

Salpeter equation in position space: Numerical solution for arbitrary confining potentials

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We present and test two new methods for the numerical solution of the relativistic wave equation

$$[(-\nabla^2 + m_1^2)^{1/2} + (-\nabla^2 + m_2^2)^{1/2} + V(r) - M]\psi(\vec{r}) = 0,$$

which appears in the theory of relativistic quark-antiquark bound states. Our methods work directly in position space, and hence have the desirable features that we can vary the potential $V(r)$ locally in fitting the $q\bar{q}$ mass spectrum, and can easily build in the expected behavior of V for $r \rightarrow 0, \infty$. Our first method converts the nonlocal square-root operators to mildly singular integral operators involving hyperbolic Bessel functions. The resulting integral equation can be solved numerically by matrix techniques. Our second method approximates the square-root operators directly by finite matrices. Both methods converge rapidly with increasing matrix size (the square-root matrix method more rapidly) and can be used in fast-fitting routines. We present some tests for oscillator and Coulomb interactions, and for the realistic Coulomb-plus-linear potential used in $q\bar{q}$ phenomenology.

I. INTRODUCTION

The discovery of the ψ and Υ resonances and their interpretation as bound quark-antiquark states ($c\bar{c}$ and $b\bar{b}$, respectively) has prompted an interest in describing such systems in terms of an effective local interaction potential. Because of the large masses of the charmed and bottom quarks, a description based on the nonrelativistic Schrödinger equation gives a plausible first approximation to the true relativistic problem, and good fits to the $c\bar{c}$ and $b\bar{b}$ spectra have been obtained with a variety of models.¹ However, relativistic effects are already important for charmonium. While some progress can be made by calculating relativistic corrections to the Schrödinger spectrum perturbatively,² relativistic effects on the wave functions are hard to treat this way.³ The resulting uncertainties affect the calculation of physically interesting quantities. Leptonic and hadronic decay widths, for example, depend on the square of the $q\bar{q}$ wave function for small quark separations where relativistic effects can be large.³ The $E1$ transition rates are also quite sensitive to small changes in the wave function.⁴ It is clear also that light-quark systems can be treated adequately only by including relativistic kinematics from the beginning.^{5,6}

The correct quantum-field-theoretic description of relativistic bound states is given by the Bethe-Salpeter-Schwinger equation.⁷ We consider here a standard approximation to this equation obtained by replacing the interaction kernel by an instantaneous local potential, and by neglecting spin and the coupling of the "large-large" and "small-small" components of the wave function. This leads to the spatial wave equation

$$[(-\nabla^2 + m_1^2)^{1/2} + (-\nabla^2 + m_2^2)^{1/2} + V(r) - M]\psi(\vec{r}) = 0, \quad (1)$$

where the kinetic terms involving the operation $(-\nabla^2 + m^2)^{1/2}$ are nonlocal and are defined in terms of their Fourier transforms. This spinless Salpeter-type equation retains the relativistic kinematics and is suitable for describing the spin-averaged spectrum of two bound fermions of masses m_1 and m_2 and total energy M .

A basic problem in the use of Eq. (1) to describe $q\bar{q}$ systems is the fact that the (effective) potential $V(r)$ is not completely known. Its short-distance behavior is determined by QCD to be approximately Coulombic, $V(r) \sim -4\alpha_s(r)/3r$, with $\alpha_s(r)$ a logarithmically varying running coupling. The long-distance behavior inferred from lattice gauge theories or the string model is linear, $V(r) \sim Br$, with B related to the string tension. While a combined Coulomb-plus-linear potential gives reasonable fits to the data,¹ the $q\bar{q}$ states are in fact sensitive to the precise form of V in the joining region, and this must be determined empirically by adjusting $V(r)$ to fit the observed spectrum. Other quantities such as decay and transition rates can then be used to test the model.

Unfortunately, neither of the two techniques used in the past for solving Eq. (1) numerically is well adapted for efficient variation of the potential. The first is to Fourier transform the equation and work in momentum space.⁵ The kinetic-energy terms in Eq. (1) are then diagonal, and the equation can be solved as an integral equation using standard matrix techniques. However, the transformed potential $\tilde{V}(p)$ appears nonlocally in momentum space, which lessens our intuition on how it should be varied. In

addition, $\tilde{V}(p)$ must either be specified analytically in terms of a few parameters, or the entire (large) potential matrix must be recalculated at each step in the fitting procedure. The second method⁶ is to expand the wave functions in some complete set of basis states for which the kinetic terms in Eq. (1) are simple (e.g., harmonic-oscillator or trigonometric functions), compute the overlap integrals of the potential, and solve the resulting eigenvalue problem for the energies and expansion coefficients. Because the overlap integrals have to be calculated, this method again requires either that the form of the potential be given analytically, or that large matrices be varied. With

$$[M_n - V(r_q)]u_{nl}(r) = \frac{2}{\pi} \int_0^\infty dr' G_l(m_q r, m_q r') \left[-\frac{d^2}{dr'^2} + \frac{l(l+1)}{r'^2} + m_q^2 \right] u_{nl}(r'), \quad (2)$$

where

$$\psi_{nlm}(\vec{r}) = (1/r)u_{nl}(r)Y_{lm}(\hat{r}),$$

and $G_l(x, x')$ is an expression involving hyperbolic Bessel functions. For $l=0$,

$$G_0(x, x') = K_0(|x - x'|) - K_0(x + x'). \quad (3)$$

To solve this equation numerically for confining potentials, we map x onto a finite interval, approximate the second derivative by finite differences and the integral by a weighted sum, and solve the resulting matrix eigenvalue problem. This method is quite flexible and allows us to build in known information about the behavior of $u_{nl}(x)$ for $x \rightarrow 0$, but requires care in the construction of the integration coefficients because of the logarithmic divergence of $G(x, x')$ for $x \rightarrow x'$.

In our second method for solving Eq. (1), we construct a symmetric parity-conserving matrix \hat{D} representing the positive operator

$$D = \left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + m^2 \right]. \quad (4)$$

Using the eigenvalues and eigenvectors of this matrix, we then construct a matrix \hat{A} such that $\hat{A}^2 = \hat{D}$. Equation (1) can be written formally as

$$[M_n - V(r)]u_{nl}(x) = 2 \left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + m_q^2 \right]^{1/2} u_{n,l}(x). \quad (5)$$

We find that replacing the square-root operator by the matrix \hat{A} yields essentially the same results as obtained with the integral version of the operator described above. This method has the advantage that one less numerical approximation is required than in the integral scheme (since no integrals appear) so the convergence with increasing matrix size is faster. It is also easier to implement for arbitrary angular momenta.

