Solving the radial Dirac equations: a numerical odyssey

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Abstract
We discuss, in a pedagogical way, how to solve for relativistic wavefunctions from the radial Dirac equations. We first solve the equations for a linear Lorentz scalar potential, \( V_s(r) \), that provides for confinement of a quark; the case of massless \( u \) and \( d \) quarks is necessarily relativistic. We use an iterative 'shooting and matching' procedure to find the eigenenergies and the upper and lower component wavefunctions. Solutions for the massive quarks (\( s \), \( c \), and \( b \)) are also presented. We then consider the Coulomb potential \( V_v(r) \). We re-derive, numerically, the (analytically well-known) relativistic hydrogen atom eigenenergies and wavefunctions, and later extend that to the cases of heavier one-electron atoms and muonic atoms. Finally, we solve for a combination of the \( V_s \) and \( V_v \) potentials, when both potentials are linearly confining and \( V_v \) has a color Coulombic component. We establish when these potentials give a vanishing spin–orbit interaction (as is approximately the case in quark models of the baryonic spectrum).

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Dirac formulated relativistic quantum mechanics in the late 1920s [1]. Since field theory had not yet been developed, the relativistic aspect led to a number of confusions related to currents since only total charge is conserved. With the discovery of antiparticles and the development of field theory, analogous to the transition from the canonical to the grand canonical ensemble in statistical mechanics, these issues were resolved. Nonetheless, the solution of the Dirac equation itself, ignoring these deeper aspects, has proven valuable even in more modern contexts.

For example, the MIT bag model of quark confinement [2] and the theories that evolved from it (chiral bag, cloudy bag, etc) [3] depend on solving the Dirac equation for the...
wavefunction for a particle in an effective potential. Through boundary conditions and other approximations, the Dirac equation has even been employed in this way in the study of nuclear structure [4, 5].

In particle physics, the quark model has been employed, with great success, to describe baryon and meson states and their structure. Usually this is done in a non-relativistic model [6], where the potentials follow the patterns expected by a Foldy–Wouthuysen reduction [7] of a simpler, theoretically motivated potential in the Dirac equation. We, however, wanted to see how these structures and solutions appear without the non-relativistic reduction approximations, by solving the Dirac equation itself for the simpler potential with fewer adjustable parameters.

Going back somewhat in time, very soon after Dirac’s initial formulation, Darwin [8] found an analytic solution for the radial wavefunctions for hydrogen-like atoms in terms of confluent hypergeometric functions. Since then, solutions of the Dirac equation have been important in atomic physics, even to recent times [9, 10]. For example, more complicated central potentials than $-Z\alpha/r$, the fourth component of a Lorentz four-vector, usually require finding a numerical solution. Another example is a muonic atom, in which a muon is in an $s$ state about a heavy nucleus having a realistic charge distribution [11].

Finding such numerical solutions involves solving coupled ordinary differential equations for the upper and lower components of the Dirac wavefunction [10, 12] (also see footnote 2),

$$\Psi_{jm}(r) = \left[ \begin{array}{c} \psi_a(r) Y_{jm}^l \\ -i \psi_b(r) Y_{jm}^{l'} \end{array} \right] = \frac{1}{r} \left[ \begin{array}{c} ig(r) Y_{jm}^l \\ -f(r) Y_{jm}^{l'} \end{array} \right],$$

(1)

where $l' = 2j - l$ and the $Y_{jm}^l$ are the spin–orbital angular momentum wavefunctions,

$$Y_{jm}^l(\theta, \phi) = \sum_{m_s} \langle jm | l^m \cdot m_s, m_s \rangle Y_m^l(\theta, \phi) \chi_{m_s},$$

(2)

where $\langle jm | l^m \cdot m_s, m_s \rangle$ is a Clebsch–Gordan coefficient and $\chi_{m_s}$ is a Pauli spinor.

We consider here the case of bound-state wavefunctions for a central potential with energy eigenvalue $E$. For example, for hydrogen-like atoms the potential is $V_v(r) = -Z\alpha/r$. With appropriate boundary conditions, the radial wavefunctions $g(r)$ and $f(r)$, which can be taken as real functions, are the solutions of the following coupled first-order ordinary differential equations (ODEs) [9, 12],

$$g'(r) + \frac{k}{r} g(r) - (E - V_v(r) + m) f(r) = 0,$$

(3)

$$f'(r) - \frac{k}{r} g(r) + (E - V_v(r) - m) g(r) = 0.$$  

(4)

Here the integer $k$ is determined by the angular momentum quantum numbers according to

$$k = -(l + 1) \quad \text{if} \quad j = l + \frac{1}{2},$$

$$k = l \quad \text{if} \quad j = l - \frac{1}{2}.$$  

(5)

The reason for the subscript on the potential $V_v$ in those equations is to indicate that it is the fourth component of a Lorentz four-vector, such as the Coulomb potential. However, our original motivation for this study was not so much for atomic physics applications as it was for

1 Reference [4] is henceforth abbreviated as GMSS.

2 It was on finding this paper that we were reminded of the coupled first-order radial Dirac equations.
treating mesons as $q \bar{q}$ states in a relativistic quark model. The non-relativistic quark model often assumes the confining potential for quarks to be the so-called Cornell potential [6],

$$V(r) = -\frac{\alpha_s}{r} + \kappa^2 r,$$

(6)

where $\alpha_s = g^2_s / 4\pi$, with $g_s$ being the (running) quark–gluon coupling constant, and $\kappa^2$ (or $\sigma$) is the string tension. It is the linear term in $V(r)$ that confines the quarks, corresponding to the effective potential in the relativistic bag model [2].

For a relativistic quark model, the two pieces of that non-relativistic potential have different Lorentz transformation properties. The color Coulomb potential, $\alpha_s/r$, is the fourth component of a Lorentz vector, while the confining linear potential transforms as a Lorentz scalar, which we will write as $V_s(r)$. Thus, in solving the relativistic radial Dirac equations, the two terms in the non-relativistic potential of equation (6) enter the coupled ODE’s differently. The equations to be solved are

$$g'(r) + \frac{k}{r}g(r) - (E - V_v(r) + V_s(r) + m)f(r) = 0,$$

(7)

$$f'(r) - \frac{k}{r}f(r) + (E - V_v(r) - V_s(r) - m)g(r) = 0.$$

(8)

Note that in these equations the sign for $V_v$ is opposite to that of the energy eigenvalue $E$, the fourth component of the momentum four-vector, while that for $V_s$ matches that for the fermion mass $m$, also a Lorentz scalar.

