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A Padé Extrapolated Inverse Power Method for Coupled Schrödinger-like Equations Applied to the Two-Body Relativistic Bound State Problem in Quantum Electrodynamics

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We adapt the inverse power method to the solution of the eigenvalue problem associated with recently developed forms of coupled two-body Dirac equations. A Pauli reduction of these equations leads to coupled Schrödinger-like equations which we solve using central difference methods. Our adaptation therefore requires an efficient inversion of large blocked and banded matrices and for the case of interactions derived from lowest order quantum electrodynamics we show how this method can be used, in conjunction with logarithmic scaling and Padé extrapolation techniques, to obtain numerical solutions for the positronium and muonium spectrum that agree with perturbation theory through order $m\alpha^4$ (with error on the order of $m\alpha^6$).

I. INTRODUCTION

Bona fide relativistic bound state wave equations have the feature that a nonperturbative solution (analytic or numerical) of the eigenvalue spectrum yields the same results to an appropriate order in a given coupling constant as does a perturbative treatment of these same equations. The prototype of such an equation is the one-body Dirac equation. This equation has an exact solution for a charged spin-one-half point particle in an external Coulomb field. The analytically derived spectrum agrees through order α^4 in the fine structure constant with that found by a perturbative treatment of the Darwin and spin-orbit terms obtained from the usual Pauli reduction of the Dirac equation [1]. This contrasts with the situation involving Breit's two-body Dirac equation [2]. A nonperturbative solution of this equation does not yield the same spectrum that a Pauli reduction and subsequent perturbative treatment of this equation does [3].

There has been, as far as we know, only one analytic treatment of a two-body relativistic wave equation with a spectrum correct through order $m\alpha^4$. The two-body Dirac equations of constraint dynamics [4, 5] for the e^+e^- system in the ${}^1J_J$ states [6, 7] give the total energy w in the center of momentum (c.m.) system

$$w = m\sqrt{2 + 2/\sqrt{1 + \alpha^2/(n + \sqrt{(l + \tfrac{1}{2})^2 - \alpha^2} - l - \tfrac{1}{2})^2}}$$

$$= 2m - \frac{m\alpha^2}{4n^2} - \frac{m\alpha^4}{2n^3(2l + 1)} + \frac{11}{64}\frac{m\alpha^4}{n^4} + O(\alpha^6).$$

These two-body Dirac equations have the advantage of being local equations but, with the exception of this exact solution, have not been tested numerically for QED systems until recently [7]. In previous work it was tacitly assumed (without checking) that a nonperturbative, numerical treatment of the constraint equations for standard field theoretic input would yield standard perturbative spectral results. We have shown in Ref. [7] that if the constraint equations for QED were so treated they would in fact yield the correct two-body spectrum through order $m\alpha^4$. In particular we computed energies for the $n = 1, 2, 3$ levels of fermion–antifermion systems in QED that agree with those of the perturbative treatment of these equations through order $m\alpha^4$. We treated the general unequal mass system and included only the effective potentials that arise from the single exchange diagram. We did not incorporate the influence of the virtual annihilation diagram when specializing to equal masses. This affirmative result established the constraint equations as legitimate relativistic two-body equations.

The above discussion is meant to give the physics motivation for the presentation that we shall give in this paper of the numerical technique that we developed for showing that our constraint equations yield the correct two-body spectrum for QED through order $m\alpha^4$. This numerical technique is based on the inverse power method, extending it to the coupled Schrödinger-like equations which we obtained from the two-body Dirac equations of constraint dynamics. We found that a crucial ingredient in the application of this method was the Padé approximant. Why were such techniques (the inverse power method together with Padé approximants) necessary for our problem?

In order to obtain agreement with the perturbative results through order $m\alpha^4$ our numerical results should differ from the actual perturbative results by an amount on the order of $m\alpha^6 \sim m10^{-8\text{–}9}$ (terms of order $m\alpha^5$ will not be present if loop diagrams are not included in the potential). Variational techniques using unperturbed wave functions are not adequate since the effective potentials have two important scales, one

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on the order of angstroms (corresponding to the Coulomb part of the potential) and one on the order of fermis (corresponding to the relativistic corrections to the potential). The unperturbed wave functions only display the gross scale of angstroms. This would be adequate for a perturbative treatment of the equation in which the relativistic corrections to the potentials are approximated by their singular (more attractive than $-1/4r^2$) forms, but it is not for a numerical solution of the nonsingular unapproximated potentials [5, 7]. In order to obtain the desired accuracy without the use of an unwarranted number of mesh points we find that we must employ Padé acceleration techniques [8] and logarithmic scaling. The presence of spin leads to four coupled Schrödinger-like equations. In recent work [7] we have derived these equations and presented the perturbative treatment of them and the numerical results, a subset of which we present in more detailed form in this paper for the purpose of illustrating our algorithm.

In this paper we discuss in detail how we applied the inverse power method to handle coupled Schrödinger-like equations. The inversion technique that we use in carrying out this method for the large banded and blocked matrices has not been presented in the literature as far as we can tell. Thus, for the reader who works with eigenvalue problems involving coupled second-order differential equations similar to the time-independent Schrödinger equation, the techniques that we present in this paper can be readily adapted to solve the central difference approximations to those equations.

In Section II we present a general discussion of the two-body Dirac equations of constraint dynamics and give the detailed Schrödinger-like form of the equations. In Section III we review the inverse power method and in Section IV we apply this method to two-body Klein–Gordon equations of constraint dynamics—single, uncoupled, Schrödinger-like equations. With the aid of numerical examples we uncover in this section special problems associated with the short distance behavior of the effective potentials (quasipotentials) and describe how we used Padé approximants and logarithmic scaling of the independent variable to greatly accelerate the convergence of the multiple mesh size, finite difference scheme [8]. In Section V, we solve the crucial problem of inversion of the banded matrices associated with the discretized versions of the coupled Schrödinger-like equations. We describe in detail with numerical examples how Padé approximants, together with the inverse power method and logarithmic scaling enabled us to obtain numerical agreement using our coupled equations with the standard perturbative results of QED.

II. THE TWO-BODY DIRAC EQUATIONS OF CONSTRAINT DYNAMICS

Since these equations may be unfamiliar to most readers we present below a brief background on the two-body Dirac equations of constraint dynamics. For an extensive review, we refer the reader to Refs. [5, 7] and work cited therein.

The 1960s and early 1970s saw the development of more efficient formulations of the quantum relativistic two-body bound state problem than the Bethe–Salpeter equation through various three-dimensional quasipotential reductions of this same equation [9]. At the same time, however, a manifestly covariant and canonical treatment of the classical relativistic two-body problem without a mediating field seemed to be ruled out by the "no-interaction theorem" of Curie, Jordan, and Sudarshan [10]. A resolution of this problem came with "relativistic constraint mechanics," emerging from studies of Dirac's treatment of constrained Hamiltonian systems [4]. It eliminated covariantly the troublesome variables of relative time and relative energy and reduced covariantly the number of degrees of freedom to that of the nonrelativistic problem with three-dimensional coordinates and momenta [4–5]. The constraint approach accomplishes this by introducing a generalized mass shell constraint for each of the two particles of the form $p_i^2 + m_i^2 + \Phi_i = 0$. Mathematical consistency required that these two constraint be "compatible." The quantum mechanical version of the "compatibility condition" is that the quantum versions of the constraints (two separate Klein–Gordon equations on the same wave function for spinless particles) commute with each other. The form of these two equations for the two-body relativistic bound state problem for fermions in QED is that of two Dirac equations.

For two relativistic spin-one-half particles interacting through a four-vector potential, the two compatible, 16-component Dirac equations [5–7] are

$$\mathcal{S}_1\psi = \gamma_{51}(\gamma_1 \cdot (p_1 - A_1) + m_1)\psi = 0, \tag{1.1a}$$

$$\mathcal{S}_2\psi = \gamma_{52}(\gamma_2 \cdot (p_2 - A_2) + m_2)\psi = 0. \tag{1.1b}$$

The relativistic four-vector potentials A_i^μ are two-body analogues of, and in the limit $m_1 \to \infty$ (or $m_2 \to \infty$) go over to, ordinary external vector potentials which may occur in the one-body Dirac equation. The Lorentz character of these interactions is apparent from the "minimal substitution" form of the equations. The general form of the covariant spin-dependent terms in the constituent vector potentials are nonperturbative consequences of the constraint approach, in particular of the compatibility condition

$$[\mathcal{S}_1, \mathcal{S}_2]\psi = 0. \tag{1.2}$$

These wave operators in the above equations operate on a single 16-component spinor. We write the 16-component Dirac spinor as

$$\psi = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}, \tag{1.3}$$

where ψ_i are four component spinors.

Equations (1.1a)–(1.1b) have several properties [5, 7] that we list without proof:

(1) They are manifestly covariant.

(2) They reduce to the ordinary one-body Dirac equation in the limit when one of the particles becomes infinitely heavy.

(3) They can be combined to give [5, 7] coupled Schrödinger-like equations for the 16 component Dirac spinors. In the center of momentum (c.m.) system these equations resemble ordinary Schrödinger-like equations with interactions including central potential, Darwin terms, spin–orbit, spin–spin, and tensor terms with additional coupling between the upper–upper (ψ_1) and lower–lower (ψ_4) four component spinor portions of the full 16-component Dirac spinor. The interactions are local and dependent on the total energy w in the c.m. frame. Other important properties are listed in Refs. [5, 7].

The general c.m. form of the coupled Schrödinger-like equations is

$$(-\nabla^2 + \Phi_1(\mathbf{r}, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, w))\psi_1 + \Phi_2(\mathbf{r}, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, w)\psi_4 = b^2(w)\psi_1 \tag{1.4a}$$

$$(-\nabla^2 + \Phi_3(\mathbf{r}, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, w))\psi_4 + \Phi_4(\mathbf{r}, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, w)\psi_1 = b^2(w)\psi_4. \tag{1.4b}$$

There are similar equations involving ψ_2 and ψ_3 but one can use Eqs. (1.1a)–(1.1b) to determine ψ_2 and ψ_3 in terms of ψ_1 and ψ_4. However, solving for ψ_2 and ψ_3 is not necessary for our purposes; solving the coupled eigenvalue equations Eqs. (1.4a)–(1.4b) numerically is sufficient. The invariant

$$b^2(w) \equiv \varepsilon_w^2 - m_w^2 = (w^4 - 2w^2(m_1^2 + m_2^2) + (m_1^2 - m_2^2)^2)/4w^2 \tag{1.5}$$

plays the role of the energy eigenvalue in this equation. It is the c.m. value squared of the relative momentum and is a function of the invariant total c.m. energy

$$w^2 = -(p_1 + p_2)^2. \tag{1.6}$$

The additional kinematical variables of importance in the above equation are

$$m_w = m_1 m_2 / w \tag{1.7}$$

and

$$\varepsilon_w = (w^2 - m_1^2 - m_2^2)/2w, \tag{1.8}$$

the relativistic reduced mass and energy of the fictitious particle of relative motion introduced by Todorov [9, 5]. (Note that in the limit when one of the particles becomes very heavy, these variables reduce to the mass and energy of the lighter particle. Also note that in this limit, the above Schrödinger-like equations are the same as those obtained by eliminating either the lower or upper component of the one-body Dirac equation in terms of the other.)