We first review briefly in Sec. II solutions of Eq. (1) found previously for the harmonic-oscillator and pure Coulomb potentials which will serve as checks on the numerical methods employed here. In Sec. III we discuss

either method it is difficult to apply standard fitting techniques to adjust the potential.

In this paper, we describe two new methods for solving Eq. (1). These methods work in position space so that the potential remains local. Furthermore, we solve directly for the wave functions, and avoid any expansion in basis states. As a result, the potential can be varied easily. The kinetic terms, however, remain nonlocal.

In our first method, we convert Eq. (1) to an integral equation (we consider here the equal-mass case $m_1 = m_2 \equiv m_q$)

the position-space formulation of the problem. We derive the integral equation in Sec. III A and the square-root method in Sec. III B, and present a number of test results in Sec. III C. We conclude with some remarks on future applications in Sec. III D. In the Appendix, we give a new derivation of the behavior of $u_{nl}(r)$ for $r \rightarrow 0$ when the potential has a Coulomb singularity at short distances.

II. OSCILLATOR AND COULOMB POTENTIALS

It will be useful to have solutions of Eq. (1) obtained by independent means to serve as checks on the numerical methods we will employ. We will use the Salpeter equation with the oscillator potential $V(r) = \frac{1}{2}r^2$, and the pure Coulomb potential $V(r) = -\alpha/r$. The oscillator problem can be converted to Schrödinger form and solved by standard numerical techniques.³ The S -wave Coulomb problem has been solved analytically.⁸ Although the pure Coulomb potential is not confining, our methods generate many bound states before entering the continuum, so this check is useful. Also, the singular nature of the Coulomb potential leads to nonanalytic behavior of the Salpeter wave function at the origin, and we will want to take this behavior into account when calculating solutions with more interesting QCD and phenomenologically motivated potentials.

For an oscillator interaction, the Salpeter equation may be written as

$$[2(p^2 + m_q^2)^{1/2} + \frac{1}{2}r^2 - M]\psi(\vec{r}) = 0, \quad (6)$$

where we have expressed p , m_q , M , and r^{-1} in units of $k^{1/3}$, with k the spring constant of the oscillator. If we convert Eq. (6) from position to momentum space and use the substitution $r^2 \rightarrow -\nabla_p^2$, we obtain the Schrödinger-type equation

$$[-\frac{1}{2}\nabla_p^2 + 2(p^2 + m_q^2)^{1/2} - M]\tilde{\psi}(\vec{p}) = 0 \quad (7)$$

considered in Ref. 3. The momentum-space wave functions are of the form

$$\tilde{\psi}_{nlm}(\vec{p}) = \phi_{nl}(p)Y_{lm}(\hat{p}), \quad (8)$$

with normalization

$$\frac{1}{(2\pi)^3} \int_0^\infty |\phi_{nl}(p)|^2 p^2 dp = 1. \quad (9)$$

The radial wave functions $R_{n,l}(r)$ vary as r^l near the origin, and the functions $r^{-l}R_{n,l}(r)$ have the limiting values

$$(r^{-l}R_{n,l})(0) = \frac{1}{2\pi^2(2l+1)!!} \int_0^\infty \phi_{n,l}(p) p^{l+2} dp. \quad (10)$$

Equation (7) can be solved numerically using standard methods.⁹ The eigenvalues for general n, l and the value of $(r^{-l}R_{n,l})(0)$ give simple checks on the accuracy of our position-space integration of (the equivalent) Eq. (6). We could also Fourier transform $\tilde{\psi}(\vec{p})$ to obtain the complete position-space wave function, but have not found this to be necessary.

The Coulomb problem is more complicated. The S -wave Salpeter equation for the static Coulomb potential,

$$\left[2(-\nabla^2 + m_q^2)^{1/2} - \frac{\alpha}{r} - M \right] R_0(r) = 0, \quad (11)$$

was investigated analytically in Ref. 8. The exact bound-state eigenvalues are given by⁸

$$M_{n0} = \frac{2m_q}{(1 + \alpha^2/4n^2)^{1/2}}, \quad n = 1, 2, \dots \quad (12)$$

The S -state radial wave function $R_0(r)$ was furthermore shown to diverge for $r \rightarrow 0$ as $(mr)^{-\nu_0}$, where ν_0 is given exactly by

$$1 = \nu_0 + \frac{\alpha}{2} \cot \frac{\pi\nu_0}{2}. \quad (13)$$

Expanding the cotangent for $\pi\nu_0/2$ small, one obtains

$$\nu_0 \simeq \frac{\alpha}{\pi} + \frac{\alpha^2}{\pi^2} + \left[2 - \frac{\pi^2}{12} \right] \frac{\alpha^3}{\pi^3} + O\left[\frac{\alpha^4}{\pi^4} \right]. \quad (14)$$

The divergence is weak for the values of $\alpha = \frac{4}{3}\alpha_s$ of interest for $q\bar{q}$ states. For example, if we take $\alpha = 0.25$, a value appropriate for charmonium, $\nu_0 \simeq 0.086583$. This mild divergence is a consequence of our static Coulomb approximation. It is not present in the complete Bethe-Salpeter-Schwinger wave function because of radiative and retardation effects which modify the Coulomb singularity and the wave function at distances $r \lesssim m_q^{-1}$.

The analysis of the singularity of $R_{n,l}(r)$ for $r \rightarrow 0$ was extended recently to general l by Castorina, Cea, Nardulli, and Paiano.¹⁰ We give an alternative derivation of their result in the Appendix, and show that the function $r^{-l}R_l(r)$ diverges as $r^{-\nu_l}$ for $r \rightarrow 0$, with ν_l that solution of the equation

$$2\nu_l \frac{\Gamma(l - \frac{1}{2}\nu_l + \frac{3}{2})\Gamma(\frac{1}{2}\nu_l + \frac{1}{2})}{\Gamma(l - \frac{1}{2}\nu_l + 1)\Gamma(\frac{1}{2}\nu_l + 1)} = \alpha \quad (15)$$

which vanishes for $\alpha \rightarrow 0$,

$$\begin{aligned} \nu_l &= \frac{\alpha}{2\pi} \frac{\sqrt{\pi} l!}{\Gamma(l + \frac{3}{2})} + O(\alpha^2) \\ &\sim \frac{\alpha}{2\sqrt{\pi} l}, \quad l \gg 1. \end{aligned} \quad (16)$$

III. POSITION-SPACE FORMULATION

A. The integral equation

Because of the appearance of the nonlocal kinetic operator $(-\nabla^2 + m^2)^{1/2}$, it is natural to seek an integral form of Eq. (1). Many equivalent forms of this equation may be found. We choose one which avoids direct encounters with δ -function contributions and principal-value or finite-part integrals.