So, we were motivated to study solutions of equations (7) and (8). Analytic solutions of these equations have been presented by Paris [14] and by Soares de Castro and Franklin [15]. We, however, have adopted a numerical approach and, in this paper, we discuss how to go about solving these coupled ODE’s numerically. Our hope in writing this paper is that, by reading it, students might avoid some of the pitfalls we encountered and then overcame.

We solve the coupled differential equations by a ‘shooting and matching’ method, similar to that which is well-known for determining the wavefunctions and energy eigenvalues in a second-order ordinary differential equation (such as the Schrödinger equation) [17]. In this paper we confine ourselves to discussing the modifications needed for the two-coupled-equations case and the peculiarities involved with the particular potentials we consider.

It turns out that solving for a linear scalar potential [4, 16] (also see footnote 1) is quite a bit easier (numerically) than the relativistic hydrogen atom, so we treat that first in section 2. We then turn, in section 3, to the problems we had with in solving the radial equations for a Coulomb-like potential for hydrogen-like atoms and how we dealt with them. Section 4 gives a discussion of the mixed problem having both a scalar and a vector potential.

2. Linear scalar potential

For the case of massless quarks (an approximation we have made [13] for the $u$ and $d$ quarks), we want to solve the equations for a confining linear scalar potential [4, 16],

$$V_s(r) = \kappa^2 (r - r_0),$$

(9)

where (with $\hbar = c = 1$), $\kappa$ has dimensions of fm$^{-1}$. The negative offset, $-\kappa^2 r_0$, effectively gives these quarks a constituent mass [4]. It also provides a rough representation of the effect of how the short-distance color Coulomb interaction between quarks leads to quark confinement, albeit without the correct Lorentz representation properties.

3 In more usual units, $\hbar c = 0.19732$ GeV fm, which can be used for converting from 1/fm to GeV.
The case of massless quarks exhibits the role of relativity in a maximal way, meaning that the lower component $f(x)$ is comparable in size to the upper component $g(x)$. We will, later, choose an appropriate mass $m$ for the massive quark flavors, $s$, $c$, and $b$, and solve for those wavefunctions. In these cases, as the quark mass $m$ increases, $f(x)$ becomes smaller relative to $g(x)$, reflecting the transition to a non-relativistic limit where $f(x)$ vanishes. Also, as will be seen, with increasing mass $m$, the heavier quark radial wavefunctions are progressively narrower than in the massless case.

It simplifies the equations if we convert the ODEs to dimensionless form, dividing through by $\kappa$ and defining a dimensionless distance $x = \kappa r$:

\begin{align}
 g'(x) + \frac{k}{x} g(x) - (\tilde{E} + V_s(x) + \tilde{m}) f(x) &= 0, \\
 f'(x) - \frac{k}{x} f(x) + (\tilde{E} - V_s(x) - \tilde{m}) g(x) &= 0,
\end{align}

where $g(x)$, $f(x)$, $\tilde{E} = E/\kappa$, $V_s(x) = x - x_0$, and $\tilde{m} = m/\kappa$ are all dimensionless.

Numerical integrations of these equations can be done by one or another of the Runge–Kutta methods \[18\]. To integrate these two first-order ODEs one needs to specify two boundary conditions (BCs) at the place where one begins the integration. However, as the radial wavefunctions eventually need to satisfy a normalization condition,

\[ \int_{0}^{\infty} x^2 \mathrm{d}x \left[ \psi_a^2(x) + \psi_b^2(x) \right] = \int_{0}^{\infty} \mathrm{d}x \left[ g^2(x) + f^2(x) \right] = 1, \]

this will determine one of the BCs, for example, the scale of the wavefunctions at asymptotically large distances.

In the shoot-and-match procedure, we shoot both outwards from the origin to a point in the middle, $x_{\text{match}}$, and inwards from some large asymptotic $x_{\text{max}}$ back to $x_{\text{match}}$. The two values for $g_{\text{out}}(x_{\text{match}})$ and $g_{\text{in}}(x_{\text{match}})$, and also $f_{\text{out}}(x_{\text{match}})$ and $f_{\text{in}}(x_{\text{match}})$, will generally differ. So, one must find values of the eigenenergy $\tilde{E}$ and BC values that reduce these gaps to zero. We will outline an iterative method for doing just that.

### 2.1. Shooting outwards

The first problem in integrating away from the origin is the singularity at $x = 0$. This singularity, however, is easily avoided by starting instead at a small value of $x = \epsilon$ away from the origin.

For the starting values of the BCs we can invoke the expected non-relativistic power-law behaviors of $\psi_a(x)$ and $\psi_b(x)$ near the origin for their known orbital angular momenta $l$ and $l'$. For example, if $j = l + \frac{1}{2}$ and $l' = l + 1$, one can choose

\[ g(\epsilon) = a_0 \epsilon^{l+1}, \quad f(\epsilon) = b_0 \epsilon^{l+2}, \]

where $\psi_a \to \Psi_{\text{NR}} \sim r^l$ at small $r$. Substituting this $f(\epsilon)$ into the second ODE allows us to determine $b_0$:

\[ f(\epsilon) = -a_0(\tilde{E} - V_s(\epsilon) - \tilde{m}) \epsilon^{l+2}/(2l + 3). \]

The parameter $a_0$ is to be determined by the iterative matching procedure. The ODE solver for almost all initial guesses for $\tilde{E}$ will have the well-known problem that the calculated $g(r)$ and $f(r)$ very soon blow up exponentially, either positively or negatively, which is why we stop the integration at $x_{\text{match}}$. 
2.2. Shooting inwards

At large distances the ODEs simplify, for this linear potential, to
\begin{align}
g'(x) - xf(x) &= 0, \quad f'(x) - xg(x) = 0, \quad (15) \\
g(x_{\text{max}}) &= a_1 e^{-x_{\text{max}}^2/2}, \quad f(x_{\text{max}}) = -a_1 e^{-x_{\text{max}}^2/2}. \quad (16)
\end{align}

Note that this asymptotic behavior is the same as that of the non-relativistic simple harmonic oscillator wavefunctions \[16\]. These forms will be used as starting values (BCs) for the inward integration of the full ODEs from \(x_{\text{max}}\). The value of \(a_1\) can be taken as arbitrary for now, to be later fixed by the normalization condition, equation (12).

2.3. Matching

After shooting both outwards from \(x = \epsilon\) and inwards from \(x_{\text{max}}\) to \(x_{\text{match}}\), we need to find a way to iteratively vary \(\tilde{E}\) and \(a_0\) to reduce the two gaps, \(\Delta g\) and \(\Delta f\), to zero. (The asymptotic parameter \(a_1\) is not to be varied, but should be of a size that makes the initial determination of the gaps at \(x_{\text{match}}\) reasonably small.)

