^2}\approx mc\frac{\zeta}{\hbar N}. \tag{36}$$

In order to be more compatible with the nonrelativistic treatments, it will be convenient to introduce the nonrelativistic energy $E_{\rm nr}\equiv-\zeta^2mc^2/2N^2$ $(E_{\rm nr}<0)$ and define

$$\mathcal{K}^2\equiv-\frac{8mE_{\rm nr}}{\hbar^2}=\frac{4m^2c^2\zeta^2}{\hbar^2N^2}\approx 4k^2. \tag{37}$$

That is, in the nonrelativistic limit we have to put simply $\rho=2kr\to\mathcal{K}r$.

We can now study the nonrelativistic behavior of the wave functions. Perhaps the easiest way to do that is to start from Eq. (32a). Following the same reasoning as above, we easily find for the nonrelativistic limit of A_n and B_n:

$$A_n=(\tau_j+s+n-\zeta\nu^{-1})^{1/2}\approx[(\epsilon-1)(j+1/2)-n]^{1/2},$$
$$B_n=(n+2s)(\tau_j+s+n-\zeta\nu^{-1})^{-1/2}$$
$$\approx[(\epsilon-1)(j+1/2)-n]^{-1/2}. \tag{38}$$

We need to study two cases depending on whether $j=l+1/2$ or $j=l-1/2$. Let us start with the case $j=l+1/2$ $(\epsilon=-1)$. In this case, $A_n\approx i[n+2(j+1/2)]^{1/2}$ and $B_n=-i[n+2(j+1/2)]^{-1/2}$. The i is just a phase factor, unimportant for the point at hand, and means only that the relativistic conventions used by us are slightly different than the nonrelativistic ones. From (32a) we get

$$F(kr)\approx|C_{\rm nr}|r^{j+1/2}e^{-kr}[\mathcal{L}_n^{2(j+1/2)}(2kr)-\mathcal{L}_{n-1}^{2(j+1/2)}(2kr)]$$
$$=|C_{\rm nr}|r^{j+1/2}e^{-kr}\mathcal{L}_n^{2(j+1/2)-1}(2kr), \tag{39}$$

where the last step follows from the second recurrence relation in (A5) and $|C_{\rm nr}|$ is a normalization constant that can be obtained from (A9) in the same way as we did for the relativistic case. Since $j=l+1/2$, we have that $j+1/2=l+1$ and $2(j+1/2)-1=2l+1$. Also, from $N=j+1/2+n$ we obtain that $n=N-l-1$. Putting all this together we get

$$F(kr)\approx|C_{\rm nr}|r^{l+1}e^{-(\mathcal{K}/2)r}\mathcal{L}_{N-l-1}^{2l+1}(\mathcal{K}r). \tag{40}$$

This is precisely the nonrelativistic solution we were looking for.[20]

The case $j=l-1/2$, $(\epsilon=1)$ is a little bit more involved. In this case we have $A_n \approx in^{1/2}$ and $B_n \approx -in^{-1/2}[n+2(j+1/2)]$. Again, except for unimportant phases we get from (32a) that

$$\begin{aligned} F(kr) &\approx |C_{\rm nr}| r^{j+1/2} e^{-kr} [n \mathcal{L}_n^{2(j+1/2)}(2kr) \\ &\quad -[n+2(j+1/2)] \mathcal{L}_{n-1}^{2(j+1/2)}(2kr)] \\ &= |C_{\rm nr}| r^{j+1/2} e^{-kr} \mathcal{L}_n'^{2(j+1/2)}(2kr) \\ &= -|C_{\rm nr}| r^{j+1/2} e^{-kr} \mathcal{L}_{n-1}^{2(j+1/2)+1}(2kr). \end{aligned} \tag{41}$$

The second step above follows from the second recurrence relation in (A2) and the third one follows from $\mathcal{L}_n'^{\alpha}(2kr) = -\mathcal{L}_{n-1}^{\alpha+1}(2kr)$. This last relation in turn follows by taking the derivative in the second recurrence relation in (A5). Here $l=j+1/2$ and $N-l-1=n-1$. Again, the minus sign is just a phase, so we can put the following for the radial function $F(kr)$:

$$F(kr) \approx |C_{\rm nr}| r^{l+1} e^{-(\mathcal{K}/2)r} \mathcal{L}_{N-l-1}^{2l+1}(\mathcal{K}r). \tag{42}$$

So, as expected, we find again the same wave function as for the $j=l+1/2$ case.

