RELATIVISTIC RESONANCES AND CONFINEMENT FOR SPIN-1/2 PARTICLES

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Committee Members:

Zoltán Papp, Ph.D.
Thomas Klähn, Ph.D.
Michael Peterson, Ph.D.

College Designee:

Prashanth Jaikumar, Ph.D.

By Derek Orion Wingard

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ABSTRACT

The aim of this thesis is to calculate bound and resonant states using the spin-0 and spin-$1/2$ theories within both non-relativistic and relativistic Quantum Mechanics, as well as confinement states for quark-antiquark pairs. The available theories are Schrödinger, Klein-Gordon, Dirac, Feynman and Gell-man, and Feshbach-Villars for spin-0 and spin-$1/2$. For the theories with a second order time derivative, an analytic continuation of the angular momentum allows one to easily solve them using standard Schrödinger procedures. Similarly, the Feshbach-Villars equation is already in Schrödinger form, thereby allowing the same non-relativistic procedure to apply. These equations are evaluated on a finite Coulomb-Sturmian basis which has been shown to provide an analytic solution to the Coulomb system [Z. Papp, Phys. Rev. A **74**, 1 (2006)]. A Gaussian potential is taken as a simple case for evaluation of bound states using each equation. A Yukawa potential modeling a typical nucleon-nucleon interaction is then taken to find the bound and resonant state using the Schrödinger, Feshbach-Villars spin-0 and Feshbach-Villars spin-$1/2$ equations. Finally, linear and quadratic confinement potentials are evaluated using the Schrödinger, Feshbach-Villars spin-0 and spin-$1/2$ equations.

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CHAPTER 1

INTRODUCTION

The Feshbach–Villars linearization procedure casts the usual Klein–Gordon and Dirac equations into a true Hamiltonian form, with multi-component wave functions. These components explicitly exhibit the underlying particle-antiparticle symmetry of relativistic Quantum Mechanics, and in the spin-$1/2$ case, the chiral symmetry. The Feshbach–Villars spin-0 equation comes from applying a linearization procedure to the Klein-Gordon equation. The Feshbach–Villars spin-$1/2$ equation is a result of the same procedure applied to the Feynman–Gell-Mann equation, which appears as two spin coupled Feshbach–Villars spin-0 equations. However, due to the complexity of the equations, they have been scarcely used in practical calculations. The aim of this thesis is to develop a method for solving the Feshbach–Villars equation for spin-$1/2$ particles. Due to the difficulty related to boundary conditions, we adopt a method where they are automatically incorporated. We do this by solving a Lippmann–Schwinger-type equation. This requires us to evaluate the associated Green's operator, which can be represented by continued fractions. Previous studies revealed that this method works with the Feshbach–Villars equation for spin-0 particles to evaluate bound and resonant states of a Coulomb plus short range potential, as well as bound states in confining potentials. Since the Feshbach–Villars equations are multi-component, the continued fraction becomes a matrix continued fraction. In this thesis, the Feshbach–Villars spin-$1/2$ equation is used to evaluate bound and resonant states of a short range potential, as well as bound states in a confining potential.

CHAPTER 2

FOUNDATIONS OF QUANTUM THEORY

In order to present a self-contained thesis, we feel it is important to review the mathematical foundation of quantum theory, the transition to its relativistic form, and the equations relevant to this work.

Hilbert Spaces

Quantum Mechanics “happens" in a Hilbert Space $\mathscr{H}$. These are complex vector spaces equipped with a scalar product operation $\langle\phi|\psi\rangle$ between any two vectors ϕ and ψ as defined by

$$\langle\phi|\psi\rangle = \int \phi^{\dagger}\psi. \tag{2.1}$$

The dagger operator † implies a complex conjugate transpose, which maps a vector to a linear functional in the dual space $\mathscr{H}^{*}$. Here, $|\psi\rangle$ is a column vector and $\langle\phi|$ is a dual of $|\phi\rangle$, meaning the linear functional in $\mathscr{H}^{*}$. It is defined through scalar product as its action on a vector $|\psi\rangle$ produces a scalar. The scalar product, or inner product, obeys the following properties:

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^{*}$$

$$\langle\phi+\chi|\psi\rangle = \langle\phi|\psi\rangle + \langle\chi|\psi\rangle$$

$$\langle\lambda\phi|\psi\rangle = \lambda\langle\phi|\psi\rangle$$

$$\langle\phi|\phi\rangle > 0 \ , \ \forall\phi \neq 0 \, .$$

By using the definition of the scalar product, we may construct a pre-Hilbert space, with the following properties for any vectors ϕ, ψ, or χ:

$$\langle \phi + \chi | \psi \rangle = \langle \phi | \psi \rangle + \langle \chi | \psi \rangle$$

$$\langle \phi | \lambda \psi \rangle = \lambda^* \langle \phi | \psi \rangle$$

$$\langle 0 | \psi \rangle = \langle \phi | 0 \rangle = 0$$

$$\langle \phi - \chi | \psi \rangle = \langle \phi | \psi \rangle - \langle \chi | \psi \rangle$$
$$\langle \phi | \psi - \chi \rangle = \langle \phi | \psi \rangle - \langle \phi | \chi \rangle$$

If $\langle \phi | \chi \rangle = \langle \psi | \chi \rangle$ for all χ,
then necessarily $\phi = \psi$.