We need to define the gaps \(\Delta g\), etc, at the match point. It is better to scale them relative to their average value, e.g.,
\[
\Delta g(\tilde{E}, a_0) = \frac{2[g_{\text{out}}(x_{\text{match}}) - g_{\text{in}}(x_{\text{match}})]}{g_{\text{out}}(x_{\text{match}}) + g_{\text{in}}(x_{\text{match}})}, \quad (17)
\]
and likewise for \(\Delta f(\tilde{E}, a_0)\).

2.4. Zeroing the gaps

The two gaps can be driven to zero by using a generalized Newton–Raphson method. For our problem with two functions, equation (17), from Taylor expansions (to first order) we obtain a two-by-two linear system for new values of the parameters, \(\tilde{E}_{\text{new}}\) and \(a_{0,\text{new}}\):

\[
0 = \Delta g + \left(\frac{\partial \Delta g}{\partial \tilde{E}}\right)(\tilde{E}_{\text{new}} - \tilde{E}_{\text{old}}) + \left(\frac{\partial \Delta g}{\partial a_0}\right)(a_{0,\text{new}} - a_{0,\text{old}}) \\
0 = \Delta f + \left(\frac{\partial \Delta f}{\partial \tilde{E}}\right)(\tilde{E}_{\text{new}} - \tilde{E}_{\text{old}}) + \left(\frac{\partial \Delta f}{\partial a_0}\right)(a_{0,\text{new}} - a_{0,\text{old}}). \quad (18)
\]

The partial derivatives here are to be calculated numerically. The procedure is to iterate solutions of these equations for \(\tilde{E}_{\text{new}}\) and \(a_{0,\text{new}}\) until the last gaps are sufficiently small.

To solve this linear system in equation (18), it is convenient to define a matrix
\[
M = \begin{bmatrix}
\frac{\partial \Delta g}{\partial \tilde{E}} & \frac{\partial \Delta g}{\partial a_0} \\
\frac{\partial \Delta f}{\partial \tilde{E}} & \frac{\partial \Delta f}{\partial a_0}
\end{bmatrix} \quad (19)
\]
and a column vector containing the gaps and partials obtained using the old parameters \(\tilde{E}_{\text{old}}\) and \(a_{0,\text{old}}\),
\[
C_{\text{old}} = \begin{bmatrix}
\left(\frac{\partial \Delta g}{\partial \tilde{E}}\right) \tilde{E}_{\text{old}} + \left(\frac{\partial \Delta g}{\partial a_0}\right) a_{0,\text{old}} - \Delta g_{\text{old}} \\
\left(\frac{\partial \Delta f}{\partial \tilde{E}}\right) \tilde{E}_{\text{old}} + \left(\frac{\partial \Delta f}{\partial a_0}\right) a_{0,\text{old}} - \Delta f_{\text{old}}
\end{bmatrix}. \quad (20)
\]

Multiplying \(C_{\text{old}}\) by the inverse matrix \(M^{-1}\) then provides us with a column vector containing the improved parameters for the next iteration:
\[
P_{\text{new}} = M^{-1}C_{\text{old}} = [\tilde{E}_{\text{new}}, a_{0,\text{new}}]^T. \quad (21)
\]
It turns out that this iterative procedure works very well, with the gaps in the slopes of 
\( g(x) \) and \( f(x) \) at the match point also going to zero.

At this point we should remark that others might have done this calculation by zeroing 
the gaps in the logarithmic derivatives, such as \( \left( \frac{dg(x)}{dx} \right)/g(x) \). This has the advantage 
of removing the scale dependence of the functions \( g \) and \( f \), but our choice of defining the 
gaps as relative, as in equation (17), is essentially equivalent, as it also involves (semi-)local 
differences divided by the (semi-)local value.

2.5. The 1s radial wavefunctions

We implemented the iterative numerical process discussed above using Mathematica [19],
but any reasonable programming language (e.g., Fortran, C++, Maple, etc) could be used 
instead. Here, we describe the calculation of the ground state radial wavefunctions for the 
GMSS potential of equation (9).

For the 1s, \( j = \frac{1}{2} \) ground state, \( l = 0, l' = 1 \), and thus \( k = -1 \). For the cases discussed 
here and below, we have fixed the constants in the GMSS potential at \( \kappa^2 = 0.9 \) GeV \text{ fm}^{-1} 
(i.e. \( \kappa = 2.14 \) fm\(^{-1} \)), and \( r_0 = 0.705 \) fm. For the dimensionless equations this linear scalar 
potential simplifies to \( \tilde{V}_s(x) = x - x_0 \), where \( x_0 = \kappa r_0 = 1.506 \).

For dimensionless distances we chose \( \epsilon = 10^{-6}, x_{\text{match}} = 1.0, \) and \( x_{\text{max}} = 6.0 \). We 
also define a small increment \( \delta = 0.0001 \), which will be used when we calculate the partial 
derivatives in equation (19) numerically and for testing when the gaps to be zeroed are small 
enough. Reducing \( \delta \) further does not significantly affect the results.

The two integrations, inwards and outwards, were done using Mathematica’s \texttt{NDSolve} 
function, but one could use any standard Runge–Kutta procedure [18]. To proceed, we need 
the four boundary conditions (BCs) from equation (13) and equation (16). In this case, we 
already had a good idea [4] (also see footnote 1) of what the energy eigenvalue \( \tilde{E} \) is for the 1s 
ground state. After some fiddling, we found an initial choice of parameters

\[
\tilde{E} = 0.82, \quad a_0 = 0.2, \quad a_1 = 1000.0 
\]

(22)

for which the resulting outwards and inwards integrations yielded curves for \( g(x) \) and \( f(x) \) 
having only relatively small \( \Delta g \) and \( \Delta f \). From these integrations one can now calculate the 
values of \( g(x) \) and \( f(x) \) at the match point \( x_{\text{match}} \) and their gaps scaled as in equation (17). 
Also, from similar integrations involving \( \delta \) increments of \( \tilde{E} \) and \( a_0 \), we can calculate the four 
partial derivatives in the two-by-two matrix \( M \) of equation (19) numerically.

We can now solve the two-by-two linear system of equation (18) for improved values of 
the parameters \( \tilde{E} \) and \( a_0 \). Manipulating arrays is a bit tricky in a programming language such 
as Fortran or C, but in Mathematica one can simply define the matrix \( M \) in equation (19) as 
a list of lists. The column vector \( \mathbf{C}_{\text{old}} \) is a simple list. Mathematica also provides a built-in 
function to invert the matrix \( M \), so the evaluation of the right-hand side of equation (21) is 
easy.