With these preliminaries out of the way we proceed directly to the set of coupled equations that relate to the main purpose of this paper. We obtain those by a further reduction of Eqs. (1.4a)–(1.4b) into coupled radial equations [7, 11]. The quantum numbers mentioned below refer to the largest component of the 16-component wave function, namely the upper–upper part ψ_1. The general wave function is of the form

$$\psi_i = \sum_{l,s} c_{i,l,s} R_{ilsj} \mathcal{Y}_{lsjm}, \tag{1.9}$$

where $R_{ilsj} = u_{ilsj}/r$ is the associated radial wave function. For singlet states ($j = l$, $s = 0$) (1.4a) becomes [7, 11] ($\ln'(\ ) \equiv (d/dr)\ln(\ )$)

$$\left\{ -\frac{d^2}{dr^2} + \frac{j(j+1)}{r^2} + 2\varepsilon_w \mathcal{A} - \mathcal{A}^2 + \ln'(\chi_1\chi_2)\frac{d}{dr} - \frac{3}{2}\partial^2\mathcal{G} + \frac{5}{2}(\mathcal{G}')^2 + \frac{3}{2}\ln'(\chi_1\chi_2)\mathcal{G}' - \frac{\ln'(\chi_1\chi_2)}{r} \right\} u_{1j0j} - \frac{\ln'(\chi_1/\chi_2)}{r}\sqrt{(l(l+1)}u_{1j1j} + \left\{ \frac{1}{2}\ln'(\chi_1\chi_2)\mathcal{G}' + \frac{3}{2}(\mathcal{G}')^2 - \frac{1}{2}\partial^2\mathcal{G} \right\} u_{4j0j} = b^2(w)u_{1j0j}. \tag{1.10a}$$

This is coupled to the equation for the lower–lower component u_{4j0j},

$$\left\{ -\frac{d^2}{dr^2} + \frac{j(j+1)}{r^2} + 2\varepsilon_w \mathcal{A} - \mathcal{A}^2 + \ln'(\bar{\chi}_1\bar{\chi}_2)\frac{d}{dr} - \frac{3}{2}\partial^2\mathcal{G} + \frac{5}{2}(\mathcal{G}')^2 + \frac{3}{2}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}' - \frac{\ln'(\bar{\chi}_1\bar{\chi}_2)}{r} \right\} u_{4j0j} - \frac{\ln'(\bar{\chi}_1/\bar{\chi}_2)}{r}\sqrt{(l(l+1)}u_{4j1j} + \left\{ \frac{1}{2}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}' + \frac{3}{2}(\mathcal{G}')^2 - \frac{1}{2}\partial^2\mathcal{G} \right\} u_{1j0j} = b^2(w)u_{4j0j}. \tag{1.10b}$$

For unequal masses and non-s states, these two coupled equations are coupled further to the $j = l$, $s = 1$ components u_{1j1j}, u_{4j1j}:

$$\left\{ -\frac{d^2}{dr^2} + \frac{j(j+1)}{r^2} + 2\varepsilon_w \mathcal{A} - \mathcal{A}^2 + \ln'(\chi_1\chi_2)\frac{d}{dr} \right.$$

$$-\frac{1}{2}\partial^2\mathcal{G}+\frac{1}{2}(\mathcal{G}')^2+\frac{1}{2}\ln'(\chi_1\chi_2)\mathcal{G}'-\frac{\ln'(\chi_1\chi_2)}{r}+\frac{\ln'(\chi_1\chi_2)+\mathcal{G}'}{r}\Bigg\}u_{1j1j}-\frac{\ln'(\chi_1/\chi_2)}{r}\sqrt{(l(l+1)}u_{1j0j}+\Bigg\{\Bigg[-\frac{1}{2}\ln'(\chi_1\chi_2)\mathcal{G}'-\frac{1}{2}(\mathcal{G}')^2+\frac{1}{2}\partial^2\mathcal{G}\Bigg]-\frac{\mathcal{G}'}{r}\Bigg\}u_{4j1j}=b^2(w)u_{1j1j}\tag{1.11a}$$

$$\Bigg\{-\frac{d^2}{dr^2}+\frac{j(j+1)}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\bar{\chi}_1\bar{\chi}_2)\frac{d}{dr}-\frac{1}{2}\partial^2\mathcal{G}+\frac{1}{2}(\mathcal{G}')^2+\frac{1}{2}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'-\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)}{r}+\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)+\mathcal{G}'}{r}\Bigg\}u_{4j1j}-\frac{\ln'(\bar{\chi}_1/\bar{\chi}_2)}{r}\sqrt{(l(l+1)}u_{4j0j}+\Bigg\{\Bigg[-\frac{1}{2}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'-\frac{1}{2}(\mathcal{G}')^2+\frac{1}{2}\partial^2\mathcal{G}\Bigg]-\frac{\mathcal{G}'}{r}\Bigg\}u_{1j1j}=b^2(w)u_{4j1j}.\tag{1.11b}$$

Next we write the coupled equation for the two triplet states $j = l \pm 1$. For the triplet equations ($s = 1$, $l = j - 1$) (1.4a)–(1.4b) become [7]

$$\Bigg\{-\frac{d^2}{dr^2}+\frac{j(j-1)}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\chi_1\chi_2)\frac{d}{dr}-\frac{\partial^2\mathcal{G}}{2(2j+1)}+\frac{1}{2}(\mathcal{G}')^2+\frac{\ln'(\chi_1\chi_2)\mathcal{G}'}{2(2j+1)}-\frac{\ln'(\chi_1\chi_2)}{r}-(j-1)\frac{\ln'(\chi_1\chi_2)+\mathcal{G}'/(2j+1)}{r}\Bigg\}u_{1j-1j}+\Bigg\{\frac{\sqrt{j(j+1)}}{2j+1}\Bigg[-\Bigg(\mathcal{G}''-\frac{\mathcal{G}'}{r}\Bigg)+\ln'(\chi_1\chi_2)\mathcal{G}'\Bigg]\Bigg\}u_{1j+1j}+\Bigg\{-\frac{\ln'(\chi_1\chi_2)\mathcal{G}'}{2(2j+1)}-\frac{1}{2}(\mathcal{G}')^2+\frac{\partial^2\mathcal{G}}{2(2j+1)}+\frac{(j-1)}{(2j+1)}\frac{\mathcal{G}'}{r}\Bigg\}u_{4j-1j}+\Bigg\{\frac{\sqrt{j(j+1)}}{2j+1}\Bigg[-\ln'(\chi_1\chi_2)\mathcal{G}'+\Bigg(\mathcal{G}''-\frac{\mathcal{G}'}{r}\Bigg)\Bigg]\Bigg\}u_{4j+1j}=b^2(w)u_{1j-1j}\tag{1.12a}$$

and

$$\Bigg\{-\frac{d^2}{dr^2}+\frac{j(j-1)}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\bar{\chi}_1\bar{\chi}_2)\frac{d}{dr}-\frac{\partial^2\mathcal{G}}{2(2j+1)}+\frac{1}{2}(\mathcal{G}')^2+\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'}{2(2j+1)}-\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)}{r}-(j-1)\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)+\mathcal{G}'/(2j+1)}{r}\Bigg\}u_{4j-1j}+\Bigg\{\frac{\sqrt{j(j+1)}}{2j+1}\Bigg[-\Bigg(\mathcal{G}''-\frac{\mathcal{G}'}{r}\Bigg)+\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'\Bigg]\Bigg\}u_{4j+1j}+\Bigg\{-\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'}{2(2j+1)}-\frac{1}{2}(\mathcal{G}')^2+\frac{1}{2(2j+1)}\partial^2\mathcal{G}+\frac{(j-1)}{(2j+1)}\frac{\mathcal{G}'}{r}\Bigg\}u_{1j-1j}+\Bigg\{\frac{\sqrt{j(j+1)}}{2j+1}\Bigg[-\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'+\Bigg(\mathcal{G}''-\frac{\mathcal{G}'}{r}\Bigg)\Bigg]\Bigg\}u_{1j+1j}=b^2(w)u_{4j-1j}.\tag{1.12b}$$

These couple to the triplet equations ($s = 1$, $l = j + 1$)

$$\Bigg\{-\frac{d^2}{dr^2}+\frac{(j+1)(j+2)}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\chi_1\chi_2)\frac{d}{dr}+\frac{\partial^2\mathcal{G}}{2(2j+1)}+\frac{1}{2}(\mathcal{G}')^2-\frac{\ln'(\chi_1\chi_2)\mathcal{G}'}{2(2j+1)}-\frac{\ln'(\chi_1\chi_2)}{r}+(j+2)\frac{\ln'(\chi_1\chi_2)-\mathcal{G}'/(2j+1)}{r}\Bigg\}u_{1j+1j}+\Bigg\{\frac{\sqrt{j(j+1)}}{2j+1}\Bigg[-\Bigg(\mathcal{G}''-\frac{\mathcal{G}'}{r}\Bigg)+\ln'(\chi_1\chi_2)\mathcal{G}'\Bigg]\Bigg\}u_{1j-1j}+\Bigg\{+\frac{\ln'(\chi_1\chi_2)\mathcal{G}'}{2(2j+1)}-\frac{1}{2}(\mathcal{G}')^2-\frac{\partial^2\mathcal{G}}{2(2j+1)}+\frac{(j+2)}{(2j+1)}\frac{\mathcal{G}'}{r}\Bigg\}u_{4j+1j}+\Bigg\{\frac{\sqrt{j(j+1)}}{2j+1}\Bigg[-\ln'(\chi_1\chi_2)\mathcal{G}'+\Bigg(\mathcal{G}''-\frac{\mathcal{G}'}{r}\Bigg)\Bigg]\Bigg\}u_{4j-1j}=b^2(w)u_{1j+1j}\tag{1.12c}$$

and

$$\Bigg\{-\frac{d^2}{dr^2}+\frac{(j+1)(j+2)}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\bar{\chi}_1\bar{\chi}_2)\frac{d}{dr}+\frac{\partial^2\mathcal{G}}{2(2j+1)}+\frac{1}{2}(\mathcal{G}')^2-\frac{1}{2(2j+1)}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'-\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)}{r}+(j+2)\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)+\mathcal{G}'/(2j+1)}{r}\Bigg\}u_{4j+1j}$$

$$+\left\{\frac{\sqrt{j(j+1)}}{2j+1}\left[-\left(\mathcal{G}''-\frac{\mathcal{G}'}{r}\right)+\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'\right]\right\}u_{4j-1|j}$$

$$+\left\{+\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'}{2(2j+1)}-\frac{1}{2}(\mathcal{G}')^2-\frac{\partial^2\mathcal{G}}{2(2j+1)}\right.$$

$$\left.+\frac{(j+2)}{(2j+1)}\frac{\mathcal{G}'}{r}\right\}u_{1j+1|j}+\left\{\frac{\sqrt{j(j+1}}{2j+1}\left[-\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'\right.\right.$$

$$\left.\left.+\left(\mathcal{G}''-\frac{\mathcal{G}'}{r}\right)\right]\right\}u_{1j-1|j}=b^2(w)u_{4j+1|j}. \tag{1.12d}$$

For the $^3P_0$ equations we have simply

$$\left\{-\frac{d^2}{dr^2}+\frac{2}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\chi_1\chi_2)\frac{d}{dr}+\frac{1}{2}\partial^2\mathcal{G}\right.$$

$$+\frac{1}{2}(\mathcal{G}')^2-\frac{1}{2}\ln'(\chi_1\chi_2)\mathcal{G}'-\frac{\ln'(\chi_1\chi_2)}{r}$$

$$\left.+2\frac{\ln'(\chi_1\chi_2)-\mathcal{G}'}{r}\right\}u_{1110}+\left\{\frac{1}{2}\ln'(\chi_1\chi_2)\mathcal{G}'-\frac{1}{2}(\mathcal{G}')^2\right.$$

$$\left.-\frac{1}{2}\partial^2\mathcal{G}+2\frac{\mathcal{G}'}{r}\right\}u_{4101}=b^2(w)u_{1110} \tag{1.13a}$$

coupled to

$$\left\{-\frac{d^2}{dr^2}+\frac{2}{r^2}+2\varepsilon_w\mathcal{A}-\mathcal{A}^2+\ln'(\bar{\chi}_1\bar{\chi}_2)\frac{d}{dr}+\frac{1}{2}\partial^2\mathcal{G}\right.$$

$$+\frac{1}{2}(\mathcal{G}')^2-\frac{1}{2}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'-\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)}{r}$$

$$\left.+2\frac{\ln'(\bar{\chi}_1\bar{\chi}_2)-\mathcal{G}'}{r}\right\}u_{4110}+\left\{\frac{1}{2}\ln'(\bar{\chi}_1\bar{\chi}_2)\mathcal{G}'-\frac{1}{2}(\mathcal{G}')'\right.$$

$$\left.+\frac{1}{2}\partial^2\mathcal{G}+2\frac{\mathcal{G}'}{r}\right\}u_{1110}=b^2(w)u_{4110}. \tag{1.13b}$$