The kinetic operator may be defined in terms of its Fourier transform,

$$\begin{aligned} &(-\nabla^2 + m^2)^{1/2} \psi(\vec{r}) \\ &= \int d^3r' \int \frac{d^3p}{(2\pi)^3} e^{i\vec{p} \cdot (\vec{r} - \vec{r}')} (p^2 + m^2)^{1/2} \psi(\vec{r}'). \end{aligned} \quad (17)$$

We rewrite this equation by extracting the operator $(-\nabla^2 + m^2)$ from the right-hand side of Eq. (17) and performing the integration over the momenta, and find that

$$\begin{aligned} &(-\nabla^2 + m^2)^{1/2} \psi(\vec{r}) \\ &= \frac{m}{2\pi^2} (-\nabla_r^2 + m_q^2) \int d^3r' \frac{K_1(m|\vec{r} - \vec{r}'|)}{|\vec{r} - \vec{r}'|} \psi(\vec{r}'). \end{aligned} \quad (18)$$

Here $K_1(x)$ is the modified (hyperbolic) Bessel function of the second kind of order one, with the asymptotic behavior

$$K_\nu(x) \sim (\pi/2x)^{1/2} e^{-x}, \quad x \gg \nu^2. \quad (19)$$

An application of Green's theorem yields the form we shall use,

$$\begin{aligned} &(-\nabla^2 + m^2)^{1/2} \psi(\vec{r}) \\ &= \frac{m}{2\pi^2} \int d^3r' \frac{K_1(m|\vec{r} - \vec{r}'|)}{|\vec{r} - \vec{r}'|} (-\nabla_{r'}^2 + m^2) \psi(\vec{r}'). \end{aligned} \quad (20)$$

This form shows clearly the nonlocality of the operator over regions of extent $\sim m^{-1}$.

By using Eq. (20) and the integral representation

$$K_\nu(z) = \frac{1}{2} \left[\frac{z}{2} \right]^\nu \int_0^\infty \frac{dt}{t^{\nu+1}} e^{-t - z^2/4t}, \quad (21)$$

we can write Eq. (1) in the form

$$[M - V(r)] \psi(\vec{r}) = \frac{m_1^2}{8\pi^2} \int_0^\infty dt \frac{e^{-t}}{t^2} \int d^3r' \exp \left[-\frac{m_1^2}{4t} (r^2 + r'^2) + \frac{m_1^2}{2t} \vec{r} \cdot \vec{r}' \right] (-\nabla_{r'}^2 + m_1^2) \psi(\vec{r}') + (m_1 \rightarrow m_2). \quad (22)$$

We can now separate the angular dependence of $\psi(\vec{r})$ by using the identity

$$e^{a\vec{r}\cdot\vec{r}'} = 4\pi \sum_{l,m} i_l(arr') Y_{lm}(\theta, \phi) Y_{lm}^*(\theta', \phi'), \quad (23)$$

where

$$i_l(z) = (\pi/2z)^{1/2} I_{l+1/2}(z)$$

is the modified spherical Bessel function of the first kind of order l . The solutions of Eq. (22) are clearly of the form $\psi_{lm}(\vec{r}) = R_l(r) Y_{lm}(\hat{r})$. By using Eq. (23), the relation

$$\nabla^2 R_l(r) Y_{lm}(\hat{r}) = \left[\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} \right] R_l(r) Y_{lm}(\hat{r}), \quad (24)$$

and making the change of variable $u = 1/t$, we finally obtain the radial equation

$$\begin{aligned} [M - V(r)] R_l(r) = \frac{m_1^2}{2\pi} \int_0^\infty dr' r'^2 \int_0^\infty du \exp \left[-\frac{1}{u} - \frac{m_1^2}{4} (r^2 + r'^2) u \right] i_l(\frac{1}{2} m_1^2 r r') \\ \times \left[-\frac{1}{r'^2} \frac{d}{dr'} r'^2 \frac{d}{dr'} + \frac{l(l+1)}{r'^2} + m_1^2 \right] R_l(r') + (m_1 \rightarrow m_2). \end{aligned} \quad (25)$$

We may evaluate the integral over u easily by writing the Bessel function i_l as

$$i_l(tu) = \left[\frac{t}{u} \right]^l \left[\frac{1}{t} \frac{d}{dt} \right]^l \frac{\sinh tu}{tu}. \quad (26)$$

The result is

$$[M - V(r)] u_l(r) = \frac{m_1^2}{\pi} \int_0^\infty dr' G_l(m_1 r, m_1 r') \left[-\frac{d^2}{dr'^2} + \frac{l(l+1)}{r'^2} + m_1^2 \right] u_l(r') + (m_1 \rightarrow m_2), \quad (27)$$

where we have introduced $u_l(r) = r R_l(r)$ and a kernel G_l given by

$$G_l(x, x') = 2^l z^{l+1} \left[\frac{1}{z} \frac{\partial}{\partial z} \right]^l \frac{1}{z} [(y-z)^{l/2} K_l((y-z)^{1/2}) - (y+z)^{l/2} K_l((y+z)^{1/2})], \quad (28)$$

with

$$y = x^2 + x'^2, \quad z = 2xx'. \quad (29)$$

The kernels $G_l(x, x')$ for the three lowest l values are

$$G_0(x, x') = K_0(|x - x'|) - K_0(x + x'), \quad (30a)$$

$$G_1(x, x') = K_0(|x - x'|) + K_0(x + x') - \frac{1}{xx'} [|x - x'| K_1(|x - x'|) - (x + x') K_1(x + x')], \quad (30b)$$

$$\begin{aligned} G_2(x, x') = \left[\frac{3(x-x')^2}{x^2 x'^2} + 1 \right] K_0(|x - x'|) - \left[\frac{3(x+x')^2}{x^2 x'^2} + 1 \right] K_0(x + x') + \frac{3}{xx'} \left[\frac{2}{xx'} - 1 \right] |x - x'| K_1(|x - x'|) \\ - \frac{3}{xx'} \left[\frac{2}{xx'} + 1 \right] (x + x') K_1(x + x'). \end{aligned} \quad (30c)$$

In each case, $G_l(x, x')$ has a logarithmic singularity for $x' = x$.