The small components go to zero because $mc^2 \gg E$, as can be seen in (32a). The radial function is given by $R(r) = (1/r)F(\mathcal{K}r)$, where $F(\mathcal{K}r)$ is given by (40) and (or) (42). The complete, nonrelativistic solution is then just simply

$$\psi(r,\theta,\phi) = R(r)\mathcal{Y}_{l-\epsilon/2m}(\theta,\phi). \tag{43}$$

This last equation means that in the nonrelativistic limit the angular part is a spherical spinor with $l=j+\epsilon/2$.

VI. CONCLUSIONS

In this paper we found that the solution of the relativistic hydrogen atom is given in terms of Laguerre functions of noninteger index. These functions are handled in exactly the same way as the Laguerre functions of integer index, and are in fact a natural extension of those used in the nonrelativistic limit. This point of view gives the student more powerful tools than in the series approach used elsewhere. He or she can use recurrence relations, Rodrigues formula, generating functions, etc. We illustrate this point by calculating the normalization constant and the nonrelativistic behavior of the solution. This approach also gives the student a more unified point of view of the quantum hydrogen atom, since in both cases (relativistic and nonrelativistic), Laguerre functions are involved in the solution.

A final remark concerns Eq. (15). This equation is valid for any central potential $V(r)$ and is completely equivalent to

$$\begin{aligned} &\left[-\hbar \frac{d}{dr} + \frac{\hbar\epsilon}{r}\left(j+\frac{1}{2}\right)\right] G(r) = [E-mc^2-V(r)]F(r), \\ &\left[\hbar \frac{d}{dr} + \frac{\hbar\epsilon}{r}\left(j+\frac{1}{2}\right)\right] F(r) = [E+mc^2-V(r)]G(r). \end{aligned} \tag{44}$$

We can then use it as a departure equation in any central potential system, including perturbation theory problems.

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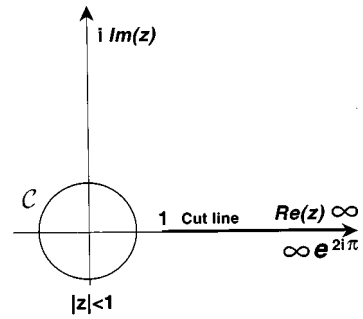

Fig. 1. The generating function $g(x,t)$ is not single valued, but we can choose a cut line from 1 to ∞ over the real line. The integration contour is given by the circle $\mathcal{C}$ of radius $|z|<1$.

APPENDIX

The purpose of this Appendix is to study some of the more important properties of Laguerre polynomials of noninteger index and to use our result to calculate the normalization constant, which is not always an easy task. We start from the generating function $g(x,t)$:

$$g(x,t) \equiv \frac{e^{-xt/(1-t)}}{(1-t)^{\alpha+1}} = \sum_{n=0}^{\infty} t^n \mathcal{L}_n^{\alpha}(x), \tag{A1}$$

which is simply a generalization to the noninteger index of the usual Laguerre generating function. If we differentiate $g(x,t)$ with respect to x and with respect to t, we obtain the recurrence relations

$$\begin{aligned} &\mathcal{L}_{n-1}^{\alpha}(x) = \mathcal{L}_{n-1}'^{\alpha}(x) - \mathcal{L}_n'^{\alpha}(x), \\ &x\mathcal{L}_n'^{\alpha}(x) = n\mathcal{L}_n^{\alpha}(x) - (n+\alpha)\mathcal{L}_{n-1}^{\alpha}(x), \\ &(2n+\alpha+1-x)\mathcal{L}_n^{\alpha}(x) = (n+\alpha)\mathcal{L}_{n-1}^{\alpha}(x) + (n-1)\mathcal{L}_{n+1}^{\alpha}(x), \end{aligned} \tag{A2}$$

where the prime means derivative with respect to x. These recurrence relations are exactly the same as those obtained in the integer index case. The generating function is not single valued, but we can choose a cut line in the complex plane to try to invert (A1). From Fig. 1, we can conclude that

$$\mathcal{L}_n^{\alpha}(x) = \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{e^{-xz/(1-z)}}{(1-z)^{\alpha+1} z^{n+1}} dz. \tag{A3}$$