In programming the iterative loop, we need to decide when the gaps are small enough to 
stop the iteration. Thus we defined a test function which returns a boolean \texttt{True} if \texttt{any} of the 
four gaps, \( \Delta g \) and \( \Delta f \) as well as their slopes \( \Delta g' \) and \( \Delta f' \), is greater than \( \delta \). The iterations 
will stop when the boolean becomes \texttt{False}.

For the starting parameters used above, \( \tilde{E} = 0.82 \) and \( a_0 = 0.2 \), we find that our 
program closes the gaps in four iterations. The final parameter values are \( \tilde{E} = 0.727102 \) and 
\( a_0 = 0.194709 \). That \( \tilde{E} \) corresponds, in more conventional units, to an energy of \( E = 0.306 \) 
GeV. The lower component \( f(x) \) has a peak value of about two-thirds that of \( g(x) \), showing

4 Mathematica is a software product of Wolfram Research, \url{http://www.wolfram.com}.
Figure 1. The normalized radial wavefunctions $\psi_a(x)$ (solid curves) and $-\psi_b(x)$ (dashed curves) for massless quarks in the GMSS linear potential for fitting $q\bar{q}$ mesons. (a) 1s ground state, (b) 2s excited state, (c) $2p_{\frac{1}{2}}$ excited state, (d) $2p_{\frac{3}{2}}$ excited state.

the importance of relativity in this case of massless quarks. Figure 1(a) shows the plots for $\psi_a(x) = g(x)/x$ and $-\psi_b(x) = -f(x)/x$. (We have plotted the $\psi$’s in figure 1(a) this way to compare with GMSS’s figure 2.) As one ought to expect for a ground state wavefunction, the upper component $\psi_a(x)$ has no nodes and the $p$-wave lower component $\psi_b(x)$ has one (at the origin).

2.6. Some excited states

The procedure outlined in the previous sub-section can be applied to calculate the energy eigenvalues and wavefunctions for excited states. One expects that the first excited state is the $2s_{\frac{1}{2}}$ state. This state also has $l = 0$, $l' = 1$ and $k = -1$, so the BCs at $x = \epsilon$ are the same as for the 1s case. The upper component wavefunction $g(x)$ should now have a new node, i.e. cross the $x$-axis somewhere between the origin and infinity. Thus, if it is desirable to have $g(x)$ start off from the origin going positive, one should choose the asymptotic normalization parameter $a_1$ to be negative.

In view of the asymptotic behavior here being similar to that of a simple harmonic oscillator, we might expect that the energy eigenvalue of this state is roughly twice that of the ground state. Choosing the parameters needed for the initial integrations to be

$$\tilde{E} = 2.1, \quad a_0 = 0.3, \quad a_1 = -4000.0,$$

we find that the iterative loop again converges in four iterations. The final parameters are $\tilde{E} = 1.91897$ (i.e. 0.809 GeV) and $a_0 = 0.378981$. Plots of $\psi_a(x)$ and $-\psi_b(x)$ are displayed in figure 1(b). For the $2s_{\frac{1}{2}}$ state, $\psi_a(x)$ has the expected one node and $\psi_b(x)$ has two.

Why are we counting nodes, anyway? Because a state with more nodes has more energy. Qualitatively, more nodes means more curvature, and that means a bigger contribution from $\nabla^2$, which in turn means a bigger kinetic energy.
Besides the 2s$^{1/2}$ state, there are also two nearby p-wave excited states. The 2p$^{3/2}$ state also has $j = l + 1/2$, but now with $l = 1$, $l' = 2$, and thus $k = -2$. The BCs near the origin are given by equations (13) and (14), but otherwise the coding is very similar to (basically, it can be copied from) the 1s$^{1/2}$ and 2s$^{1/2}$ cases. Starting this time with

$$\tilde{E} = 2.1, \quad a_0 = 3.0, \quad a_1 = -4000.0, \quad (24)$$

the gaps close in four iterations, with final parameters $\tilde{E} = 2.23003$ (i.e. 0.940 GeV) and $a_0 = 1.577 84$. The 2p$^{3/2}$ wavefunctions $\psi_a(x)$ and $-\psi_b(x)$ are shown in figure 1(d). In contrast to the 2s case, here both $\psi_a(x)$ and $\psi_b(x)$ have two nodes, reflecting a higher energy eigenvalue.

The other p-wave state, 2p$^{1/2}$, is qualitatively different. This is the first case for which $j = l - 1/2$, and $k$ is now a positive integer. In a sense, this switches the roles of $g(x)$ and $f(x)$. The boundary conditions for the outward integration when $j = l - 1/2$ are different from those of equation (13): 

$$f(\epsilon) = a_0 \epsilon^l, \quad g(\epsilon) = b_0 \epsilon^{l+1}. \quad (25)$$

Substituting $g(\epsilon)$ into the first ODE allows us to determine this $b_0$, so

$$g(\epsilon) = a_0 (\tilde{E} + V_s(\epsilon) + \tilde{m}) \epsilon^{l+1}/(2l + 1). \quad (26)$$

That is, if $a_0 > 0$, both $g(x)$ and $f(x)$ start out from the origin with positive slopes.

Starting for this 2p$^{1/2}$ case with initial parameters

$$\tilde{E} = 2.1, \quad a_0 = 3.0, \quad a_1 = -4000.0, \quad (27)$$

the iterative procedure converges on the fifth iteration, with final parameter values $\tilde{E} = 2.37846$ (i.e. 1.002 GeV) and $a_0 = 0.171483$. The 2p$^{1/2}$ $\psi$'s are plotted in figure 1(c). Here also both component wavefunctions have two nodes.

We note in passing that the higher spin state of this pair has the lower energy, contrary to the well-known case for the Coulomb potential. This is a common feature for nuclear states (even ground states) and reflects the presence of an effective scalar potential as found in many nuclear potential models [20].

The energy difference between the 2p$^{3/2}$ and 2p$^{1/2}$ states, 62 MeV, is due to a spin–orbit interaction. However, there is evidence in the baryon spectrum that the spin–orbit interaction is suppressed [21]. Page, Goldman, and Ginocchio (PGG) [22] claim this reflects a cancellation between a scalar potential $V_s$ and a vector potential, $V_v$, having the same linear slope at large distances. We will return to this point in section 4.