In the case of equal quark masses, $m_1 = m_2 = m_q$, we can remove the quark mass entirely from the kinetic energy term on the right-hand side of Eq. (27) by using a scaled radial variable $x = m_q r$, with the result

$$\frac{1}{2m_q} \left[M - V \left[\frac{x}{m_q} \right] \right] u_l(x) = \frac{1}{\pi} \int_0^\infty dx' G_l(x, x') \left[-\frac{d^2}{dx'^2} + \frac{l(l+1)}{x'^2} + 1 \right] u_l(x'). \quad (31)$$

This form of the equation is especially useful when the quark mass is to be varied, since the complicated kinetic energy operator needs to be calculated only once.

We will be primarily interested in QCD-motivated potentials in actual applications, that is, potentials which are of Coulomb-type near the origin. The wave functions $u_l(r)$ then behave as r^{l-v_l+1} for $r \rightarrow 0$, where v_l is determined by Eq. (15).¹⁰ It is convenient for numerical purposes to work instead with functions which approach constant values for $r \rightarrow 0$, and can be approximated by low-order polynomials. We therefore define functions $w_l(r)$ by

$$u_l(r) = r^{l-\nu_l+1} w_l(r), \quad (32)$$

and rewrite Eq. (27) as

$$[M - V(r)]w_l(r) = \frac{m_1^2}{\pi} \int_0^\infty dr' (r'/r)^{l-\nu_l+1} G_l(m_1 r, m_1 r') \\ \times \left[-\frac{d^2}{dr'^2} - \frac{2(l-\nu_l+1)}{r'} \frac{d}{dr'} + \frac{\nu_l(2l+1-\nu_l)}{r'^2} + m_1^2 \right] w_l(r') + (m_1 \rightarrow m_2). \quad (33)$$

The rapid variations of the wave functions near the origin are now encompassed in the kernels. For potentials without a Coulomb singularity, we set ν_l equal to zero.

To solve Eq. (33) numerically, we convert it to a matrix eigenvalue problem. We map the infinite interval $[0, \infty]$ onto the finite interval $[0, 1]$ by the change of variables $t = (1+x/b)^{-1}$, where b is a scale adjusted to keep the wave functions of interest centered in $[0, 1]$, make the space discrete by dividing the interval into $n+1$ regions with $t_j = j/(n+1)$, and approximate the derivatives in Eq. (33) by finite differences. In the work reported here, we used mainly a five-point central difference scheme, except near the end points. There we used lopsided (Markoff's forward difference) schemes so that only information about the system in the sector $r \geq 0$ appears. While one might consider using the parity of the wave functions, $w_l(-r) = w_l(r)$, to continue to $r < 0$, and then applying central difference formulas throughout, such a construction assumes that the wave functions have a continuous polynomial structure across the origin. This is not the case for the Coulomb eigenfunctions w_l which have discontinuous first derivatives at $r=0$, and using such a method would slow the rate of convergence with decreasing mesh size.

We approximate the integral in Eq. (33) by a weighted sum, typically of five-point (Bode's rule) form away from singularities. Near the logarithmic singularity of $G_l(x, x')$ and at the $r \rightarrow 0$ ($t \rightarrow 1$) edge where $r^{l-\nu_l-1}$ diverges for $l=0, 1$, we construct weights which integrate the divergent quantities exactly for $w_l(r)$ a low-order polynomial.¹¹ We consider here only the $l=0$ case, and thus construct weights such that $r^{n-\nu} G_0(mr, mr')$ is integrated exactly ($-1 \leq n \leq 3$ for a five-point scheme). Furthermore, to avoid problems at $r=0, \infty$ ($t=1, 0$) because of infinite contributions from Coulomb and confining potentials, we do not include those points explicitly, but use open-point integration schemes to include the end intervals.

These discrete approximations reduce Eq. (33) to a matrix eigenvalue equation of the form

$$\sum_{j,k} c_{ij} d_{jk} w_k + V_i w_i = M w_i, \quad (34)$$

where the c_{ij} are the integration weights incorporating the kernel, and the d_{jk} are the derivative coefficients including diagonal contributions from the ν_l dependence and the rest mass terms. The mass can be completely factored out of the kinetic matrix in the case $m_1 = m_2$, Eq. (31), so in that case the kinetic matrix need only be calculated once for a given scale b . Equation (34) can be solved using standard matrix routines. While the matrix is full, the matrix elements are large only near the diagonal, and the results are quite stable.

The present method has the advantage that as much information about the nature of the wave functions as desired can be built into the kinetic matrix. We did find that the non-Hermiticity introduced in the matrix by the Markoff forward-difference approximation for the derivatives led to spurious states appearing in the numerical solutions if the differentiation scheme was too large. These solutions had highly oscillatory wave functions and did not seem to affect neighboring states.

B. The square-root scheme

In Sec. III A we used the discrete form of the right-hand side of Eq. (33) as a numerical approximation to the operator $(-\nabla^2 + m^2)^{1/2}$. That method had the advantage that detailed information about the form of the wave functions for $r \rightarrow 0$ could be built in, improving the accuracy of the values of the wave function inside the Compton wavelength. We now develop a different approximation to this operator in which no integrals appear, reducing the number of numerical approximations by one. We will not be able to build in the type of information described above, but will nevertheless gain substantially in the rate of convergence of the eigenvalues.