We can show that (A3) is a solution of Laguerre's differential equation by substituting into Laguerre's differential equation of noninteger index [Eq. (25) plus conditions (26)]. We easily find that the differential equation is the integral of a total derivative over a closed curve, as happens to be the case for the usual Laguerre polynomials.[20] Performing the change of variable $xz/(1-z)=s-x$, we find that

$$\mathcal{L}_n^{\alpha}(x) = \frac{e^x x^{-\alpha}}{n!} \frac{d^n(x^{n+\alpha}e^{-x})}{dx^n}. \tag{A4}$$

This result is precisely the Rodrigues formula. We can use it to deduce new recurrence relations, for instance from the expression for $\mathcal{L}_{n+1}^{\alpha}(x)$ and $\mathcal{L}_n^{\alpha+1}(x)$ we find

$$\begin{aligned} &(n+1)\mathcal{L}_{n+1}^{\alpha}(x) = (n+\alpha+1)\mathcal{L}_n^{\alpha}(x) - x\mathcal{L}_n^{\alpha+1}(x), \\ &\mathcal{L}_n^{\alpha+1}(x) = \mathcal{L}_n^{\alpha}(x) + \mathcal{L}_{n-1}^{\alpha+1}(x). \end{aligned} \tag{A5}$$

The moral of the story is that we do not need to worry about the non-single-valuedness of the generating function. From Leibnitz' formula and Eq. (A4), we find the two following equivalent expressions for Laguerre polynomials:

$$\mathcal{L}_n^\alpha(x)=e^{-x}x^\alpha\sum_{k=0}^{n}\frac{(-1)^k n!\Gamma(n+\alpha+1)}{k!(n-k)!\Gamma(\alpha+k+1)}x^k$$
$$=e^{-x}x^\alpha\sum_{s=0}^{n}\frac{(-1)^{n-s} n!\Gamma(n+\alpha+1)}{s!(n-s)!\Gamma(n+\alpha-s+1)}x^{n-s}. \tag{A6}$$

That is, the solutions to the noninteger differential equation (25) together with the boundary conditions (26) (regular behavior at the origin and vanishing asymptotic value at infinity) imply that they behave as a polynomial multiplied by the factor $e^{-x}x^\alpha$.

We are now ready to study the orthogonality properties of $\mathcal{L}_n^\alpha(x)$. If $m\neq n$ we can suppose without any loss of generality that $m>n$. We use the Rodrigues formula and m-times partial integration to find

$$\int_0^\infty e^{-x}x^\alpha\mathcal{L}_n^\alpha(x)\mathcal{L}_m^\alpha(x)dx=\frac{(-1)^m}{n!m!}\int_0^\infty e^{-x}x^{\alpha+m}\frac{d^m}{dx^m}\times\left[e^x x^{-\alpha}\frac{d^n}{dx^n}(e^{-x}x^{\alpha+n})\right]dx. \tag{A7}$$

This integral converges for $\mathrm{Re}(\alpha)>-1$. We now use (A6) to write this last expression in the form

$$\frac{(-1)^m}{m!}\int_0^\infty e^{-x}x^{\alpha+m}\frac{d^m}{dx^m}\left[\sum_{k=0}^{n}\frac{(-1)^k\Gamma(n+\alpha+1)}{k!(n-k)!\Gamma(\alpha+k+1)}x^k\right]dx. \tag{A8}$$

But in this case we have to differentiate the polynomial inside the square brackets in (A8) more times than its maximum (integer) power, giving a vanishing result. In other words, if $m\neq n$ we conclude that (A7) is zero. If $m=n$, after an n-times derivation, only the last power of the polynomial survives. The result of the integral is a gamma function $\Gamma(n+\alpha+1)/n!$, giving precisely Eq. (33),

$$\int_0^\infty e^{-x}x^\alpha\mathcal{L}_n^\alpha(x)\mathcal{L}_m^\alpha(x)dx=\delta_{mn}\frac{\Gamma(n+\alpha+1)}{n!}. \tag{A9}$$

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