For lowest order QED, $\mathcal{A}=-\alpha/r$ for fermion–antifermion systems. The other (invariant) functions appearing in our Schrödinger-like equation are

$$\chi_1=\frac{E_1+m_1}{G}, \tag{1.14a}$$

$$\chi_2=\frac{E_2+m_2}{G}, \tag{1.14b}$$

$$\bar{\chi}_1=\frac{E_1-m_1}{G}, \tag{1.14c}$$

$$\bar{\chi}_1=\frac{E_2-m_2}{G}, \tag{1.14d}$$

$$E_1(\mathcal{A})=G(\varepsilon_1-\mathcal{A}), \tag{1.15a}$$

$$E_2(\mathcal{A})=G(\varepsilon_2-\mathcal{A}), \tag{1.15b}$$

$$G^2=\frac{1}{(1-2\mathcal{A}/w)}, \tag{1.16}$$

$$\mathcal{G}=\ln G, \tag{1.17}$$

$$\mathcal{G}'=\frac{d\mathcal{G}}{dr};\quad \partial^2\mathcal{G}=\frac{d^2\mathcal{G}}{dr^2}+\frac{2}{r}\frac{d\mathcal{G}}{dr}. \tag{1.18}$$

For the $^3P_0$ case (Eqs. (1.13a)–(1.13b)) and the equal mass (or $l=0$) $j=l$ case (Eqs. (1.10a)–(1.10b) or (1.11a)–(1.11b) we have just two coupled Schrödinger-like equations. They have the general form

$$\left(-\frac{d^2}{dr^2}+f(r)\frac{d}{dr}+q(r)\right)u(r)+g(r)v(r)=b^2u(r) \tag{1.19a}$$

$$\left(-\frac{d^2}{dr^2}+e(r)\frac{d}{dr}+s(r)\right)v(r)+a(r)u(r)=b^2v(r). \tag{1.19b}$$

For all other cases (that is, for the unequal mass $j=l\neq 0$ and $0\neq j=l\pm 1$ cases) we have four coupled equations of the form

$$\left(-\frac{d^2}{dr^2}+f(r)\frac{d}{dr}+q(r)\right)u(r)+g(r)v(r)+c(r)y(r)$$

$$+p(r)z(r)=b^2u(r) \tag{1.20a}$$

$$\left(-\frac{d^2}{dr^2}+f(r)\frac{d}{dr}+s(r)\right)v(r)+a(r)u(r)+h(r)y(r)$$

$$+\beta(r)z(r)=b^2v(r) \tag{1.20b}$$

$$\left(-\frac{d^2}{dr^2}+e(r)\frac{d}{dr}+\sigma(r)\right)y(r)+k(r)u(r)+l(r)v(r)$$

$$+j(r)z(r)=b^2y(r) \tag{1.20c}$$

$$\left(-\frac{d^2}{dr^2}+e(r)\frac{d}{dr}+t(r)\right)z(r)+m(r)u(r)+n(r)v(r)$$

$$+o(r)y(r)=b^2z(r). \tag{1.20d}$$

In this paper we show how we adapt the inverse power method for the solution of the eigenvalue problem for coupled equations of the form of Eqs. (1.19) and (1.20).

III. REVIEW OF THE INVERSE POWER METHOD FOR COMPUTING EIGENVALUES

We use this short review section to establish notation and to point out some unique aspects of our equations that require some adaptation of the standard procedure used in the implementing the inverse power method.

With the eigenvalue equation

$$H|u\rangle = \lambda|u\rangle, \tag{2.1}$$

the first step in the inverse power method [12] for determining the eigenvalue and eigenvectors of this equation requires an estimate of $|u\rangle$ and λ. Suppose that we are estimating λ^0, the ground state eigenvalue. Let $|\hat{u}_0\rangle$ be our estimate of $|u\rangle$ and let λ_0 be our estimate of λ^0. Let $|\hat{u}^0\rangle$ be the ground state eigenvector. The inverse-power method leads to an improved estimate of λ^0 and its eigenvector $|\hat{u}^0\rangle$ and the crucial step in this procedure is the construction of the vector

$$|u_1\rangle = (H - \lambda_0)^{-1}|\hat{u}_0\rangle. \tag{2.2}$$

Numerically this requires the inversion of a (generally very large) banded matrix. We give the standard inversion technique [12] for tridiagonal matrices appearing in Schrödinger-like equations in Section IV. We present the generalization of this technique necessary for coupled Schrödinger-like equations in Section V.

Given $|u_1\rangle$, one then computes $\langle\hat{u}_0|u_1\rangle$ and then using a complete set of states shows that the eigenvalue would be corrected to

$$\lambda_0 \to \lambda_0 + \frac{1}{\langle\hat{u}_0|u_1\rangle} \sim \lambda^0. \tag{2.3}$$

The beauty of the inverse power method is that it provides a way of turning the original vector $|\hat{u}_0\rangle$ into the direction of $|\hat{u}^0\rangle$ by an iterative procedure.

This begins with the normalization of $|u_1\rangle$ to $|\hat{u}_1\rangle$. Note that it is more important that our initial eigenvalue estimate be good than that our eigenvector guess be good. One can ascertain that our eigenvalue estimate λ_0 is closer to λ^0 than it is to any of the other λ^i, $i = 1, 2, \ldots$, by counting nodes of $\hat{u}_0(x)$). If this is so, then the new estimate of the eigenvector, $|\hat{u}_1\rangle$, is closer to $|\hat{u}^0\rangle$ than is $|\hat{u}_0\rangle$.

Each time we repeat this, the eigenvector found becomes closer to the correct result. One constructs

$$|u_2\rangle = (H - \lambda_0)^{-1}|\hat{u}_1\rangle \tag{2.16}$$

and one finds that $\langle\hat{u}_1|u_2\rangle$ is closer to $(\lambda^0 - \lambda_0)^{-1}$ than $\langle\hat{u}_0|u_1\rangle$ is. Numerically, we repeat this procedure until $\langle\hat{u}_i|u_{i+1}\rangle$ differs from $\langle\hat{u}_{i-1}|u_i\rangle$ by an amount less than some prescribed value. Once that has occurred we can correct λ_0 to $\lambda_0 + 1/\langle\hat{u}_i|u_{i+1}\rangle$. Note that we can help this process along by replacing λ_0 by $\eta\lambda_0 + (1 - \eta)/\langle\hat{u}_j|u_{j+1}\rangle$, where $0 < \eta < 1$. This may be somewhat risky since in our case the operator H (see Eqs. (1.10)–(1.13)) depends on the eigenvalue, $H = H(\lambda)$. Note that because of the nonlinearity of the eigenvalue problem, we have three overlapping avenues of approach. One can fix λ_0 in both spots in the inverse operator $(H(\lambda_0) - \lambda_0)^{-1}$ while the iteration proceeds or adjust it in the $-\lambda_0$ spot or in $H(\lambda_0)$ or in both, while the iterations are proceeding. In the next section we continue the review of the inverse power method with an application to an ordinary uncoupled Schrödinger-like equation.

IV. TWO BOUND SPINLESS PARTICLES AND THE INVERSE POWER METHOD FOR EIGENVALUES OF AN UNCOUPLED SCHRÖDINGER-LIKE EQUATION

What makes the inverse power method such a powerful tool for Schrödinger-like equations is that one can numerically invert $(H - \lambda_0)$ in the equation

$$(H - \lambda_0)|u_1\rangle = |\hat{u}_0\rangle \tag{3.1}$$

relatively simply [12]. In the case where we have an uncoupled Schödinger-like equation of the form

$$\left(-\frac{d^2}{dr^2} + q(r)\right) u(r) = \lambda u(r), \tag{3.2}$$

H will be tridiagonal if we use the simplest matrix form for $-d^2/dr^2$. In that case, Eq. (3.1) has the form

$$\mathbf{Dv} = \mathbf{u} \tag{3.3}$$

in which the tridiagonal matrix $\mathbf{D}$ represents the operator $H - \lambda_0$, the column vector $\mathbf{v}$ represents the unknown vector $|u_1\rangle$, and $\mathbf{u}$ represents the known vector $|\hat{u}_0\rangle$. Let the vector $\mathbf{d}$ be the diagonal portion of $\mathbf{D}$ and let $\mathbf{f}$ and $\mathbf{e}$ be the right and left off-diagonal portions of $\mathbf{D}$. In component form Eq. (3.3) is, for $i = 2, \ldots, M - 1$,

$$d_1 v_1 + f_1 v_2 = u_1 \tag{3.4a}$$

$$e_i v_{i-1} + d_i v_i + f_i v_{i+1} = u_i \tag{3.4b}$$

$$e_M v_{M-1} + d_M v_M = u_M. \tag{3.4c}$$

We repeat the standard inversion procedure of (3.4) as an introduction for the important generalizations given in Section IV.

First, we manipulate (3.4) to give v_i, $i = 1, \ldots, M - 1$, in terms of v_M and the known vector $\mathbf{u}$. Let $\bar{d}_1 = d_1, \bar{u}_1 = u_1$. Then

$$v_1 = \frac{1}{\bar{d}_1}(\bar{u}_1 - f_1 v_2). \tag{3.5}$$

Use the next equation to give v_2 in terms of v_3,

$$e_2 v_1 + d_2 v_2 + f_2 v_3 = \left(d_2 - \frac{e_2 f_1}{\bar{d}_1}\right) v_2 + \frac{e_2}{\bar{d}_1}\bar{u}_1 + f_2 v_3 = u_2,$$

so that

$$v_2 = \frac{1}{\bar{d}_2}(\bar{u}_2 - f_2 v_3), \tag{3.6}$$

where

$$\bar{d}_2 = d_2 - \frac{e_2 f_1}{\bar{d}_1}, \quad \bar{u}_2 = u_2 - \frac{e_2 \bar{u}_1}{\bar{d}_1}. \tag{3.7}$$

Continuing in this way we obtain from (3.4a)–(3.4b)

$$v_i = \frac{1}{\bar{d}_i}(\bar{u}_i - f_{i-1} v_{i+1}), \quad i = 1, \ldots, M-1, \tag{3.8}$$

where

$$\bar{d}_i = d_i - \frac{e_i f_{i-1}}{\bar{d}_{i-1}} \tag{3.9}$$

$$\bar{u}_i = u_i - \frac{e_i \bar{u}_{i-1}}{\bar{d}_{i-1}}. \tag{3.10}$$

We now combine the $i = M - 1$ term of (3.8) with (3.4c) to solve for v_M in terms of $\bar{u}_M$ (and thus for the whole vector $\mathbf{u}$). We have

$$v_{M-1} = \frac{1}{\bar{d}_{M_1}}(\bar{u}_{M-1} - f_{M-1} v_M). \tag{3.11}$$

Substitute this into (3.4c) and we find

$$v_M = \frac{\bar{u}_M}{\bar{d}_M}, \tag{3.12}$$

where, as with (3.9)–(3.10),

$$\bar{d}_M = d_M - \frac{e_M f_{M-1}}{\bar{d}_{M-1}} \tag{3.13}$$

and

$$\bar{u}_M = u_M - \frac{e_M \bar{u}_{M-1}}{\bar{d}_{M-1}}. \tag{3.14}$$

Starting with (3.12) and the known vector $\bar{\mathbf{u}}$, we can use (3.8) to generate the rest of the components of the vector $\mathbf{v}$. For later comparison we note that the crucial scalar product (our vectors are real)

$$\langle \hat{u}_0 | u_1 \rangle = \int_0^\infty \hat{u}_0(r) u_1(r)\, dr = \mathbf{u} \cdot \mathbf{v} = \sum_{i=1}^{N} u_i v_1.$$