We begin with the kinetic operator $(-\nabla^2 + m^2)^{1/2}$, use the fact that $\psi(\vec{r})$ is of the form $R_l(r) Y_{lm}(\hat{r})$, and expand the square-root formally. This gives

$$(-\nabla^2 + m^2)^{1/2} \psi(\vec{r}) = m \left[1 - \frac{1}{m^2} \nabla^2 \right]^{1/2} R_l(r) Y_{lm}(\hat{r}) \\ = m \sum_{k=0}^{\infty} \left[\frac{1}{2} \right] \left[\frac{1}{m^2} \right]^k (-\nabla^2)^k R_l(r) Y_{lm}(\hat{r}) \\ = m \sum_{k=0}^{\infty} \left[\frac{1}{2} \right] \left[\frac{1}{m^2} \right]^k \left[-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{l(l+1)}{r^2} \right]^k R_l(r) Y_{lm}(\hat{r}). \quad (35)$$

The radial wave functions R_l for the free wave equation $\sqrt{\cdot}\psi = M\psi$ vary as r^l at the origin. It will be convenient to use instead functions

$$v_l(r) = r^{-l+1}R_l(r)$$

which vanish linearly with r for all l . Pulling the factor r^{l-1} through the differential operators and resumming the series, we find that

$$(-\nabla^2 + m^2)^{1/2}\psi(\vec{r}) = r^{l-1}A(m, l)v_l(r)Y_{lm}(\hat{r}), \quad (36)$$

where A is the operator

$$A(m, l)$$

$$= r^{-l+1} \left[-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{l(l+1)}{r^2} + m^2 \right]^{1/2} r^{l-1}$$

$$= \left[-\frac{d^2}{dr^2} - \frac{2l}{r} \frac{d}{dr} + \frac{2l}{r^2} + m^2 \right]^{1/2}. \quad (37)$$

Equation (1) can now be written as

$$[A(m_1, l) + A(m_2, l) + V(r)]v_l(r) = Mv_l(r). \quad (38)$$

In the equal-mass case, we can again remove the m dependence from the kinetic term by using the scaled variables $x = m_q r$ ($m_1 = m_2 = m_q$).

Our objective now is to approximate the operator $A(m, l)$ by a finite matrix without going through the intermediate step of introducing integral operators as in Eq. (33). As a first step, we introduce an operator $D = A^2$,

$$D = r^{-l+1} \left[-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{l(l+1)}{r^2} + m^2 \right] r^{l-1}$$

$$= -\frac{d^2}{dr^2} - \frac{2l}{r} \frac{d}{dr} + \frac{2l}{r^2} + m^2. \quad (39)$$

The operator in brackets in the first form of this equation is positive definite and Hermitian, hence has real positive eigenvalues. The similarity transformation which gives the second form of the equation preserves this property. Let Δ be the (infinite) diagonal matrix of eigenvalues of D , and U be the corresponding matrix of eigenvectors. Then

$$D = U\Delta U^{-1}, \quad (40)$$

and A is given by

$$A = U\Delta^{1/2}U^{-1}, \quad (41)$$

where $\Delta^{1/2}$ is the diagonal matrix of positive square roots of the eigenvalues.

To obtain finite matrix approximations for D and A , we make a change of variable $r = \beta(t)$ which maps the infinite interval $0 \leq r < \infty$ to the finite interval $0 \leq t \leq 1$ [we will use $\beta(t) = bt/(1-t^2)$, which actually maps $-\infty < r < \infty$ symmetrically to $-1 \leq t \leq 1$]. In terms of t ,

$$D = -\left[\frac{1}{\beta'}\right]^2 \frac{d^2}{dt^2} + \left[\frac{\beta''}{(\beta')^3} - \frac{2l}{\beta\beta'}\right] \frac{d}{dt} + \frac{2l}{\beta^2} + m^2. \quad (42)$$

We then subdivide the interval $0 \leq t \leq 1$ and approximate

TABLE I. Test of the square-root method for the integration of the relativistic oscillator equation, Eq. (6), with $m_q = 1.310$. $E_n = M_n - 2m_q$ and m_q are given in units of $k^{1/3}$, where k is the spring constant of the oscillator. N is the size of the matrix approximation to the square-root operator. The scale size b in the mapping $r = bt/(1-t^2)$ is $b = 4$ in units of $k^{-1/3}$. The rows labeled Miller were calculated by integrating the equivalent momentum-space Schrödinger problem in Eq. (7) using Miller's method (Ref. 9) with $N = 200$.

	N	$E_{n,l}$				
		$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
$l=0$	21	1.6596	3.5283	5.1657	6.6533	8.0267
	25	1.6595	3.5282	5.1656	6.6548	8.0349
	49		3.5280	5.1654	6.6553	8.0394
	77					8.0395
	Miller	1.6595	3.5280	5.1654	6.6553	8.0394
$l=1$	21	2.6663	4.3929	5.9424	7.3659	8.6859
	25	2.6663	4.3931	5.9435	7.3706	8.7015
	49		4.3932	5.9441	7.3737	8.7122
	77					8.7125
	Miller	2.6663	4.3932	5.9441	7.3737	8.7124
$l=2$	21	3.6109	5.2261	6.6993	8.0612	9.3230
	25	3.6109	5.2265	6.7021	8.0722	9.3538
	49	3.6110	5.2268	6.7039	8.0794	9.3761
	77				8.0796	9.3766
	Miller	3.6110	5.2268	6.7039	8.0796	9.3765

the derivatives by finite differences. This construction gives a finite matrix \hat{D} as an approximation for D . It is essential that \hat{D} (like D) have real positive eigenvalues. This puts some constraints on the differentiation schemes used. We have found it satisfactory to use central difference approximations except near the end points where we used small lopsided schemes. We use the fact that the eigenfunctions of D vanish at $r=0$ to include that point in the differences, but can omit the row and column for $t=r=0$ from the matrix. We also omit the row and column for $t=1, r=\infty$, thus imposing the boundary condition that the eigenfunctions vanish there.

The rest of our construction is straightforward. We diagonalize \hat{D} using standard matrix routines, calculate the matrix of eigenfunctions \hat{U} and the diagonal matrix of positive roots of the eigenvalues $\hat{\Delta}^{1/2}$, and use Eq. (41) to obtain the approximate square-root operator

$$\hat{A} = \hat{U} \hat{\Delta}^{1/2} \hat{U}^{-1}. \quad (43)$$

The original continuum eigenvalue problem, Eq. (38), is now replaced by the finite matrix problem

$$[\hat{A}(m_1, l) + \hat{A}(m_2, l) + \hat{V}] \hat{v}_l = M \hat{v}_l, \quad (44)$$

which is readily solved.

As we will see in the next section, this method has the advantage of very rapid convergence of the eigenvalues as the size of the matrices is increased. It has the disadvantage that we cannot build in the known $r^{1-\nu_l}$ behavior of $v_l(r)$ for $r \rightarrow 0$ in the case of realistic $q\bar{q}$ potentials with Coulomb singularities at the origin. The eigenfunctions

of the free operators D and A do not have this behavior. As a result, the eigenfunctions converge slowly for $mr \ll 1$ in the presence of a Coulomb potential, and are best calculated in this (very limited) region by extrapolating from larger r , or by the use of our first (integral-equation) technique.