### 2.7. Solutions for massive quarks

The cases for the linear scalar potential $V_s(r)$ of equation (9) when the quarks are massive are computed straightforwardly using the program described above. For example, using masses appropriate for the $Q\bar{q}$ mesonic states, where $q$ stands for a massless non-strange quark ($u$ and $d$) and $Q$ for the massive strange ($s$), charmed ($c$), and bottom ($b$) quarks, we find the following eigenenergies:

$$m_u = m_d = 0.0 \text{ GeV}, \quad E_u = E_d = 0.306 \text{ GeV}, \quad (28)$$

$$m_s = 0.3445 \text{ GeV}, \quad E_s = 0.486 \text{ GeV}, \quad (29)$$

$$m_c = 1.803 \text{ GeV}, \quad E_c = 1.667 \text{ GeV}, \quad (30)$$

$$m_b = 5.298 \text{ GeV}, \quad E_b = 5.007 \text{ GeV}, \quad (31)$$
Solving the radial Dirac equations: a numerical odyssey

Figure 2. The upper (left panel) and lower (right panel) component radial wavefunctions, $\psi_a(x)$, for massless $u$ and massive $s, c$, and $b$ quarks.

by requiring a match to the appropriately weighted average of the lowest pseudoscalar and vector states [23]. Note that for the heaviest quarks the states are conventionally bound, $E_Q < m_Q$, and confinement need not be invoked to understand the stability of the state, in contrast to the situation for the light quarks.

Figure 2(a) compares the results for the $u, s, c$, and $b$ quarks for the upper components, $\psi_a(x)$, and figure 2(b) does the same for the lower components, $-\psi_b(x)$. Note that as the mass $m_q$ increases, the $Q\bar{q}$ system becomes more and more non-relativistic, i.e. the lower component wavefunction $\psi_b$ gets smaller, relative to the upper component $\psi_a$. Also, as $m_q$ gets larger, the wavefunctions are more and more concentrated near the origin.

3. Vector potential—hydrogen-like atoms

In contrast with the case of massless quarks, an electron bound in a Coulomb potential, as in the hydrogen atom, is at the opposite extreme, i.e. to a very good approximation a completely non-relativistic system. The binding energy of the ground state, $Ry = 13.6$ eV, is very small compared to the mass of the electron, $m_e = 0.511$ MeV. (In this section we will use MeV instead of GeV.) The Schrödinger equation for this problem predicts its energy levels basically correctly, missing only the fine-structure splitting, a spin–orbit effect about $10^{-4}$ times smaller than the binding of the $n = 2$ levels [24].

As noted in the introduction, the analytic solutions of the Dirac equation for the hydrogen atom were found long ago [8], and these solutions do give the fine-structure splitting as a relativistic effect. Nonetheless, it is an interesting numerical exercise to see if the program for the linear scalar potential outlined above (or something like it) can be applied to the hydrogen atom case, and with enough accuracy. We want to solve equations (3) and (4) with $V_v(r) = -Z\alpha/r$. We will initially set $Z = 1$, as these solutions are somewhat more delicate. Heavier, hydrogen-like atoms with $Z > 1$ will be treated later.

Converting to dimensionless equations by dividing through by $m_e$ (instead of $\kappa$ as before),

$$
\frac{g'(x)}{x} + \frac{k}{x} g(x) - \left(1 + \tilde{E} + \frac{Z\alpha}{x}\right) f(x) = 0,
$$

(32) $$
\frac{f'(x)}{x} - \frac{k}{x} f(x) - \left(1 - \tilde{E} - \frac{Z\alpha}{x}\right) g(x) = 0,
$$

(33)

where now $x = m_e r$ and $\tilde{E} = E/m_e$. The energy $E$ is better written as $E = m_e - B$, where $B$ is the binding energy of the level of interest (which has principal quantum number $n$ and
orbital angular momentum quantum number \( l \). Note that, because of the smallness of the binding energies, \( E \) is only slightly less than \( m_e \). Thus \( \tilde{E} \) is less than (but very close to) 1, which is why we factored out a minus sign from the third term in equation (33), relative to that in equation (4). We will use the binding energy \( \tilde{B} = B / m_e \) instead of \( \tilde{E} \) as one of the two parameters to be determined in the matching of the inwards and outwards integrations.

3.1. Boundary conditions for inward integration

For asymptotically large \( x \) the ODEs reduce to

\[
g'(x) = (1 + \tilde{E}) f(x), \quad f'(x) = (1 - \tilde{E}) g(x).
\]  

The solutions of these asymptotic equations at \( x = x_{\text{max}} \) are

\[
g(x_{\text{max}}) = a_1 e^{-\mu x_{\text{max}}}, \quad f(x_{\text{max}}) = -a_1 \left( \frac{1 - \tilde{E}}{1 + \tilde{E}} \right)^{1/2} e^{-\mu x_{\text{max}}},
\]

which will be used as the BCs (starting values) for the inwards integration with \( a_1 \) as another parameter to be determined later by the normalization condition. The coefficient in the exponential decay is small:

\[
\mu = \sqrt{1 - \tilde{E}^2} = \sqrt{2 \tilde{B} - \tilde{B}^2} \approx \sqrt{2 \tilde{B}} \approx 0.00730 \approx \alpha.
\]

The Coulomb wavefunctions are quite long-ranged, and are all the more so, the smaller the binding energy. Equation (35) also shows that, asymptotically, \( f(x) \) is very much smaller than \( g(x) \), reflecting the non-relativistic nature of the hydrogen atom.

3.2. Boundary conditions for outward integration

As before, to avoid the singularity at \( x = 0 \), we integrate outwards from \( x = \epsilon \), where \( \epsilon \) takes an appropriately small value. In this case, one might even consider taking \( \epsilon \) as the radius of the nucleus providing the Coulomb potential (but see section 3.6 for a better approach). For the boundary conditions for integrating outwards from \( x = \epsilon \) when \( j = l + \frac{1}{2} \), i.e. \( l' = l + 1 \) and \( k = -(l + 1) \), we can again assume

\[
g(\epsilon) = a_0 \epsilon^{l+1}, \quad f(\epsilon) = b_0 \epsilon^{l+2}.
\]

Substituting these in the second ODE, we can solve for \( b_0 \), finding

\[
f(\epsilon) = -a_0 \frac{Z \alpha}{2l + 3} \epsilon^{l+1} + \mathcal{O}(\epsilon^{l+2}).
\]

Noticably different is the lowering of the power behavior of \( f(x) \) due to the \( 1/x \) behavior of the potential. Note that, because of the factor of \( \alpha \approx 1/137 \), the magnitude of \( f(x) \) is much smaller than that of \( g(x) \), also here near the origin.