Before considering the more complicated examples of the coupled Schrödinger-like equations (1.19a)–(1.19b) and (1.20a)–(1.20d), we examine a simpler two-body equation, one for two spinless particles. In Ref. [13] we have shown that the two simultaneous Klein–Gordon equations for the two spinless particles in the constraint approach can be reduced to a single uncoupled Schrödinger-like equation. For mutual electromagnetic interactions it takes the form

$$\left[\mathbf{p}^2 - \frac{2\varepsilon_w \alpha}{r} - \frac{\alpha^2}{r^2} - \frac{i\alpha}{r^2(rw + 2\alpha)}\mathbf{r} \cdot \mathbf{p}\right] \psi = b^2 \psi. \tag{3.15}$$

(Note that in the limit in which one of the particles becomes very heavy, this equation reduces to the ordinary Klein–Gordon equation for a spinless particle in an external Coulomb potential.) In the coordinate representation the substitution $\psi(\mathbf{r}) = u_l(r) Y_{lm}/r$ leads to the radial form

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2\varepsilon_w \alpha}{r} - \frac{\alpha^2}{r^2} + \frac{\alpha}{r^2(rw + 2\alpha)} - \frac{\alpha}{r(rw + 2\alpha)}\frac{d}{dr}\right] u_l = b^2 u_l. \tag{3.16}$$

In that same work we showed that the ground state perturbative spectrum for the total c.m. energy w for equal masses is

$$w = m\left[2 - \frac{\alpha^2}{4} - \frac{13\alpha^4}{64}\right] \tag{3.17}$$

through order α^4. We shall use this example to establish and further review certain aspects of the inverse power method as well as to detail some of the special techniques we used to obtain a comparable accuracy numerically for $\alpha \sim \frac{1}{137}$. In this test calculation we take both masses to be that of the electron. We use the central difference method for approximating the eigenvalues and the endpoint of the calculation is taken to be 20 Å. The iterations using the inverse power method are continued until the difference in successively computed eigenvalues is less than some small fraction of $\mu\alpha^6$ (μ is the reduced mass $m/2$), much less than the accuracy we expect for our equations. Numerical errors are thus small compared to theoretical errors. All of the calculations were done on an AT(286) personal computer.

The nonrelativistic ground state energy level for our actual example Hamiltonian given in Eq. (3.17) is $-m\alpha^2/4$. Although we are not interested in comparison of our calculated spectral results with experiment, we shall use the actual values of the fine structure constant along with the electron's mass. This will provide a realistic test of our numerical scheme. In that case, the above nonrelativistic ground state energy level is numerically equal to -6.8028501603 eV. It is modified to $m[-\alpha^2/4 - 13\alpha^4/64]$ or -6.8031444973 eV by the semirelativistic

correction. For comparison $m\alpha^4 = 0.0007245221$ eV, $m\alpha^5 = 0.0000052871$ eV, and $m\alpha^6 = 0.0000000386$ eV. (This is the reason why we are including so many significant figures in our theoretical-numerical test [14].) The first numerical calculation that we performed used equal mesh sizes of approximately 0.08, 0.04, and 0.02 Å corresponding to 256, 512, and 1024 grid points with the end-point truncated to about $r_N \equiv 20$ Å. The respective eigenvalues found are -6.7934553887, -6.8014683095, and -6.8036671772 eV. As a measure of the difference between our nonperturbative numerical calculation and the perturbative analytic calculation of the binding energy we define the fractional difference as $(w_{\text{pert}} - w_{\text{nonpert}})/\mu\alpha^4$. The fractional differences (FD) corresponding to the above three values are 13.3731037, 2.3135083, and -0.7214134. Although adequate for comparison with the nonrelativistic results (for which $(w_{\text{nonrel}} - w_{\text{nonpert}})/(-m\alpha^2/4)$ yields the three values of $-.0013810$, $-.0002031$, .0001201), they are clearly not adequate for the semirelativistic results. To be truly useful the error should be on the order of $m\alpha^6$ (corresponding to $FD \sim \alpha^2 \sim 0.00005$), since without radiative corrections this would be the next order semirelativistic correction. A fixed point Padé extrapolation procedure [8] of the eigenvalue $\lambda \equiv b^2(w)$ based on the above three points using

$$\lambda(h) = \frac{A + Bh^2}{1 + Ch^2}, \tag{3.18}$$

where h is the mesh size, yields

$$\lambda(0) = \frac{5\lambda_1\lambda_3 - 4\lambda_2\lambda_3 - \lambda_1\lambda_2}{4\lambda_1 - 5\lambda_2 + \lambda_3}.$$

Using this and Eq. (1.5) we obtain

$$w(0) - 2m_e = -6.8041392832 \text{ eV} \tag{3.19}$$

or FD $= -1.3730236$, which is clearly an inadequate approximation to the correct result. The size of the difference between it and the perturbative result is 1.37 times the fine structure scale of $\mu\alpha^4$. This becomes plausible in light of the fact that the smallest mesh size is of the order 10^3 times the classical electron radius, a distance at which the denominator part of the derivative term in the interaction has a significant variation and also at which the $-\alpha^2/r^2$ becomes as important as the Coulomb term $-2\varepsilon_w\alpha/r$. In fact, in this case the extrapolated value is less accurate than the value with the smallest grid size.

As a comparison we consider Eq. (3.16) without the derivative term,

$$\left[\mathbf{p}^2 - \frac{2\varepsilon_w\alpha}{r} - \frac{\alpha^2}{r^2}\right]\psi = b^2\psi. \tag{3.20}$$

In that case the ground state binding energy can be solved exactly [6, 7], yielding

$$w = m\sqrt{2 + 2/\sqrt{1 + \alpha^2/(n + \sqrt{(l+\tfrac{1}{2})^2 - \alpha^2} - l - \tfrac{1}{2})^2}}$$
$$= 2m - \frac{m\alpha^2}{4n^2} - \frac{m\alpha^4}{2n^3(2l+1)} + \frac{11}{64}\frac{m\alpha^4}{n^4} + O(\alpha^6). \tag{3.21a}$$

For the ground state this gives

$$w - 2m = m\left[-\frac{\alpha^2}{4} - \frac{21\alpha^4}{64}\right] + O(\alpha^6)). \tag{3.21b}$$

Numerically this is -6.8033256279 eV. The respective eigenvalues found using 256, 512, and 1024 grid points are -6.7929216290, -6.80070457790, and -6.8026629524 eV corresponding to FD values of 14.3598098, 3.6176262, and 0.9146381. The simple three-point Padé extrapolated eigenvalue $\lambda(0)$ yields the extrapolated binding energy of $w(0) - 2m_e = -6.8033168749$ eV or FD $= 0.0120811$. This is clearly a much better approximation to the perturbative result, since the size of the difference is just 0.012 times the fine structure scale of $\mu\alpha^4$. Note that in this case the extrapolated result is significantly better than the value calculated at the smallest grid size. However, the accuracy with this number of grid points still leaves something to be desired as it is a factor of about 200 times the $\mu\alpha^6$ error scale we demand.

This extrapolation procedure works extraordinarily well for a purely Coulombic potential (without the additional $-\alpha^2/r^2$ fine structure-producing potential). With just

$$\left[\mathbf{p}^2 - \frac{2\varepsilon_w\alpha}{r}\right]\psi = b^2\psi, \tag{3.22}$$

the exact Coulombic bound state solution for the ground state is

$$w = \sqrt{2}m\sqrt{1 + 1/\sqrt{1+\alpha^2}}. \tag{3.23}$$

Perturbatively this corresponds to

$$w - 2m = m\left[-\frac{\alpha^2}{4} + \frac{11\alpha^4}{64}\right] + O(\alpha^6).$$

Numerically this is -6.8026011058 eV. The exact solution is -6.8026011162 eV. The respective eigenvalues found using 256, 512, and 1024 grid points are -6.7922535171, -6.8000083061, and -6.8019525430 eV, corresponding to FD values of 14.2819513, 3.5786346, and 0.8951589. The Padé extrapolated eigenvalue $\lambda(0)$ yields the extrapolated binding energy of $w(0) - 2m_e = -6.8026011158$ eV or FD $= -0.0000138$. This is an extremely accurate representation of the perturbative value and it is even a better representation of

the exact result, the size of the difference being 0.0000005 times the fine structure scale of $\mu\alpha^4$. Note that in this case the extrapolated result attests quite strongly to the value of this extrapolation procedure [8], as the difference calculated at the smallest grid size is of the order of 1.0 times the fine structure scale of $\mu\alpha^4$.

However, we are still left with relatively poor extrapolation results for Eq. (3.16) and to a lesser extent for Eq. (3.20). The problem is one of scale. For the purely Coulomb example of Eq. (3.22) there is only one scale that is of importance and that is the atomic scale of angstroms. For the cases of Eqs. (3.20), (3.22) an additional scale occurs around a few fermis, as it is at this distance that the non-Coulombic terms become about as important as the Coulomb term. Because of the importance of both scales we make a variable change to

$$x = \ln(r/r_0), \tag{3.25}$$

where r_0 is proportional to the Compton wave length. We further make a change of the dependent variable

$$\tilde{u} = e^{x/2}u, \tag{3.26}$$

so that the Hermitian part of the operator will remain Hermitian. In that case Eq. (3.16) for S-states has the form (we have dropped the tilde on u)

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{f}{r}\right)\frac{d}{dx} - \frac{3f}{2r} + q - \frac{3}{4r^2}\right)u(x) = b^2u(x), \tag{3.27}$$

where $q = -2\varepsilon_w/r - \alpha^2/r^2$ with $r = r_0e^x$ and $f = -\alpha^2/(r^2(rw + 2\alpha))$. In applying the inverse power method to Eq. (3.27) note that the crucial scalar product (we have dropped the tilde on $\hat{u}_0(x)$ and $u_1(x)$)

$$\langle\hat{u}_0|u_1\rangle = \int_{-\infty}^{\infty}\hat{u}_0(x)u_1(x)\,dx = \mathbf{u}\cdot\mathbf{v} = \sum_{i=1}^{N}u_iv_i.$$

We use the same set of numbers (256,512,1024) of grid points as with the equally spaced case but now we solve the above eigenvalue equation with equally spaced points in x space instead of r space. The range in x space is $\ln(r_0/r_N) \le x \le \ln(r_N/r_0)$, where, as before, r_0 is about a Compton wave length and r_N is about 20 Å. In r space this corresponds to $r_0(r_0/r_N) \le r \le r_N$. The step sizes vary from about $2r_0(r_0/r_N)\ln(r_N/r_0)/M$ to $r_N\ln(r_N/r_0)/M$ for $M = 256$, 512, and 1024. The perturbative value $m[-\alpha^2/4 - 13\alpha^4/64]$ of the energy we are trying to reproduce is numerically -6.8031444973 eV. At these three number of mesh points the inverse power method yields -6.7901974734, -6.7999193135, and -6.8023396923 eV, corresponding to FD values of 17.8697443, 4.4514639, and 1.1108081. From these values we obtain the fixed-point Padé value for the extrapolated binding energy of $w(0) - 2m_e = -6.8031444728$ eV. This is in excellent agreement with the perturbative value with the difference being 0.0000338 times the fine structure scale of $\mu\alpha^4$ that is consistent with the demand of errors on the order of $\mu\alpha^6$. Note that the extrapolated value is significantly better than the best unextrapolated value, as is most clearly shown by the remarkable drop in the FD value. In fact the latter is not of an acceptable accuracy, its difference being on the order of the fine structure scale itself. Which non-Coulombic term is the most troublesome in this regard? Without the derivative terms the perturbative value of the energy we are trying to reproduce is $m[-\alpha^2/4 - 21\alpha^4/64]$ or -6.8033256279 eV. At the three number of mesh points the inverse power method yields $w - 2m_e = -6.7903427169$, -6.8000913547, and -6.8025185935 eV with corresponding FD values of 17.9192764, 4.5774899, and 1.1138852. From these values we obtain the fixed-point Padé value for the extrapolated binding energy of $w(0) - 2m_e = -6.8033256715$ eV. Again this is in excellent agreement with the perturbative value we are trying to reproduce with the difference being -0.0000602 times the fine structure scale of $\mu\alpha^4$. Again the extrapolated value is significantly better than the best unextrapolated value, with the latter not being of an acceptable accuracy, its difference once again being on the order of the fine structure scale itself.