C. Numerical tests

We have applied the preceding methods for the position-space solution of Eq. (1) to problems with oscillator, Coulomb, and Coulomb-plus-linear potentials to test their speed and accuracy. The results are impressive.

The solutions for the oscillator potential are very well behaved. In Table I we show the rapid convergence of the relativistic eigenvalues with increasing matrix size using the square-root scheme, and compare our results with those obtained by integrating the equivalent momentum space equation [Eq. (7)] using Miller's method.¹⁰ The results obtained with the integral-equation method are essentially identical. The parameters used in this calculation correspond to quite relativistic particles, and the wave functions we obtain are significantly different from nonrelativistic oscillator wave functions, as discussed elsewhere.³ As shown in Table II, the convergence of the radial wave functions $r^{-l}R_{n,l}(r)$ to their limiting values at $r=0$ is also quite rapid, although less so than the convergence of the eigenvalues.

A second, more stringent, test of our methods is shown in Table III, where we compare the $l=0$ eigenvalues obtained numerically for the Coulomb potential $V = -\alpha/r$ with the exact results⁸ given by Eq. (12). The agreement

TABLE II. Test of the square-root method for the integration of the relativistic oscillator equation, Eq. (6), with $m_q = 1.310$. All lengths are in units of $k^{-1/3}$, where k is the spring constant of the oscillator. N is the size of the matrix approximation to the square-root operator. The rows labeled Miller were calculated by integrating the equivalent momentum-space Schrödinger problem in Eq. (7) using Miller's method (Ref. 9) with $N=200$ and then using Eq. (10).

	N	$(R_{n,l}/r^l)(0)$				
		$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
$l=0$	21	1.536	2.208	2.743	3.297	3.632
	25	1.533	2.189	2.716	3.165	3.656
	49	1.530	2.175	2.661	3.077	3.446
	77		2.173	2.658	3.068	3.431
	Miller	1.530	2.173	2.657	3.067	3.427
$l=1$	21	1.388	2.636	3.963	5.379	6.936
	25	1.385	2.615	3.949	5.278	7.029
	49	1.382	2.598	3.878	5.220	6.600
	77	1.381	2.597	3.874	5.209	6.592
	Miller	1.381	2.597	3.873	5.206	6.587
$l=2$	21	1.025	2.331	4.081	5.963	9.655
	25	1.021	2.321	4.026	6.138	9.017
	49	1.019	2.304	3.985	6.054	8.467
	77		2.303	3.982	6.044	8.478
	Miller	1.019	2.303	3.981	6.042	8.473

TABLE III. Numerical tests of the integral equation and square-root methods for integration of the spinless Salpeter equation, Eq. (11), for the Coulomb potential $V(r)=-\alpha/r$ for $\alpha=0.25$, $m_1=m_2=m=1.45$ GeV, and $l=0$. Here $E_n=M_n-2m$. The exact values are from Eq. (12). The scale factors b are used in the mappings $r=bt/(1-t^2)$ (square-root method) and $r=b(t^1-1)$ (integral-equation method) described in the text. The results are for a 101×101 matrix.

n	E_n , exact (GeV)	E_n , square root (GeV)	E_n , integral (GeV)	b (GeV $^{-1}$)
1	-0.022 394	-0.023 06	-0.022 51	2
2	-0.005 648	-0.005 74	-0.005 56	4
3	-0.002 514	-0.002 54	-0.002 44	8
4	-0.001 415	-0.001 43	-0.001 40	16
5	-0.000 906	-0.000 912	-0.000 85	32
6	-0.000 629	-0.000 635	-0.000 65	32
7	-0.000 462	-0.000 465	-0.000 43	64
8	-0.000 354	-0.000 358	-0.000 34	64

is quite satisfactory considering the smallness of the energies on the natural scale $2m_q=2.90$ GeV defined by the equal-mass kinetic operator $2(-\nabla^2+m_q^2)^{1/2}$. We have found in general that the eigenvalues obtained using the integral-equation method converge less rapidly to their limiting values with increasing matrix size than those obtained using the square-root method, presumably because of the extra numerical approximations involved in the evaluation of the integrals. Some evidence of this behavior appears in Table III, where the results quoted for the integral-equation scheme are already inaccurate in the second significant figure for $n \geq 5$ as judged by more extensive calculations.

We also show the scale parameters b used in the two similar, but not identical, mappings from the infinite interval $0 \leq r < \infty$ to the finite interval $0 \leq t \leq 1$ used in our procedure. It is essential for obtaining accurate energies and wave functions that all loops in a given wave function

be well represented on our finite mesh. This requires that b be increased roughly as n^2 as we look for higher states in the nonconfining Coulomb potential. The results given in Table III for the square-root method are taken from the rather wide regions of stability of the eigenvalues with respect b , e.g., $2 \leq b \leq 32$ for $n=1$, $16 \leq b$ for $n=4$. (For realistic confining potentials for the $q\bar{q}$ system, all the low states can be studied using a single value of b .) We note these energies are systematically too negative by amounts which decrease rapidly with increasing n . We attribute these small discrepancies to the failure of the polynomially behaved wave functions in the square-root scheme to account adequately for the r^{-v_0} behavior of the exact $l=0$ wave functions $R_{n,0}(r)$ for $r \rightarrow 0$. This leads to a small underestimate of the average kinetic energy. In fact, the ground-state energy is given accurately by the integral-equation method which incorporates the r^{-v_0} behavior exactly. This effect is negligible for realistic

TABLE IV. Convergence of the eigenvalues with increasing matrix size N in the square-root method for integrating the spinless Salpeter equation, Eq. (1), for $V(r)=-\alpha/r+Br$ with $\alpha=0.25$, $B=0.18$ GeV 2 , and $m_1=m_2=m=1.45$ GeV. Here $E_n=M_n-2m_q$, and b is the scale factor used in the mapping $r=bt/(1-t^2)$ described in the text.