For the \( j = l - \frac{1}{2} \) case, i.e. \( l' = l - 1 \) and \( k = l \), we let \( f(x) \) determine the nature of the boundary conditions (as in equation (25)), i.e.

\[
f(\epsilon) = a_0 \epsilon^l, \quad g(\epsilon) = b_0 \epsilon^{l+1}.
\]

Substituting these in the first ODE, we again solve for \( b_0 \) and find

\[
g(\epsilon) = a_0 \frac{Z \alpha}{2l + 1} \epsilon^l + \mathcal{O}(\epsilon^{l+1}).
\]

Again, for this case, \( g(x) \) and \( f(x) \) start off with the same slope, as in equation (26). And again, there is a lower power behavior of \( g(x) \) due to the \( 1/x \) in the potential, as in equation (38).
3.3. The 1s ground state

The natural unit of length for the hydrogen atom problem is the Bohr radius, \( a_B = \frac{h^2}{m_e \alpha} = 0.529 \ \text{Å} = 0.529 \times 10^2 \ \text{fm} \). Thus a natural scale for \( x \) is in units of the dimensionless Bohr radius, \( x_B = a_B m_e / \hbar c \), which is \( 1/\alpha \) in \( \hbar = c = 1 \) units.

In view of the slow exponential decay in equation (35) (i.e. the smallness of \( \mu \)), for our calculations we chose \( x_{\text{max}} = 7x_B \), along with \( x_{\text{match}} = 0.5x_B \). Fixing \( a_1 = 10 \) (recall, it is arbitrary before normalization) and the starting values of the parameters to be tuned, \( B = 12 \times 10^{-6} \ \text{MeV} \) (less than the expected 13.6 eV) and \( a_0 = 0.015 \), we found the 2 × 2 matrix of partial derivatives to be

\[
M = \begin{bmatrix}
-108.877 & 107.348 \\
-320.810 & 107.494
\end{bmatrix}.
\] (41)

This shows a big sensitivity of the hydrogen atom wavefunctions to the choice of binding energy. Nonetheless, the iterative process of refining \( \bar{B} \) and \( a_0 \) proceeds nicely to a solution with \( B = 13.6059 \ \text{eV} \) and \( a_0 = 0.0104306 \). As expected, \( f(x) \) is smaller than \( g(x) \) by a factor approximately equal to \( \alpha \).

We do not plot the corresponding \( \psi_a(x) \) and \( \psi_b(x) \) radial wavefunctions as they are already known analytically. They are both purely decaying exponentials proportional to \( e^{-\mu x} \). This is not surprising for the upper component, \( \psi_a(x) \), since that is just what the Schrödinger equation predicts for the hydrogen atom ground state. It may not be so obvious, however, that the lower component, \( \psi_b(x) \), has the same form. That it has no node at the origin (in contrast to figure 1(a)) is a consequence of the \( Z\alpha/x \) potential changing the presumed \( x^4 \)-dependence of \( f(x) \) near the origin to an \( x^{4+1} \)-dependence.

3.4. Some excited states

The \( n = 2 \) excited states of hydrogen are done in a very similar manner to the 1s ground state calculation. The major difference is that, from the Balmer formula [24], we expect the binding energy \( B \) for these states to be about \( 1/n^2 = 1/4 \) times the ground state binding energy. Also, based on equation (36), we expect the wavefunctions will extend outwards about twice as far, so, for our calculations we chose \( x_{\text{max}} = 16a_B \) instead of \( 7a_B \).

For the 2s\(^{1}\) state, starting with initial parameters \( B = 3.2 \ \text{eV} \) (which we expected to be low), \( a_0 = 0.0007 \), and (fixed) \( a_1 = -10.0 \), the program converges in four iterations to give final \( B = 3.40085 \ \text{eV} \) and \( a_0 = 0.00071905 \). As expected on general grounds, unlike the ground state, \( \psi_a(x) \) and \( \psi_b(x) \) each have one node.

For the 2p\(_{\frac{1}{2}}\) state, starting with initial parameters \( B = 3.2 \ \text{eV} \) (also low), \( a_0 = 0.0004 \), and (fixed) \( a_1 = 100.0 \), the program converged in four iterations to give final \( B = 3.40086 \ \text{eV} \) and \( a_0 = 0.000393546 \). In fact, the 2s\(_{\frac{1}{2}}\) and 2p\(_{\frac{1}{2}}\) levels are degenerate [24] as a result of an \( O(4) \) symmetry hiding in the equations. The small difference in the converged \( B \)'s we find here is within the numerical precision of our Mathematica program. However, the 2s\(_{\frac{1}{2}}\) and 2p\(_{\frac{1}{2}}\) wave functions are very different. Here also, \( \psi_a \) and \( \psi_b \) each have one node.

For the 2p\(_{\frac{3}{2}}\) state, starting this time with initial parameters \( B = 3.2 \ \text{eV} \), \( a_0 = 0.000015 \), and \( a_1 = 100.0 \), the program converged in four iterations to give final \( B = 3.40144 \ \text{eV} \) and \( a_0 = 0.0000141876 \). The difference we find between the \( j = \frac{1}{2} \) and \( j = \frac{3}{2} \) energy levels, 0.58 meV, is the spin–orbit splitting, an intrinsically relativistic effect. The analytic value of this splitting is 0.453 meV [9, 24] and the difference here is again due to the limited machine precision used in our Mathematica program. For the 2p\(_{\frac{3}{2}}\) state also, \( \psi_a \) and \( \psi_b \) each have one node. The \( \psi_a(x) \)'s for the 2p\(_{\frac{1}{2}}\) and 2p\(_{\frac{3}{2}}\) states are very similar, but the lower component
Table 1. Numerical results for the 1s ground state binding energies $B$ for hydrogen-like atoms with nuclear charge $Z$. The second column displays the non-relativistic eigenenergy and the third the result of the numerical integrations. For comparison, the analytic eigenenergies from equation (42) are given in the fourth column. Energies here are in keV.

| $Z$ | $Z^2$ Ry | $B$ (numerical) | $B$ (analytic) |
|-----|---------|----------------|--------------|
| 10  | 1.360   | 1.3624         | 1.3624       |
| 100 | 136.0   | 161.6          | 161.6        |
| 136 | 251.546 | 433.8          | 448.3        |

ψ(x)s are quite different, reflecting the fact that the lower components and the difference are both entirely due to relativity.

3.5. Hydrogen-like atoms with $Z > 1$

There are no big surprises here, as table 1 shows. From equation (36), the exponential fall-off of the wave functions is faster, as $\mu \sim \sqrt{B} \sim Z$, so we adjust the values of $x_{\text{match}}$ and $x_{\text{max}}$ accordingly by dividing the hydrogenic values by $Z$. Running the code for the 1s ground state for $V_\nu(r) = 2a_0/r$ works well for $Z \leq 100$. As $Z$ grows larger, the relativistic corrections to the energy become increasingly important.