If we choose to drop the $-\mathcal{A}^2 = -\alpha^2/r^2$ term, instead of the derivative term, then the perturbative value of the energy we are trying to reproduce is $m[-\alpha^2/4 + 9\alpha^4/64]$ or -6.8024199753 eV. At the three number of mesh points the inverse power method yields $= -6.7894788647$, -6.7991964040, and -6.8016157089 eV, corresponding to FD = 17.8615827, 4.4492383, and 1.1100648. From these values we obtain the fixed-point Padé value for the extrapolated binding energy of $w(0) - 2m_e = -6.8024201320$ eV. This is in excellent agreement with the perturbative value we are trying to reproduce with the difference being -0.0002163 times the fine structure scale of $\mu\alpha^4$. Again the extrapolated value is significantly better than the best unextrapolated value, with the latter not being of an acceptable accuracy, its difference once again being on the order of the fine structure scale itself. What we learn from this and the analysis of the previous paragraph is that both relativistic perturbations are equally difficult to reproduce numerically without the fixed-point Padé extrapolation scheme, even with the logarithmic scaling of the independent variable in the eigenvalue equation. This is clearly demonstrated by the steep drop in the FD value from about 18 to nearly α.

V. TWO BOUND SPIN-ONE-HALF PARTICLES AND THE INVERSE POWER METHOD FOR EIGENVALUES OF COUPLED SCHRÖDINGER-LIKE EQUATIONS

The general discussion on the inverse power method given in Section III applies here as well. The difficult task is the

inversion of $H - \lambda$. We first seek a method for this inversion when $H|u\rangle = \lambda|u\rangle$ is represented by the coupled radial Schrödinger-like equations (see Eqs. (1.19a)–(1.19b)) of the form ($|u\rangle$ is represented by the functions $u(r)$ and $v(r)$)

$$\left(\frac{-d^2}{dr^2} + f(r)\frac{d}{dr} + q(r)\right) u(r) + g(r)v(r) = \lambda u(r), \tag{4.1a}$$

$$\left(\frac{-d^2}{dr^2} + e(r)\frac{d}{dr} + s(r)\right) v(r) + h(r)u(r) = \lambda v(r), \tag{4.1b}$$

In the finite difference approach the system (4.1a)–(4.1b) corresponds to a matrix in block form. The two diagonal blocks are banded tridiagonal matrices while the off-diagonal blocks are diagonal matrices. In matrix form the equations corresponding Eq. (3.1) are

$$\mathbf{Dv} + \mathbf{Gx} = \mathbf{u}, \tag{4.2a}$$

$$\mathbf{Hv} + \mathbf{Sx} = \mathbf{w}; \tag{4.2b}$$

$\mathbf{v}$ and $\mathbf{x}$ represent the unknown vector $|u_1\rangle$ (or $u_1(r)$, $v_1(r)$) of Eq. (3.1) and $\mathbf{u}$ and $\mathbf{w}$ represent the known vector $|\hat{u}_0\rangle$ (or $\hat{u}_0(r)$, $\hat{v}_0(r)$). $\mathbf{D}$ and $\mathbf{S}$ are the tridiagonal matrices representing the coefficients of $u(r)$ and $v(r)$, respectively, in Eqs. (4.1a)–(4.1b) while $\mathbf{G}$ and $\mathbf{H}$ are diagonal matrices representing the functions $g(r)$ and $h(r)$. The three bands that make up $\mathbf{D}$ are represented by the vector $\mathbf{d}$ along the diagonal, and $\mathbf{e}$ and $\mathbf{f}$ are the right and left off-diagonal portions. The corresponding three bands that make up $\mathbf{S}$ are η, $\mathbf{s}$, and ζ. The elements of the diagonal matrix $\mathbf{G}$ and $\mathbf{H}$ are represented by the vectors $\mathbf{g}$ and $\mathbf{h}$. In component form we have

$$d_1v_1 + f_1v_2 + g_1x_1 = u_1 \equiv \bar{u}_1 \tag{4.3a}$$

$$h_1v_1 + s_1x_1 + \zeta_1x_2 = w_1 \equiv \bar{w}_1 \tag{4.3b}$$

and for $i = 2, \ldots, M - 1$,

$$e_iv_{i-1} + d_iv_i + f_iv_{i+1} + g_ix_i = u_i \tag{4.3c}$$

$$h_iv_i + \eta_ix_{i-1} + s_ix_i + \zeta_ix_{i+1} = w_i \tag{4.3d}$$

and, finally,

$$e_Mv_{M-1} + d_Mv_M + g_Mx_M = u_M \tag{4.3e}$$

$$h_Mv_M + \eta_Mx_{M-1} + s_Mx_M = w_M. \tag{4.3f}$$

We rewrite Eqs. (4.3a)–(4.3b) as

$$\bar{d}_1v_1 + \bar{g}_1x_1 = \bar{u}_1 - f_1v_2 \tag{4.4a}$$

$$\bar{h}_1v_1 + \bar{s}_1x_1 = \bar{w}_1 - \zeta_1x_2, \tag{4.4b}$$

where

$$\bar{d}_1 = d_1, \quad \bar{g}_1 = g_1, \quad \bar{s}_1 = s_1, \quad \bar{h}_1 = h_1. \tag{4.5}$$

Solve (4.4a)–(4.4b) for v_1 and x_1,

$$v_1 = \frac{(\bar{u}_1 - f_1v_2)}{\tilde{d}_1} + \frac{(\bar{w}_1 - \zeta_1x_2)}{\tilde{h}_1}, \tag{4.6a}$$

$$x_1 = \frac{(\bar{w}_1 - \zeta_1x_2)}{\tilde{s}_1} + \frac{(\bar{u}_1 - f_1v_2)}{\tilde{g}_1}, \tag{4.6b}$$

where

$$\tilde{d}_1 = (\bar{d}_1\bar{s}_1 - \bar{g}_1\bar{h}_1)/\bar{s}_1 \tag{4.7a}$$

$$\tilde{g}_1 = (\bar{g}_1\bar{h}_1 - \bar{d}_1\bar{s}_1)/\bar{h}_1 \tag{4.7b}$$

$$\tilde{s}_1 = (\bar{d}_1\bar{s}_1 - \bar{g}_1\bar{h}_1)/\bar{d}_1 \tag{4.7c}$$

$$\tilde{h}_1 = (\bar{g}_1\bar{h}_1 - \bar{d}_1\bar{s}_1)/\bar{g}_1. \tag{4.7d}$$

For $i = 2$, the next two equations (4.3c)–(4.3d) are

$$e_2v_1 + d_2v_2 + f_2v_3 + g_2x_2 = u_2 \tag{4.8a}$$

$$h_2v_2 + \eta_2x_1 + s_2x_2 + \zeta_2x_3 = w_2. \tag{4.8b}$$

In analogy with (4.4a)–(4.4b) they can be written as

$$\bar{d}_2v_2 + \bar{g}_2x_2 = \bar{u}_2 - f_2v_3 \tag{4.10a}$$

$$\bar{h}_2v_2 + \bar{s}_2x_2 = \bar{w}_2 - \zeta_2x_3, \tag{4.10b}$$

where

$$\bar{d}_2 = d_2 - \frac{e_2f_1}{\tilde{d}_1}, \quad \bar{g}_2 = g_2 - \frac{e_2\zeta_1}{\tilde{h}_1} \tag{4.11a}$$

$$\bar{h}_2 = h_2 - \frac{\eta_2f_1}{\tilde{g}_1}, \quad \bar{s}_2 = s_2 - \frac{\eta_2\zeta_1}{\tilde{s}_1} \tag{4.11b}$$

$$\bar{u}_2 = u_2 - \frac{e_2\bar{u}_1}{\tilde{d}_1} - \frac{e_2\bar{w}_1}{\tilde{h}_1} \tag{4.11c}$$

$$\bar{w}_2 = w_2 - \frac{\eta_2\bar{w}_1}{\tilde{s}_1} - \frac{\eta_2\bar{u}_1}{\tilde{g}_1}. \tag{4.11d}$$

Solving (4.10a)–(4.10b) in analogy to (4.4a)–(4.4b) yields

$$v_2 = \frac{(\bar{u}_2 - f_2v_3)}{\tilde{d}_2} + \frac{(\bar{w}_2 - \zeta_2x_3)}{\tilde{h}_2} \tag{4.12a}$$

$$x_2 = \frac{(\bar{w}_2 - \zeta_2x_3)}{\tilde{s}_2} + \frac{(\bar{u}_2 - f_2v_3)}{\tilde{g}_2}, \tag{4.12b}$$

where

$$\tilde{d}_2 = (\bar{d}_2\bar{s}_2 - \bar{g}_2\bar{h}_2)/\bar{s}_2 \tag{4.13a}$$

$$\tilde{g}_2 = (\bar{g}_2\bar{h}_2 - \bar{d}_2\bar{s}_2)/\bar{h}_2 \tag{4.13b}$$

$$\tilde{s}_2 = (\bar{d}_2\bar{s}_2 - \bar{g}_2\bar{h}_2)/\bar{d}_2 \tag{4.13c}$$

$$\tilde{h}_2 = (\bar{g}_2\bar{h}_2 - \bar{d}_2\bar{s}_2)/\bar{g}_2. \tag{4.13d}$$

This process is repeated so that in general we have for $i = 2, 3, \ldots, M-1$,

$$v_i = \frac{(\bar{u}_i - f_i v_{i+1})}{\tilde{d}_i} + \frac{(\bar{w}_i - \zeta_i x_{i+1})}{\tilde{h}_i} \tag{4.14a}$$

$$x_i = \frac{(\bar{w}_i - \zeta_i x_{i+1})}{\tilde{s}_i} + \frac{(\bar{u}_i - f_i v_{i+1})}{\tilde{g}_i}, \tag{4.14b}$$

where

$$\bar{u}_i = u_i - \frac{e_i\bar{u}_{i-1}}{\tilde{d}_{i-1}} - \frac{e_i\bar{w}_{i-1}}{\tilde{h}_{i-1}} \tag{4.15a}$$

$$\bar{w}_i = w_i - \frac{\eta_i\bar{w}_{i-1}}{\tilde{s}_{i-1}} - \frac{\eta_i\bar{u}_{i-1}}{\tilde{g}_{i-1}} \tag{4.15b}$$

and

$$\tilde{d}_i = (\bar{d}_i\bar{s}_i - \bar{g}_i\bar{h}_i)/\bar{s}_i \tag{4.16a}$$

$$\tilde{g}_i = (\bar{g}_i\bar{h}_i - \bar{d}_i\bar{s}_i)/\bar{h}_i \tag{4.16b}$$

$$\tilde{s}_i = (\bar{d}_i\bar{s}_i - \bar{g}_i\bar{h}_i)/\bar{d}_i \tag{4.16c}$$

$$\tilde{h}_i = (\bar{g}_i\bar{h}_i - \bar{d}_i\bar{s}_i)/\bar{g}_i \tag{4.16d}$$

with

$$\bar{d}_i = d_i - \frac{e_i f_{i-1}}{\tilde{d}_{i-1}}, \quad \bar{g}_i = g_i - \frac{e_i\zeta_{i-1}}{\tilde{h}_{i-1}} \tag{4.17a}$$

$$\bar{h}_i = h_i - \frac{\eta_i f_{i-1}}{\tilde{g}_{i-1}}, \quad \bar{s}_i = s_i - \frac{\eta_i\zeta_{i-1}}{\tilde{s}_{i-1}}. \tag{4.17b}$$

To repeat, the above equations are for $i = 2, 3, \ldots, M-1$. We combine the $i = M-1$ equations for v_{M-1} and x_{M-1} in terms of v_M and x_M with (4.3e)–(4.3f) to obtain

$$v_M = \frac{\bar{u}_M}{\tilde{d}_M} + \frac{\bar{w}_M}{\tilde{h}_M} \tag{4.18a}$$

$$x_M = \frac{\bar{w}_M}{\tilde{s}_M} + \frac{\bar{u}_M}{g_M}, \tag{4.18b}$$

where $\bar{u}_M$, $\tilde{u}_M$, and $\tilde{d}_M$, $\tilde{g}_M$, $\tilde{s}_M$, $\tilde{h}_M$, are given by (4.15)–(4.17) with $i = M$. Then (4.18) gives v_M and x_M in terms of the entire vectors **u** and **w** and we use (4.14) and (4.6) to backtrack to the remaining components of **v** and **x** for $i = M-1, M-2, \ldots, 2, 1$.