	N	$E_{n,l}$ (GeV)				
		$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
$l=0$ $b=7$ GeV $^{-1}$	25	0.4924	1.0022	1.3925	1.7252	2.0205
	33				1.7258	2.0228
	41				1.7259	2.0234
	49				1.7260	2.0236
	77					2.0237
$l=1$ $b=8$ GeV $^{-1}$	25	0.8345	1.2481	1.5960	1.9033	2.1793
	33			1.5962	1.9042	2.1838
	41			1.5962	1.9044	2.1845
	49			1.5963	1.9045	2.1848
	77					2.1850
$l=2$ $b=9$ GeV $^{-1}$	25	1.0962	1.4601	1.7792	2.0663	2.3264
	33		1.4602	1.7796	2.0681	2.3330
	41			1.7797	2.0685	2.3344
	49				2.0686	2.3348
	77				2.0687	2.3350

TABLE V. Convergence of the wave functions $w_{n,l}(0) = (m_q r)^{\nu_l} r^{-l} \times R_{n,l}(r) |_{r=0}$ with increasing matrix size N in the square-root method for integrating the spinless Salpeter equation, Eq. (1), for $V(r) = -\alpha/r + Br$ with $\alpha=0.25$, $B=0.18$ GeV², and $m_1=m_2=m_q=1.45$ GeV. b is the scale factor used in the mapping $r = bt/(1-t^2)$. $w_{n,l}(0)$ is determined by extrapolation as described in the text.

	N	$n=1$	$w_{n,l}(0)$ (GeV ^{$l+3/2$})			
			$n=2$	$n=3$	$n=4$	$n=5$
$l=0$ $b=7$ GeV ⁻¹	25	0.777	0.773	0.790	0.808	0.788
	49	0.780	0.775	0.789	0.805	0.825
	77	0.779	0.774	0.788	0.803	0.819
	101	0.779	0.773	0.787	0.803	0.819
$l=1$ $b=8$ GeV ⁻¹	25	0.265	0.365	0.445	0.524	0.523
	49	0.264	0.364	0.443	0.511	0.577
	77	0.264	0.365	0.442	0.510	0.572
	101	0.264	0.364	0.442	0.510	0.572
$l=2$ $b=9$ GeV ⁻¹	25	0.0683	0.115	0.159	0.212	0.223
	49	0.0681	0.144	0.159	0.203	0.248
	77	0.0680	0.144	0.159	0.203	0.247
	101	0.0680	0.114	0.158	0.203	0.247

confining potentials.

In Tables IV and V, we show the rate of convergence of the eigenvalues and the wave functions at the origin obtained with the square-root method for a realistic Coulomb-plus-linear potential for the $c\bar{c}$ system. The final results obtained for the two methods for $N=101$ are compared in Table VI. The convergence of the eigenvalues with increasing matrix size is very rapid in the square-root scheme, and matrices of size $N=25$ or 33 give energies accurate enough for phenomenological purposes (accuracy ~ 1 MeV or better in total masses > 3 GeV). This method is easy to implement, and is quite fast. Once

TABLE VI. Comparison of the integral equation and square-root methods for integrating the spinless Salpeter equation, Eq. (1), for $V(r) = -\alpha/r + Br$ with $\alpha = -0.25$, $B = 0.18$ GeV², $m_1 = m_2 = m_q = 1.45$ GeV, and $l=0$, using a scale parameter $b=7$ GeV⁻¹, and matrix size $N=101$. Here $E_n = M_n - 2m_q$ and $w_{n,0}(0) = (m_q r)^{\nu_0} \times R_{n,0}(r) |_{r=0}$ in the relativistic case, and $w_{n,0}(0) = R_{n,0}(0)$ in the Schrödinger theory. The results obtained using $V(r)$ in the nonrelativistic Schrödinger equation are shown for comparison.

n	Integral equation	Square root E_n (GeV)	Schrödinger
1	0.4925	0.4924	0.5166
2	1.0023	1.0022	1.0556
3	1.3928	1.3925	1.4779
4	1.7263	1.7260	1.8451
5	2.0240	2.0237	2.1768
		$w_{n,0}(0)$ (GeV ^{3/2})	
1	0.780	0.779	0.699
2	0.774	0.773	0.639
3	0.787	0.787	0.617
4	0.803	0.803	0.604
5	0.819	0.819	0.595

the kinetic matrix \hat{A} is set up, the potential matrix may be added and the eigenvalues determined in less than 1 sec of CPU (central processing unit) time,¹² certainly adequate for potential fitting.

The convergence of the wave functions at the origin shown in Table V is less rapid than the convergence of the energies, but results sufficiently accurate for practical purposes can again be obtained using rather small matrices. Because the square-root method does not treat the wave functions quite right for $r \rightarrow 0$, we obtained the values of $(r^{\nu_l - l} R_{n,l})(0)$ shown in Table V by least-squares extrapolation from larger r , omitting the smallest two to four values of r depending on the matrix size. This procedure is satisfactory as shown by the comparison with the corresponding integral-equation results in Table VI. We should perhaps emphasize that, because of the Coulomb singularity, the rate of convergence of the wave functions is *slowest* near the origin. The wave functions for $r \gtrsim m_q^{-1}$ converge rapidly, and are essentially identical in the two methods.

Finally, in Table VI we compare relativistic results for the energies and wave functions at the origin with the nonrelativistic (Schrödinger) results for the same potential. The relativistic corrections to the spectrum are quite large even though the $c\bar{c}$ system is usually considered to be fairly nonrelativistic. As a result, empirical potentials adjusted to fit the *observed* spectrum will differ in the relativistic and nonrelativistic treatments, with the relativistic potentials being more confining as observed in Ref. 3. We note also that the trends of the relativistic and nonrelativistic wave functions are markedly different, an effect which is significant for leptonic widths.³

D. Future applications

We are currently using the square-root matrix method for solving the Salpeter equation to fit the spin-averaged spectra and leptonic decay widths of the $c\bar{c}$ and $b\bar{b}$ sys-

tems, and will ultimately include light-quark systems. Our initial objective is to obtain a good empirical potential which incorporates linear asymptotic behavior at large r and the expected Coulomb term with an r -dependent running coupling at small r , and is adjusted between to fit the observed spectra and leptonic widths. The square-root scheme is well suited for this problem since reliable energies may be obtained from small matrix sizes, and we may vary $V(r)$ quite freely (a problem in other methods^{5,6}). To simplify the calculations further, we use a relation between the value of the wave functions at the origin and the inverse density of states derived elsewhere³ to calculate the leptonic widths (including radiative corrections), and only use the wave functions as needed to correct this relation.