As $Z$ approaches $1/\alpha = 137.036$, however, the numerical solutions become inaccurate and, eventually, unstable. This can be seen in the rapid increase in the value of the parameter $a_0$. The value of $Z = 1/\alpha$ is where the Klein paradox [25] comes into play, since the analytic result for this state is [12]

$$E(1s) = m(1 - Z^2\alpha^2)^{1/2}$$

and the eigenenergy becomes complex beyond that point. The resolution of this paradox is, as has been well-known for a long time, the creation of electron–positron pairs from the Dirac–Fermi sea when $Z > 1/\alpha$ [26].

3.6. Muonic atoms

When a negatively-charged muon slows down in matter, sometimes it is captured by the Coulomb potential of an atomic nucleus before it decays. If so, it then quickly cascades down through its hydrogen-like levels to the 1s ground state, emitting x-rays along the way. From there it then either decays or can be be captured by the nucleus, both of which are weak interaction processes. The capture process depends sensitively upon the value of the 1s wavefunction at the origin.

The numerical coding for muonic atom ground states for values of $Z$ of interest goes pretty much as for the electronic atom case for such a $Z$. The differences come from replacing the mass of the electron (0.511 MeV) with that of the muon (105.66 MeV). This must be done for the ‘muonic Bohr radius’, $a_{B\mu} = a_B(m_\mu/m_e) = 255.8$ fm, and consequently in the choices of $x_{\text{match}}$ and $x_{\text{max}}$ which are now proportional to $a_{B\mu}/Z$. Also, the non-relativistic binding energy $B$ is now $Z^2(m_\mu/m_e)$Ry.

Calculating, as above, the ground state for muonic $^{40}$Ca ($Z = 20$), starting with $B = 1.1$ MeV and $a_0 = 0.1$, the iterations converge to final values of $B = 1.13136$ MeV and $a_0 = 0.239462$. However, this initial calculation used a value of $\epsilon = 10^{-4}$ (dimensionless), or a cut-off at the origin of 0.000 187 fm, rather smaller than the size of the $^{40}$Ca nucleus [27],

$$R_{\text{Ca}} \approx r_0A^{1/3} = 1.2 \times 40^{1/3} = 4.1 \text{ fm.}$$

(43)
The nuclear charge is not a point charge, of course, but has a charge density distribution, \( \rho(r) \), which is spread out over the volume of the nuclear sphere. In fact, one of the major reasons for having studied muonic atoms in the past, through the last \( 2p \rightarrow 1s \) x-ray, is for determining this charge density [11].

As a simple example, suppose the nucleus is a sphere of radius \( R \) and charge \( eZ \) with a charge density \( \rho \) which is constant out to its surface and zero for \( r > R \). We need to find the potential seen by the negative muon for \( r < R \). If it were sitting exactly at the center of the nucleus, it would (by symmetry) feel no force. That is, there is no term in the potential linear in \( r \), as the force at the origin is \( \frac{dV_{\text{nuc}}}{dr} \big|_{r=0} = 0 \). This suggests that we can take \( V_{\text{nuc}}(r) = A + Br^2 \). The coefficient \( B \) can be fixed from the requirement that the slopes \( \frac{dV_{\text{nuc}}}{dr} \) and \( \frac{dV_{\text{Coul}}}{dr} \) match at \( r = R \). The coefficient \( A \) in turn is fixed by the requirement of continuity at \( r = R \). Thus a potential reasonably appropriate for such a muonic atom is

\[
V_v(r) = \begin{cases} 
\frac{\alpha Z(r^2 - 3R^2)}{2R^3} & \text{for } r \leq R, \\
-\frac{\alpha Z}{r} & \text{for } r > R.
\end{cases}
\]

(44)

This potential no longer has the \( 1/r \) singularity at the origin, so the BCs for the outgoing integration for the \( 1s \) state are more like those in equations (13) and (14) for \( l = 0 \):

\[
g(\epsilon) = a_0 \epsilon, \quad \text{and} \quad f(\epsilon) = a_0 (1 - \tilde{E}) \epsilon^2 / 3,
\]

(45)

bearing in mind that we here are making the equations dimensionless by setting \( m_\mu = 1 \) and that the eigenenergy of the bound state is less than \( m_\mu \). Unlike the pure Coulomb case, here \( f(r) \) will have curvature near \( r = 0 \), where it will vanish.

Running the numerical integrations with potential \( V_v(r) \) for \(^{40}\text{Ca} \) gives a binding energy \( B = 1.0706 \) keV, some 60 keV smaller than the pure Coulomb result for this nucleus. Figure 3 displays the difference between the \( \psi_a(x) \)'s and \( \psi_b(x) \)'s for the case with this nuclear charge distribution and the pure Coulomb case.

It is interesting that, very recently [28], a laser-spectroscopic experiment on muonic hydrogen (a bound state of a proton and a negative muon) has measured the charge radius of...
the proton with unprecedented precision: \( r_p = 0.841 \ 84(67) \) fm. That experiment’s value is in disagreement with the long-accepted values obtained by electron scattering and spectroscopy of ordinary hydrogen by five standard deviations. If this discrepancy survives the test of time, then the accepted value of the Rydberg constant, \( R_y \), will have to be significantly changed. Or, perhaps even more drastically, reconsideration of the fundamentals of the theory of quantum electrodynamics may be necessary, such as a new short-range interaction.

4. Combining the two potentials

We now consider the solution of the radial Dirac equations, equations (7) and (8), when both potentials, the Lorentz scalar \( V_s(x) \) and Lorentz vector \( V_v(x) \), come into play. We will assume both potentials \( V_s(x) \) and \( V_v(x) \) are linearly confining and have the same slopes (i.e. have the same string tension \( \kappa \)). We also assume that \( V_v(x) \) has a color-Coulomb attraction near the origin. The two potentials are displaced from each other with \( V_s(x) \) lying above \( V_v(x) \), as in figure 4:

\[
V_s(x) = x + x_s, \quad V_v(x) = -\alpha_s/x + x - x_v, \quad (46)
\]

or, more appropriately, the smeared version of \( V_v(x) \) similar to that described above in section 3.6. Here \( x_s \) and \( x_v \) are parameters to be adjusted to get some desired eigenenergy. They give rise to a separation between the two asymptotic potentials of \( x_d = x_s + x_v \).