Our next task is to seek an inverse of $H - \lambda$ in which $H|U\rangle = \lambda|u\rangle$ is represented by four coupled radial Schrödinger-like equations (see (1.20a)–(1.20d) of the forms $|u\rangle$ is represented by the functions $u(r)$, $v(r)$, $y(r)$, and $z(r)$)

$$\left(-\frac{d^2}{dr^2} + f(r)\frac{d}{dr} + q(r)\right)u(r) + g(r)v(r) + c(r)y(r) + p(r)z(r) = b^2u(r) \tag{4.19a}$$

$$\left(-\frac{d^2}{dr^2} + f(r)\frac{d}{dr} + s(r)\right)v(r) + a(r)u(r) + h(r)y(r) + \beta(r)z(r) = b^2v(r) \tag{4.19b}$$

$$\left(-\frac{d^2}{dr^2} + e(r)\frac{d}{dr} + \sigma(r)\right)y(r) + k(r)u(r) + l(r)v(r) + j(r)z(r) = b^2y(r) \tag{4.19c}$$

$$\left(-\frac{d^2}{dr^2} + e(r)\frac{d}{dr} + t(r)\right)z(r) + m(r)u(r) + n(r)v(r) + o(r)y(r) = b^2z(r). \tag{4.19d}$$

In the finite difference approach the above system of equations corresponds to a matrix in 4×4 block form. In matrix form the equations corresponding to Eqs. (3.1) are

$$\mathbf{Dv} + \mathbf{Gx} + \mathbf{Cz} + \mathbf{Pa} = \mathbf{u} \tag{4.20a}$$

$$\mathbf{Hv} + \mathbf{Sx} + \mathbf{Qz} + \mathbf{Ba} = \mathbf{w} \tag{4.20b}$$

$$\mathbf{Kv} + \mathbf{Lx} + \mathbf{Rz} + \mathbf{Ja} = \mathbf{y} \tag{4.20c}$$

$$\mathbf{Mv} + \mathbf{Nx} + \mathbf{Oz} + \mathbf{Ia} = \mathbf{t}. \tag{4.20d}$$

The four diagonal blocks **D**, **S**, **R**, **I** are banded tridiagonal matrices while the 12 off-diagonal blocks **G**, **C**, **P**, **H**, **Q**, **B**, **K**, **L**, **J**, **M**, **N**, **O** are diagonal matrices. The elements of these 12 diagonal matrices are represented by vectors with lower case symbols corresponding to upper case diagonal matrices. The tridiagonal matrices **D** and **S** are represented as before by the respective set of vectors **e**, **d**, **f**, and η, **s**, ζ. The other tridiagonal matrices **R** and **I** are represented by the set of vectors γ, **r**, α and ν, **i**, μ, respectively. The vectors **v**, **x**, **z**, **a** represent the unknown vector $|u_1\rangle$ while the four vectors **u**, **w**, **y**, **t** represent the known vector $|\hat{u}_0\rangle$. In component form the first row of each row of blocks is

$$d_1v_1 + g_1x_1 + c_1z_1 + p_1a_1 = u_1 - f_1v_2 \equiv \bar{u}_1 - f_1v_2 \tag{4.21a}$$

$$h_1v_1 + s_1x_1 + q_1z_1 + b_1a_1 = w_1 - \zeta_1x_2 \equiv \bar{w}_1 - \zeta_1x_2 \tag{4.21b}$$

$$k_1v_1 + l_1x_1 + r_1z_1 + j_1a_1 = y_1 - \alpha_1z_2 \equiv \bar{y}_1 - \alpha_1z_2 \tag{4.21c}$$

$$m_1v_1 + n_1x_1 + o_1z_1 + i_1a_1 = t_1 - \mu_1a_2 \equiv \bar{t}_1 - \mu_1a_2 \tag{4.21d}$$

and for $i = 2, 3, \ldots, M-1$ we have

$$d_i v_i + g_i x_i + c_i z_i + p_i a_i = u_i - f_i v_{i+1} - e_i v_{i-1} \quad (4.22a)$$

$$h_i v_i + s_i x_i + q_i z_i + b_i a_i = w_i - \zeta_i x_{i+1} - \eta_i x_{i-1} \quad (4.22b)$$

$$k_i v_i + l_i x_i + r_i z_i + j_i a_i = y_i - \alpha_i z_{i+1} - \gamma_i z_{i-1} \quad (4.22c)$$

$$m_i v_i + n_i x_i + o_i z_i + i_i a_i = t_i - \mu_i a_{i+1} - \nu_i a_{i-1} \quad (4.22d)$$

and

$$d_M v_M + g_M x_M + c_M z_M + p_M a_M = u_M - e_M v_{M-1} \quad (4.23a)$$

$$h_M v_M + s_M x_M + q_M z_M + b_M a_M = w_M - \eta_M x_{M-1} \quad (4.23b)$$

$$k_M v_M + l_M x_M + r_M z_M + j_M a_M = y_M - \gamma_M z_{M-1} \quad (4.23c)$$

$$m_M v_M + n_M x_M + o_M z_M + i_M a_M = t_M - \nu_M a_{M-1}. \quad (4.23d)$$

By solving the four equations (4.21a)–(4.21d) for v_1, x_1, z_1, a_1 and substituting into the $i = 2$ equations etc., we find that the $i = 2, 3, \ldots, M-1$ equations can be written as

$$\bar{d}_i v_i + \bar{g}_i x_i + \bar{c}_i z_i + \bar{p}_i a_i = \bar{u}_i - f_i v_{i+1} \quad (4.24a)$$

$$\bar{h}_i v_i + \bar{s}_i x_i + \bar{q}_i z_i + \bar{b}_i a_i = \bar{w}_i - \zeta_i x_{i-1} \quad (4.24b)$$

$$\bar{k}_i v_i + \bar{l}_i x_i + \bar{r}_i z_i + \bar{j}_i a_i = \bar{y}_i - \alpha_i z_{i+1} \quad (4.24c)$$

$$\bar{m}_i v_i + \bar{n}_i x_i + \bar{o}_i z_i + \bar{i}_i a_i = \bar{t}_i - \mu_i a_{i+1}, \quad (4.24d)$$

where

$$\bar{d}_i = d_i - e_i f_{i-1}/\tilde{d}_{i-1}, \quad \bar{g}_i = g_i - e_i \zeta_{i-1}/\tilde{h}_{i-1} \quad (4.25a)$$

$$\bar{c}_i = c_i - e_i \alpha_{i-1}/\tilde{k}_{i-1}, \quad \bar{p}_i = p_i - e_i \mu_{i-1}/\tilde{m}_{i-1} \quad (4.25b)$$

$$\bar{u}_i = u_i - e_i(u_{i-1}/\tilde{d}_{i-1} + w_{i-1}/\tilde{h}_{i-1} + y_{i-1}/\tilde{k}_{i-1} + t_{i-1}/\tilde{m}_{i-1}), \quad (4.25c)$$

$$\bar{h}_i = h_i - e_i f_{i-1}/\tilde{g}_{i-1}, \quad \bar{s}_i = s_i - \eta_i \zeta_{i-1}/\tilde{s}_{i-1} \quad (4.25d)$$

$$\bar{q}_i = q_i - e_i \alpha_{i-1}/\tilde{l}_{i-1}, \quad \bar{b}_i = b_i - \eta_i \mu_{i-1}/\tilde{n}_{i-1} \quad (4.25e)$$

$$\bar{w}_i = w_i - \eta_i(u_{i-1}/\tilde{g}_{i-1} + w_{i-1}/\tilde{s}_{i-1} + y_{i-1}/\tilde{l}_{i-1} + t_{i-1}/\tilde{n}_{i-1}), \quad (4.25f)$$

$$\bar{k}_i = k_i - \gamma_i f_{i-1}/\tilde{c}_{i-1}, \quad \bar{l}_i = l_i - \gamma_i \zeta_{i-1}/\tilde{q}_{i-1} \quad (4.25g)$$

$$\bar{r}_i = r_i - \gamma_i \alpha_{i-1}/\tilde{r}_{i-1}, \quad \bar{j}_i = j_i - \gamma_i \mu_{i-1}/\tilde{o}_{i-1} \quad (4.25h)$$

$$\bar{y}_i = y_i - \gamma_i(u_{i-1}/\tilde{c}_{i-1} + w_{i-1}/\tilde{q}_{i-1} + y_{i-1}/\tilde{r}_{i-1} + t_{i-1}/\tilde{o}_{i-1}), \quad (4.25i)$$

$$\bar{m}_i = m_i - \gamma_i f_{i-1}/\tilde{p}_{i-1}, \quad \bar{n}_i = n_i - \nu_i \zeta_{i-1}/\tilde{b}_{i-1} \quad (4.25j)$$

$$\bar{o}_i = o_i - \gamma_i \alpha_{i-1}/\tilde{j}_{i-1}, \quad \bar{i}_i = i_i - \nu_i \mu_{i-1}/\tilde{i}_{i-1} \quad (4.25k)$$

$$\bar{t}_i = t_i - \nu_i(u_{i-1}/\tilde{p}_{i-1} + w_{i-1}/\tilde{b}_{i-1} + y_{i-1}/\tilde{j}_{i-1} + t_{i-1}/\tilde{i}_{i-1}). \quad (4.25l)$$

In order to define the tilde variables let

$$\bar{d}_1 = d_1, \quad \bar{g}_1 = g_1, \quad \bar{c}_1 = c_1, \quad \bar{p}_1 = p_1 \quad (4.26a)$$

$$\bar{h}_1 = h_1, \quad \bar{s}_1 = s_1, \quad \bar{q}_1 = q_1, \quad \bar{b}_1 = b_1 \quad (4.26b)$$

$$\bar{k}_1 = k_1, \quad \bar{l}_1 = l_1, \quad \bar{r}_1 = r_1, \quad \bar{j}_1 = j_1 \quad (4.26c)$$

$$\bar{m}_1 = m_1, \quad \bar{n}_1 = n_1, \quad \bar{o}_1 = o_1, \quad \bar{i}_1 = i_1 \quad (4.26d)$$

and (for $i = 1, \ldots, M$)

$$DSHG_i = \bar{d}_i \bar{s}_i - \bar{h}_i \bar{g}_i, \quad RIOJ_i = \bar{r}_i \bar{i}_i - \bar{o}_i \bar{j}_i, \quad (4.27a)$$

$$GKDL_i = \bar{g}_i \bar{k}_i - \bar{d}_i \bar{l}_i, \quad QIOB_i = \bar{q}_i \bar{i}_i - \bar{o}_i \bar{b}_i, \quad (4.27b)$$

$$DNMG_i = \bar{d}_i \bar{n}_i - \bar{m}_i \bar{g}_i, \quad QJRB_i = \bar{q}_i \bar{j}_i - \bar{r}_i \bar{b}_i, \quad (4.27c)$$

$$HLKS_i = \bar{h}_i \bar{l}_i - \bar{k}_i \bar{s}_i, \quad CIOP_i = \bar{c}_i \bar{i}_i - \bar{o}_i \bar{p}_i, \quad (4.27d)$$

$$SMHN_i = \bar{s}_i \bar{m}_i - \bar{h}_i \bar{n}_i, \quad CJRP_i = \bar{c}_i \bar{j}_i - \bar{r}_i \bar{p}_i, \quad (4.27e)$$

$$NKML_i = \bar{n}_i \bar{k}_i - \bar{m}_i \bar{l}_i, \quad CBQP_i = \bar{c}_i \bar{b}_i - \bar{q}_i \bar{p}_i. \quad (4.27f)$$