Our methods are easily applied also to the unequal-mass case, and by introducing spin-dependent terms in the potential we hope to extend our analysis to most $q\bar{q}$ and $q\bar{Q}$ systems.

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APPENDIX

We will show here that the solution of Eq. (27) for a pure Coulomb potential behaves near the origin as

$$R_l(r) \sim r^{l-\nu_l} [1 + ar + \dots], \quad (\text{A1})$$

where ν_l is given by Eq. (15) and a is determined below, Eq. (A11). The leading behavior for $l=0$ was established in Ref. 8, and that result was recently generalized to arbitrary l by Castorina, Cea, Nardulli, and Paiano.¹⁰ The derivation here is somewhat different from those given previously.

We begin with Eq. (25) with $V(r) = -\alpha/r$,

$$\left[M + \frac{\alpha}{r} \right] R_l(r) = \frac{m_1^2}{2\pi} \int_0^\infty dr' r'^2 \int_0^\infty du \exp \left[-\frac{1}{u} - \frac{m_1^2}{4} (r^2 + r'^2) u \right] i_l \left(\frac{1}{2} m_1^2 r r' \right) \\ \times \left[-\frac{1}{r'^2} \frac{d}{dr'} r'^2 \frac{d}{dr'} + \frac{l(l+1)}{r'^2} + m_1^2 \right] R_l(r') + (m_1 \rightarrow m_2). \quad (\text{A2})$$

The terms on the left- and right-hand sides of this equation which are most singular for $r \rightarrow 0$ have no natural scale. As a result, the equation can only be satisfied if $R_l(r)$ behaves as a power for $r \rightarrow 0$. We assume the behavior in Eq. (A1), substitute in Eq. (A2), and retain only the most singular terms. The result is an equation which determines ν_l ,

$$\alpha r^{l-\nu_l-1} = \nu_l(2l+1-\nu_l) \frac{m_1^2}{2\pi} \int_0^\infty dr' r'^{l-\nu_l} \int_0^\infty du \exp \left[-\frac{1}{u} - \frac{m_1^2}{4} (r^2 + r'^2) u \right] i_l \left(\frac{1}{2} m_1^2 r r' \right) + (m_1 \rightarrow m_2). \quad (\text{A3})$$

We next make the substitutions $r' = r e^\theta$, $v = \frac{1}{2} m^2 r^2 e^\theta u$ in the two terms on the right and scale an overall power of r out of the equation to obtain the relation

$$\alpha = \frac{2}{\pi} \nu_l(2l+1-\nu_l) \int_{-\infty}^\infty d\theta e^{(l-\nu_l)\theta} \int_0^\infty dv e^{-v \cosh \theta} i_l(v) (e^{-m_1^2 r^2 e^\theta / 2v} + e^{-m_2^2 r^2 e^\theta / 2v}). \quad (\text{A4})$$

The exponentials in the last factor can now be replaced by unity for $r \rightarrow 0$. The integral over v can be evaluated,¹³

$$\int_0^\infty dv e^{-v \cosh \theta} i_l(v) = Q_l(\cosh \theta), \quad (\text{A5})$$

and we find that

$$\alpha = \frac{8}{\pi} \nu_l(2l+1-\nu_l) \int_0^\infty d\theta Q_l(\cosh \theta) \cosh(l-\nu_l)\theta. \quad (\text{A6})$$

The final integral can be identified as a special case of a product formula for Legendre functions¹⁴

$$\int_0^\infty d\theta Q_l(\cosh \theta) \cosh m\theta d\theta \\ = \frac{\Gamma(l-m+1)}{\Gamma(l+m+1)} Q_l^m(0+i\epsilon) Q_l^m(0-i\epsilon) \\ = \frac{\pi}{4} \frac{\Gamma(\frac{1}{2}l + \frac{1}{2}m + \frac{1}{2}) \Gamma(\frac{1}{2}l - \frac{1}{2}m + \frac{1}{2})}{\Gamma(\frac{1}{2}l + \frac{1}{2}m + 1) \Gamma(\frac{1}{2}l - \frac{1}{2}m + 1)}. \quad (\text{A7})$$

The result is an equation which determines ν_l in terms of α ,¹⁰

$$\alpha = 2\nu_l \frac{\Gamma(l - \frac{1}{2}\nu_l + \frac{3}{2}) \Gamma(\frac{1}{2}\nu_l + \frac{1}{2})}{\Gamma(l - \frac{1}{2}\nu_l + 1) \Gamma(\frac{1}{2}\nu_l + 1)}, \quad (\text{A8})$$

where the proper solution is the one which vanishes for $\alpha \rightarrow 0$,

$$\nu_l = \frac{\alpha}{2\pi} \frac{\sqrt{\pi} l!}{\Gamma(l + \frac{3}{2})} + O(\alpha^2). \quad (\text{A9})$$

We remark that the right-hand side of Eq. (A7) is convex upward between zeros at $\nu_l = 0$ and $\nu_l = 2l + 2$, is symmetric under the substitution $\nu_l \rightarrow 2l + 2 - \nu_l$, and has poles at $\nu = 2l + 3 + 2n$. There are no positive solutions for ν_l compatible with the boundary conditions on Eq. (A2) except that given by Eq. (A8), and none at all for $\alpha > \alpha_c$, where α_c corresponds to $\nu_l = l + 1$,¹⁰

$$\alpha_c = 4 \left[\frac{\Gamma(\frac{1}{2}l + 1)}{\Gamma(\frac{1}{2}l + \frac{1}{2})} \right]^2. \quad (\text{A10})$$

The first negative solution occurs for

$$\nu_l^- \approx -2 + \frac{\alpha(l+1)!}{\sqrt{\pi} \Gamma(l + \frac{5}{2})} + O(\alpha^2), \quad (\text{A11})$$

corresponding to a term in $R_l(r)$ roughly of order r^2 relative to the leading term.

It is straightforward to extend the calculation above to obtain the coefficient a in Eq. (A1) [but no higher terms: the powers ν_l^- intervene, and the exponentials in the last factor in Eq. (A4) cannot be replaced by unity]. The result is

$$a = -\frac{\alpha M}{8} \left/ \left[\frac{1}{8} \alpha^2 + l + 1 - \nu_l \left(l - \frac{1}{2} \nu_l + \frac{3}{2} \right) \right] \right. . \quad (\text{A12})$$

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