The reason for giving the potentials the same asymptotic slopes is to check that the spin–orbit interaction disappears as claimed in [22]. In doing so, we have changed the earlier offset of \(-x_0\) in \( V_s \) to \(+x_s\) since, in GMSS (where only a Lorentz scalar potential was used), the negative offset \(-x_0\) represented a reasonable approximation the one-gluon-exchange attraction, roughly an average of the two potentials as shown in the figure.
Now, however, the BC’s at large distances are changed from those in equation (16), since, in the equation for $g(x)$, equation (7), the difference of the dimensionless $V_v(x)$ and $V_a(x) \rightarrow x$ has its $x$-dependence cancel. We need to solve the large-$x$ equations

$$g'(x) - (\tilde{E} + x_d + \tilde{m}) f(x) = 0, \quad f'(x) - 2x g(x) = 0,$$

from which

$$g''(x) - 2(\tilde{E} + x_d + \tilde{m}) x g(x) = 0.$$  \hspace{1cm} (48)

This is a minor modification of the differential equation for the Airy functions [30]. Since we require decaying solutions at our starting point $x_{\text{max}}$ for the inwards integrations, we discard the runaway $Bi$ solution for $g(x)$. The BC’s at large $x = x_{\text{max}}$ are then

$$g(x_{\text{max}}) = a_1 Ai[2^{1/3}(\tilde{E} + x_d + \tilde{m})^{1/3} x_{\text{max}}],$$

$$f(x_{\text{max}}) = a_1 \left[ \frac{2}{(\tilde{E} + x_d + \tilde{m})^{1/3}} \right]^{1/3} Ai'[2^{1/3}(\tilde{E} + x_d + \tilde{m})^{1/3} x_{\text{max}}].$$  \hspace{1cm} (49)

Despite appearances, $g(x_{\text{max}})$ and $f(x_{\text{max}})$ still start off with the opposite slopes, as in equation (16), since, for $t > 0$, $Ai(t) > 0$ and $Ai'(t) < 0$.

For calculations, we simplified the displacement between the two potentials by setting $x_0 = 0$, giving us one less parameter to worry about. The first wavefunction we want to compute is the ground state for the massless quark case, $m_q = 0$, starting out with $\alpha_s = 0$ and then adjusting both $x_d = x_s$ and $\alpha_s$ until we get the desired eigenenergy, noted above in equation (28).

It turns out that to do so is trickier than in the $V_v$ only case, presumably because of the cancellation between $V_v(x)$ and $V_a(x)$ in the differential equation for $g'(x)$. Our first iterative search with $\alpha_s = 0$ found a highly excited state with $\tilde{E} = 7.975$, not the desired 0.7263, for which $\psi_d(x)$ had six nodes! After some hand-searching on $x_s$, we found we could get a ground state solution, i.e. a $\psi_d(x)$ with no nodes, looking like the $b$-quark $\psi_d(x)$ of figure 2(a). This solution started with $x_s = 4.0$ (very large!) and converged, in six iterations, to $\tilde{E} = 5.735$ (about eight times too large).

From this $\alpha_s = 0$ solution we were able to march down, in small steps in $x_s$ (still with $\alpha_s = 0$, to $x_s = 0.20$, with the energy now smaller, $\tilde{E} = 2.779$, but still a factor of 4 too large. (For smaller values of $x_s$ the iterative procedure would not converge, with the matrix of equation (19) becoming singular.) The wavefunction $\psi_d(x)$ for this solution was broader than that for the $x_s = 4.0$ case, and the $\psi_d(x)$ was relatively larger in comparison with $\psi_d$.

At this point we began marching the value of $\alpha_s$ in small steps up from zero, i.e. we began turning on the Coulomb attraction. As expected this attraction lowers the energy, and we were able to achieve the desired massless quark eigenenergy of 0.306 GeV with the following values:

$$x_s = 0.20, \quad \alpha_s = 1.103, \quad \tilde{E} = 0.7263.$$  \hspace{1cm} (50)

The long marches did achieve the factor of 8 reduction in the ground state eigenenergy. Because of the Coulomb attraction, $\psi_d(x)$ begins to resemble the hydrogen-atom ground state $\psi_d(x)$, and it is much narrower than that shown in figure 1(a).

The ground state solution says nothing about the PGG claim that, for $V_v(x)$ and $V_a(x)$ having equal slopes, the spin–orbit interaction vanishes. To check this we need to find, at a minimum, the eigenenergies of the $2p_{\frac{1}{2}}$ and $2p_{\frac{3}{2}}$ excited states. For the same values of $x_s$ and $\alpha_s$ as in equation (50) and after some searching for good starting values for the iterative procedure, we obtained the three $n = 2$ wavefunctions which are narrower and more hydrogen-like than in the $V_v$ only case (see figure 1). The eigenenergies, in GeV, for these states are

$$E_{2s} = 1.020, \quad E_{2p_{\frac{1}{2}}} = 0.674, \quad E_{2p_{\frac{3}{2}}} = 1.008.$$  \hspace{1cm} (51)
The $2p^\frac{1}{2}$ state is nearly degenerate with the $2s$ state, some 200 MeV higher than in section 2.6, but this degeneracy is probably accidental. There is, however, a huge spin–orbit splitting between the $2p^\frac{1}{2}$ and $2p^\frac{3}{2}$ states, not what is expected from the claim made by PGG [22].

This difference, of course, is due entirely to the presence of the Coulomb attraction term in $V_v(x)$. If we set $\alpha_s = 0$, then (again for $x_s = 0$) we find the following $n = 2$ eigenenergies (in GeV):

$$E_{2s} = 1.757, \quad E_{2p^\frac{1}{2}} = 1.523, \quad E_{2p^\frac{3}{2}} = 1.523. \quad (52)$$

The wavefunctions in this case are similar to above but are, of course, somewhat broader and less peaked near the origin. These results show the expected PGG symmetry (zero spin–orbit splitting). Note, incidentally, that the $2s$ state is higher in energy than the $2p$ states, as in the experimental charmonium spectrum [23]. Clearly, having a significant Coulomb contribution in $V_v(x)$ will destroy the PGG symmetry.

5. Summary

In this paper we have discussed, pedagogically, three increasingly more sensitive cases for solving the radial Dirac equations numerically.

1. A Lorentz scalar potential, $V_s$, which is linearly confining for quarks. The case of massless quarks is necessarily relativistic. As the mass of the quark increases, the wavefunction solutions become more and more non-relativistic.

2. A Lorentz vector potential, $V_v$, whose time-like component is a Coulomb potential. We first treated, numerically, the hydrogen atom, which is basically a non-relativistic problem. We do, however, obtain the relativistic spin–orbit splitting between the $2p^\frac{1}{2}$ and $2p^\frac{3}{2}$ states (at the edge of our machine precision).

3. The combination of scalar and vector potentials, aiming at a relativistic quark model of mesons. Of particular interest is when we do (and do not) get a relativistic spin–orbit splitting.

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