Thus defining

$$DET_i = DSHG_i \times RIOJ_i + GKDL_i \times QIOB_i + DNMG_i \times QJRB_i + HLKS_i \times CIOP_i + SMHN_i \times CJRP_i + NKML_i \times CBQP_i \quad (4.28)$$

for $i = 1, 2, \ldots, M$, we have

$$\tilde{d}_i = DET_i/[\bar{s}_i(RIOJ_i) - \bar{l}_i(QIOB_i) + \bar{n}_i(QJRB_i)], \quad (4.29a)$$

$$\tilde{h}_i = DET_i/[-\bar{g}_i(RIOJ_i) + \bar{l}_i(CIOP_i) - \bar{n}_i(CJRP_i)], \quad (4.29b)$$

$$\tilde{k}_i = DET_i/[\bar{g}_i(QIOB_i) - \bar{s}_i(\mathrm{CIOP}_i) + \bar{n}_i(CBQP_i)], \quad (4.29c)$$

$$\tilde{m}_i = DET_i/[-\bar{g}_i(QJRB_i) + \bar{s}_i(CJRP_i) - \bar{l}_i(CBQP_i)], \quad (4.29d)$$

$$\tilde{g}_i = DET_i/[-\bar{h}_i(RIOJ_i) + \bar{k}_i(QIOB_i) - \bar{m}_i(CJRP_i)], \quad (4.29e)$$

$$\tilde{s}_i = DET_i/[\bar{d}_i(RIOJ_i) - \bar{k}_i(\mathrm{CIOP}_i) - \bar{m}_i(CBQP_i)], \quad (4.29f)$$

$$\tilde{l}_i = DET_i/[-\bar{d}_i(QIOB_i) + \bar{h}_i(CIOP_i) - \bar{m}_i(CBQP_i)], \quad (4.29g)$$

$$\tilde{n}_i = DET_i/[\bar{d}_i(QJRB_i) - \bar{h}_i(CJRP_i) + \bar{k}_i(CBQP_i)], \quad (4.29h)$$

$$\tilde{c}_i = DET_i/[\bar{i}_i(HLKS_i) + \bar{j}_i(MSHN_i) + \bar{b}_i(NKML_i)], \quad (4.29i)$$

$$\tilde{q}_i = DET_i/[\bar{i}_i(GKDL_i) + \bar{j}_i(DNMG_i) - \bar{p}_i(NKML_i)], \quad (4.29j)$$

$$\tilde{r}_i = DET_i/[\bar{i}_i(DSHG_i) - \bar{b}_i(DNMG_i) - \bar{p}_i(SMHN_i)], \quad (4.29k)$$

$$\tilde{o}_i = DET_i/[-\bar{j}_i(DSHG_i) - \bar{b}_i(KGDL_i) - \bar{p}_i(HLKS_i)], \quad (4.29l)$$

$$\tilde{p}_i = DET_i/[-\bar{o}_i(HLKS_i) - \bar{r}_i(SMHN_i) - \bar{q}_i(NKML_i)], \quad (4.29m)$$

$$\tilde{b}_i = DET_i/[-\bar{o}_i(GKDL_i) - \bar{r}_i(DNMG_i) + \bar{c}_i(NKML_i)], \quad (4.29n)$$

$$\tilde{j}_i = DET_i/[-\bar{o}_i(DSHG_i) + \bar{q}_i(DNMG_i) + \bar{c}_i(SMHN_i)], \quad (4.29o)$$

$$\tilde{i}_i = DET_i/[\bar{r}_i(DSHG_i) + \bar{q}_i(GKDL_i) + \bar{c}_i(HLKS_i)]. \quad (4.29p)$$

Finally we reach the last set of equations

$$\bar{d}_M v_M + \bar{g}_M x_M + \bar{c}_M z_M + \bar{p}_M a_M = \bar{u}_M, \tag{4.30a}$$

$$\bar{h}_M v_M + \bar{s}_M x_M + \bar{q}_M z_M + \bar{b}_M a_M = \bar{w}_M, \tag{4.30b}$$

$$\bar{k}_M v_M + \bar{l}_M x_M + \bar{r}_M z_M + \bar{j}_M a_M = \bar{y}_M, \tag{4.30c}$$

$$\bar{m}_M v_M + \bar{n}_M x_M + \bar{o}_M z_M + \bar{i}_M a_M = \bar{t}_M, \tag{4.30d}$$

where

$$\bar{d}_M = d_M - e_M f_{M-1}/\tilde{d}_{M-1}, \quad \bar{g}_M = g_M - e_M \zeta_{M-1}/\tilde{h}_{M-1}, \tag{4.31a}$$

$$\bar{c}_M = c_M - e_M \alpha_{M-1}/\tilde{k}_{M-1}, \quad \bar{p}_M = p_M - e_M \mu_{M-1}/\tilde{m}_{M-1}, \tag{4.31b}$$

$$\bar{u}_M = u_M - e_M(u_{M-1}/\tilde{d}_{M-1} + w_{M-1}/\tilde{h}_{M-1} + y_{M-1}/\tilde{k}_{M-1} + t_{M-1}/\tilde{m}_{M-1}), \tag{4.31c}$$

$$\bar{h}_M = h_M - e_M f_{M-1}/\tilde{g}_{M-1}, \quad \bar{s}_M = s_M - \eta_M \zeta_{M-1}/\tilde{s}_{M-1}, \tag{4.31d}$$

$$\bar{q}_M = q_M - e_M \alpha_{M-1}/\tilde{l}_{M-1}, \quad \bar{b}_M = b_M - \eta_M \mu_{M-1}/\tilde{n}_{M-1}, \tag{4.31e}$$

$$\bar{w}_M = w_M - \eta_M(u_{M-1}/\tilde{g}_{M-1} + w_{M-1}/\tilde{s}_{M-1} + y_{M-1}/\tilde{l}_{M-1} + t_{M-1}/\tilde{n}_{M-1}), \tag{4.31f}$$

$$\bar{k}_M = k_M - \gamma_M f_{M-1}/\tilde{c}_{M-1}, \quad \bar{l}_M = l_M - \gamma_M \zeta_{M-1}/\tilde{q}_{M-1}, \tag{4.31g}$$

$$\bar{r}_M = r_M - \gamma_M \alpha_{M-1}/\tilde{r}_{M-1}, \quad \bar{j}_M = j_M - \gamma_M \mu_{M-1}/\tilde{o}_{M-1}, \tag{4.31h}$$

$$\bar{y}_M = y_M - \gamma_M(u_{M-1}/\tilde{c}_{M-1} + w_{M-1}/\tilde{q}_{M-1} + y_{M-1}/\tilde{r}_{M-1} + t_{M-1}/\tilde{o}_{M-1}), \tag{4.31i}$$

$$\bar{m}_M = m_M - \gamma_M f_{M-1}/\tilde{p}_{M-1}, \quad \bar{n}_M = n_M - \nu_M \zeta_{M-1}/\tilde{b}_{M-1}, \tag{4.31j}$$

$$\bar{o}_M = o_M - \gamma_M \alpha_{M-1}/\tilde{j}_{M-1}, \quad \bar{i}_M = i_M - \gamma_M \alpha_{M-1}/\tilde{i}_{M-1}, \tag{4.31k}$$

$$\bar{t}_M = t_M - \nu_M(u_{M-1}/\tilde{p}_{M-1} + w_{M-1}/\tilde{b}_{M-1} + y_{M-1}/\tilde{j}_{M-1} + t_{M-1}/\tilde{i}_{M-1}). \tag{4.31l}$$

The above equations can be solved for v_M, x_M, z_M, a_M, leading us to

$$v_M = \bar{u}_M/\tilde{d}_M + \bar{w}_M/\tilde{h}_M + \bar{y}_M/\tilde{k}_M + \bar{t}_M/\tilde{m}_M, \tag{4.32a}$$

$$x_M = \bar{u}_M/\tilde{g}_M + \bar{w}_M/\tilde{s}_M + \bar{y}_M/\tilde{l}_M + \bar{t}_M/\tilde{n}_M, \tag{4.32b}$$

$$z_M = \bar{u}_M/\tilde{c}_M + \bar{w}_M/\tilde{q}_M + \bar{y}_M/\tilde{r}_M + \bar{t}_M/\tilde{o}_M, \tag{4.32c}$$

$$a_M = \bar{u}_M/\tilde{p}_M + \bar{w}_M/\tilde{b}_M + \bar{y}_M/\tilde{j}_M + \bar{t}_M/\tilde{i}_M; \tag{4.32d}$$

then we determine the rest of the components of the above indicated vectors,

$$v_i = (\bar{u}_i - f_i v_{i+1})/\tilde{d}_i + (\bar{w}_i - \zeta_i x_{i+1})/\tilde{h}_i + (\bar{y}_i - \alpha_i z_{i+1})/\tilde{k}_i + (\bar{t}_i - \mu_i a_{i+1})/\tilde{m}_i, \tag{4.33a}$$

$$x_i = (\bar{u}_i - f_i v_{i+1})/\tilde{g}_i + (\bar{w}_i - \zeta_i x_{i+1})/\tilde{s}_i + (\bar{y}_i - \alpha_i z_{i+1})/\tilde{l}_i + (\bar{t}_i - \mu_i a_{i+1})/\tilde{n}_i, \tag{4.33b}$$

$$z_i = (\bar{u}_i - f_i v_{i+1})/\tilde{c}_i + (\bar{w}_i - \zeta_i x_{i+1})/\tilde{q}_i + (\bar{y}_i - \alpha_i z_{i+1})/\tilde{r}_i + (\bar{t}_i - \mu_i a_{i+1})/\tilde{o}_i, \tag{4.33c}$$

$$a_i = (\bar{u}_i - f_i v_{i+1})/\tilde{p}_i + (\bar{w}_i - \zeta_i x_{i+1})/\tilde{b}_i + (\bar{y}_i - \alpha_i z_{i+1})/\tilde{j}_i + (\bar{t}_i - \mu_i a_{i+1})/\tilde{i}_i, \tag{4.33d}$$

for $i = M - 1, \ldots, 2, 1$. Thus the inversion is accomplished.

Based on our experience with the spinless uncoupled Schrödinger-like equation the actual form for the equations used in our numerical work should be scaled by $x = \ln(r/r_0)$, where r_0 is proportional to the Compton wave length. In that case our general set of equations has the form

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{f(r)}{r}\right)\frac{d}{dx} - \frac{f(r)}{2r} + q(r) - \frac{3}{4r^2}\right)u(x) + g(r)v(x) = b^2 u(x) \tag{4.34a}$$

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{e(r)}{r}\right)\frac{d}{dx} - \frac{e(r)}{2r} + s(r) - \frac{3}{4r^2}\right)v(x) + a(r)u(x) = b^2 v(x) \tag{4.34b}$$

for the case of two coupled equations and

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{f(r)}{r}\right)\frac{d}{dx} - \frac{f(r)}{2r} + q(r) - \frac{3}{4r^2}\right)u(x) + g(r)v(x) + c(r)y(x) + p(r)z(x) = b^2 u(x) \tag{4.35a}$$

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{f(r)}{r}\right)\frac{d}{dx} - \frac{f(r)}{2r} + s(r) - \frac{3}{4r^2}\right)v(x) + a(r)u(x) + h(r)y(x) + \beta(r)z(x) = b^2 v(x) \tag{4.35b}$$

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{e(r)}{r}\right)\frac{d}{dx} - \frac{e(r)}{2r} + \sigma(r) - \frac{3}{4r^2}\right)y(x) + k(r)u(x) + l(r)v(x) + j(r)z(x) = b^2 y(x) \tag{4.35c}$$

$$\left(-\frac{1}{r^2}\frac{d^2}{dx^2} + \left(\frac{2}{r^2} + \frac{e(r)}{r}\right)\frac{d}{dx} - \frac{e(r)}{2r} + t(r) - \frac{3}{4r^2}\right)z(x) + m(r)u(x) + n(r)v(x) + o(r)y(x) = b^2 z(x) \tag{4.35d}$$

for the case of four coupled equations. Also included in the above equations is a scale change in the dependent variables. The tildes (see Eq. (3.26)) are suppressed in the above functions. For the case of only two coupled equations, the crucial scalar product is

$$\langle \hat{u}_0 | u_1 \rangle = \int_{-\infty}^{\infty} dx\, (\hat{u}_0(x)u_1(x) + \hat{v}_0(x)v_1(x)) = \mathbf{u}\cdot\mathbf{v} + \mathbf{w}\cdot\mathbf{x} = \sum_{i=1}^{N} (u_i v_i + w_i x_i). \tag{4.36}$$

For the case of four coupled equations that scalar product is

$$\begin{aligned}\langle \hat{u}_0|u_1\rangle &= \int_{-\infty}^{\infty} dx\,(\hat{u}_0(x)u_1(x) + \hat{v}_0(x)v_1(x) + \hat{y}_0(x)y_1(x) \\ &\quad + \hat{z}_0(x)z_1(x)) \\ &= \mathbf{u}\cdot\mathbf{v} + \mathbf{w}\cdot\mathbf{x} + \mathbf{y}\cdot\mathbf{z} + \mathbf{t}\cdot\mathbf{a} \\ &= \sum_{i=1}^{N} (u_iv_i + w_ix_i + y_iz_i + t_ia_i).\end{aligned} \tag{4.37}$$

We describe the details of the two most important test cases just as we did in the examples in Section IV. In particular we will discuss in detail here the $^1S_0$ and $^3S_1$ states of positronium. (We are not, however, including the effects of the annihilation diagram for the latter in the tests presented below.) As mentioned in the beginning of this paper, our equations have an exact solution for singlet positronium. As shown elsewhere [6], our singlet equation is identical in form to Eq. (3.15) for spinless particles without the derivative term, that is, to Eq. (3.20). The perturbative spectrum is given in Eq. (3.21a) and, as in the discussion below that equation, our nonperturbative numerical treatment yields that perturbative result with errors on the order of $\mu\alpha^6$ if Padé approximates are teamed with logarithmic scaling. It was shown in Refs. [6, 7, 11] that Eq. (3.20) can be derived from Eqs. (1.4a)–(1.4b) with the aid of the additional combinations of the first-order form of our equations for $\mathcal{A} = -\alpha/r$. That allows us to express the lower–lower portion of the wave function in terms of the upper–upper portion. If we choose not to perform that reduction then we obtain the two coupled equations (1.10a)–(1.10b), the appropriate radial counterparts of Eqs. (1.4a)–(1.4b). Unfortunately, we have not been able to perform this by taking one-half the number of coupled equations for triplet ($j \neq l$) positronium. We thus remain with Eqs. (1.12a)–(1.12d) in that case. (We can reduce the $^3P_0$ equations Eqs. (1.23a)–(1.23b) to a single equation and we can reduce the four coupled equations (1.10a)–(1.11b) for the unequal mass, non-s-states to two coupled equations involving only the upper–upper portions of the $j = l$ singlet and triplet equations.)

As a check on our equations in the singlet case and for more confidence building for the more complicated case of four coupled equations in the triplet case, we solve for the singlet spectrum nonperturbatively by solving the coupled equations (1.10a)–(1.10b). As a preliminary step in this calculation and to show the importance (in nonperturbative calculations) of the coupling of the lower–lower component we first solve for the spectrum using just Eq. (1.10a). Using 256,512, and 1024 grid points and the scaling given by Eqs. (3.25)–(3.26) the inverse power method yields for $w(0) - 2m_e$ the values -6.7903764082, -6.8000704745, and -6.802483754 eV. These correspond to FD values of 17.8727750, 4.4928286, and 1.1619701. The fixed point Padé extrapolation procedure of the eigenvalue $\lambda \equiv b^2(w)$, based on the above three points, yields $w(0) - 2m_e = -6.8032861579$ eV. Compared to the perturbatively correct value of -6.8033256279 eV the error is on the order of 5% of $\mu\alpha^4$ (FD = 0.0544773), much larger than the order $\mu\alpha^6$ error expected.

On the other hand, using the coupled set of two equations (1.10a)–(1.10b) the inverse power method yields for $w(0) - 2m_e$ the values -6.7904137751, -6.8001094449, and -6.80252313203 eV (corresponding to FD = 17.8212004, 4.4390408, and 1.1076210). The fixed point Padé extrapolation procedure of the eigenvalue $\lambda \equiv b^2(w)$, based on the above three points, yields $w(0) - 2m_e = -6.8033256719$ eV. Compared to the perturbatively correct value of -6.8033256279 eV the error is on the order of 0.006% of $\mu\alpha^4$ (FD = -0.0000607) which is on the order of the $\mu\alpha^6$ error expected. (Note that the exact result given in the first part of Eq. (3.21) is numerically equal to -6.8033256816 eV and is in fact, as it should be, closer to our nonperturbative numerical result than the perturbative result). This demonstrates the importance of the inclusion of the lower–lower component, as well as providing an important application of the inverse-power method for two coupled Schrödinger-like equations.

For the $^3S_1$ state, we will compare the numerical results of four sets of equations. The first is the uncoupled form of Eq. (1.12a) in which we ignore the coupling to the upper–upper $^3D_1$ states and the lower–lower components of both the $^3S_1$ and $^3D_1$ states. The inverse power method yields for $w(0) - 2m_e$ the values -6.7899230859, -6.7995982298, and -6.80200670225 eV corresponding to FD values of 17.8317929, 4.4779636, and 1.1537412. The fixed point Padé extrapolation procedure of the eigenvalue $\lambda \equiv b^2(w)$, based on the above three points, yields $w(0) - 2m_e = -6.8028074990$ eV. Compared to the perturbatively correct value of [7] $m[-\alpha^2/4 + 1\alpha^4/192] + O(\alpha^6)$ or -6.8028426132 eV, the error is on the order of 5% of $\mu\alpha^4$ (FD = 0.0484653) which is much larger than the order of the $\mu\alpha^6$ error expected.

If we use the coupled set of Eqs. (1.12a)–(1.12b), neglecting the coupling to the $^3D_1$ states, then the inverse power method on the three different mesh sizes plus the Padé extrapolation procedure yields $w(0) - 2m_e = -6.8028082195$ eV. Compared to the perturbatively correct value of -6.8028426132 eV the error is again, on the order of 5% of $\mu\alpha^4$, no improvement on the previous result. If we ignore the coupling to the lower–lower components but include the coupling to the upper–upper $^3D_1$ component (Eqs. (1.12a), (1.12c)) the results improve somewhat, but not significantly, to $w(0) - 2m_e = -6.8028239499$ eV, representing an error on the order of 2.6% of $\mu\alpha^4$.

Finally, using the fully coupled set of four equations (1.12a)–(1.12d) the inverse power method yields for $w(0) - 2m_e$ the values -6.7899565162, -6.7996329559, and -6.8020417571 eV or FD = 17.7856518, 4.4300339, and 1.1053577. The fixed-point Padé extrapolation procedure of the eigenvalue $\lambda \equiv b^2(w)$, based on the above three points, yields $w(0) - 2m_e = -6.8028426638$ eV. Compared to the perturbatively correct value of -6.8028426131 eV the error is on the order of 0.007% of $\mu\alpha^4$ (FD = -0.0000698) which is on the order of the $\mu\alpha^6$ error expected. This demonstrates the

importance of the inclusion of the lower–lower as well as the $^3D_1$ component and provides an important application of the inverse-power method for four coupled Schrödinger-like equations. (Note that in the perturbative treatment of the singlet and triplet equations this coupling played no role whatsoever [7].) The tabulated results for radial, as well as orbital exications, and those for muonium are presented in Ref. [7].

In summary we have extended the inverse power method combined with Padé extrapolated bound state eigenvalues from one Schrödinger-like equation to two and then four coupled Schrödinger-like equations. We have presented an inversion technique for large banded and blocked matrices analogous to that presented in textbooks [12] for unblocked and banded matrices. We have seen just as with earlier [8] work with uncoupled Schrödinger-like equation that Padé approximants were crucial in order to obtain high order accuracy with just the set of mesh points (here 256,512,1024). We also found that scaling was essential to obtain these accurate results when two length scales (angstroms and fermis) were present. (When the only length scale present was angstroms, Padé approximants were sufficient without the use of scaling). These results establish these two-body Dirac equations as reliable relativistic bound state equations; they are capable of reproducing perturbative results when treated nonperturbatively. They share this feature in common with the one-body Dirac equations. No other relativistic two-body bound state equations (including the Breit and Bethe–Salpeter equations) have been successfully tested in this way.

Furthermore, the method that we have presented in this paper is applicable to any set of coupled set of equations that are Schrödinger-like and thus can be applied in physical problems other than the one which we chose here.

REFERENCES

1. J. J. Sakurai, *Advanced Quantum Mechanics* (Addison-Wesley, Reading, MA, 1967, p. 213.
2. H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron A* (Springer-Verlag, Berlin, 1957).
3. W. Krolikowski, *Acta Phys. Polon. B* **12,** 891 (1981).
4. P. A. M. Dirac, *Lectures on Quantum Mechanics* (Yeshiva Univ., New York, 1964); P. Van Alstine, Ph.D. dissertation, Yale University, 1976; M. Kalb and P. Van Alstine, Yale Report Nos. C00-3075-146, C00-3075-156, 1976; I. T. Todorov, Dubna Joint Institute for Nuclear Research No. E2-10175, 1976; *Ann. Inst. H. Poincaré A* **28,** 207 (1978), A. Komar, *Phys. Rev. D* **18,** 1881, 1887 (1978), L. P. Horwitz and F. Rohrlich, *Phys. Rev. D* **24,** 1528 (1981).
5. P. Van Alstine and H. W. Crater, *J. Math. Phys.* **23,** 1697 (1982), H. W. Crater and P. Van Alstine, *Ann. Phys. (N.Y.)* **148,** 57 (1983); *Phys. Rev. D* **36,** 3007 (1987).
6. P. Van Alstine and H. W. Crater, *Phys. Rev. D* **34,** 1932 (1986).
7. H. W. Crater, R. L. Becker, C. Y. Wong, and P. Van Alstine, *Phys. Rev. D* **46,** 5117 (1992).
8. H. W. Crater and G. W. Reddien, *J. Comput. Phys.* **19,** 236 (1975).
9. See, for example, R. Blankenbecler and R. Sugar, *Phys. Rev.* **142,** 1051 (1966) and I. T. Todorov, in *Properties of the Fundamental Interactions,* edited by A. Zichichi (Editrice Compositori, Bologna, 1973), Vol. 9, part C, p. 953; *Phys. Rev. D* **3,** 2351 (1971).
10. D. G. Currie, T. F. Jordan, and E. C. G. Sudarshan, *Rev. Mod. Phys.* **35,** 350, 1032 (1963).
11. H. W. Crater, R. L. Becker, C. Y. Wong, and P. Van Alstine, Report No. ORNL/TM-12112, 1992 (unpublished).
12. E. Isaacson, *Analysis of Numerical Methods,* (Wiley, New York, 1966).
13. H. W. Crater and P. Van Alstine, *Phys. Rev. D* **30,** 2585 (1984).
14. We use the value $\alpha = 0.007297353$ and the electron mass $m = 0.51099916$ MeV. Note, further, that all of the equations in this paper are in natural units (with $c = \hbar = 1$). Using these numerical values for m and α in the equations in the text allows one to reproduce the numerical results given (without conversion to S.I. units). Note that the success of our method does not depend on the exact value of α or the electron mass that we chose to use. It is the smallness of the value of α that makes a comparison between the perturbative and numerical results more meaningful. If we had chosen $\alpha = 0.1$ then the numerical distinction between $O(m\alpha^4)$ and $O(m\alpha^6)$ would not have been as clear. For example, the relativistic correction to the ground state of triplet positronium due to the exchange diagram is $m\alpha^4/192$. It would be difficult to distinguish this from $O(m\alpha^6)$ for a numerical test with $\alpha = 0.1$.