Pre-Hilbert spaces are also equipped with a norm, given by $\|\phi\| = \sqrt{\langle \phi | \phi \rangle}$, which has the properties:

$$\|\lambda \phi\| = |\lambda| \ \|\phi\|$$

$\|\phi\| > 0$ when $\phi \neq \mathbf{0}$;
$\|\phi\| = 0$ when $\phi = \mathbf{0}$.

Using this norm, further properties are established. There is the Parallelogram Identity,

$$\|\phi + \psi\|^2 + \|\phi - \psi\|^2 = 2\|\phi\|^2 + 2\|\psi\|^2, \tag{2.2}$$

the polarization identity,

$$\langle \phi | \psi \rangle = \frac{1}{4} \left(\|\phi + \psi\|^2 + \|\phi - \psi\|^2 + i\|\phi + i\psi\|^2 - i\|\phi - i\psi\|^2 \right), \tag{2.3}$$

the Cauchy-Schwarz inequality,

$$|\langle \phi | \psi \rangle| \leq \|\phi\| \ \|\psi\|, \tag{2.4}$$

and the triangular identity,

$$\|\phi + \psi\| \leq \|\phi\| + \|\psi\|. \tag{2.5}$$

The idea of a distance between any two vectors must also be established, meaning we must define

the essential properties of a metric space for the pre-Hilbert space. This operation, given by $d(\phi, \psi) = \|\phi - \psi\|$, is positive definite, symmetric, and obeys the Triangular Identity.

The essential properties we require of a pre-Hilbert space have now been established, so the notion of completeness may be shown to move to a proper Hilbert space $\mathscr{H}$. A sequence of points ϕ_n is said to converge to ϕ if $d(\phi_n, \phi) \to 0$ as $n \to \infty$. ϕ can thus be referred to as the limit of ϕ_n. In a stricter case, a sequence ϕ_n is said to be a *Cauchy* sequence if $d(\phi_n, \phi_m) \to 0$ as $m, n \to \infty$. If every Cauchy sequence in the pre-Hilbert space is convergent, the space is said to be *complete*. A complete pre-Hilbert space is called a *Hilbert space*.

There is one final property often required of Hilbert spaces to be of use for Quantum Mechanics, the *separability*. This states that the only non-zero inner product between any two vectors in the set is with itself, $\langle \phi_n | \phi_n \rangle > 0$, unless it is the zero vector, for which the result is $\langle 0|0\rangle = 0$. This is equivalent to saying $\mathscr{H}$ possesses an *orthogonal basis*.

Schrödinger Quantum Mechanics

A normalized vector ψ of $\mathscr{H}$ is used to establish the validity of the probabilistic interpretation,

$$\langle \psi | \psi \rangle = \int \psi^\dagger(z)\psi(z)\mathrm{d}z = +1. \tag{2.6}$$

This vector is referred to as the wave function. In the non-relativistic theory, it satisfies the Schrödinger equation,

$$\hat{H}\psi = \left[\frac{\hat{p}^2}{2m} + \hat{V}\right]\psi = E\psi. \tag{2.7}$$

In the position representation, one applies the correspondence principle by making the substitutions

$$\hat{p} \to -i\hbar\nabla \tag{2.8}$$

and

$$E \to i\hbar\partial_t, \tag{2.9}$$

to arrive at the usual form

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}\right]\psi = i\hbar\partial_t\psi. \tag{2.10}$$

This is the basic equation of non-relativistic quantum mechanics. It has been derived from the classical mechanical Hamiltonian and the correspondence principle.

Klein-Gordon Equation

If we wish to derive a relativistic theory, we should apply the correspondence principle to the length of a 4-momentum vector p_μ, which is a Lorentz scalar. p_μ is given by

$$p_\mu = \left(\frac{E}{c}, -\mathbf{p}\right), \tag{2.11}$$

where **p** is the usual 3-vector momentum of the Schrödinger theory. This connects the energy and momentum. The invariant length is given by

$$E^2 - p^2c^2 = m^2c^4. \tag{2.12}$$

Now adopting natural units where $\hbar = c = 1$, p_μ can in turn be treated as an operator by

$$p_\mu = i\left(\partial_t, \partial_x, \partial_y, \partial_z\right), \qquad p^\mu p_\mu = p^\mu \eta_{\mu\nu} p^\nu = E^2 - \mathbf{p}\cdot\mathbf{p} = -\frac{\partial^2}{\partial t^2} + \nabla^2, \tag{2.13}$$

where the Einstein summation convention is assumed and $\eta^{\mu\nu} = \text{Diag}(+,-,-,-)$ is the Minkowski metric. ∂_μ^2 similarly becomes

$$\partial^\mu\partial_\mu = dt^2 - \nabla^2, \tag{2.14}$$

where the notation means $\frac{\partial}{\partial x_\mu} = \partial_\mu$. It is also customary to redefine $(t, x, y, z) \to (0, 1, 2, 3)$. In a relativistic setting, the energy momentum dispersion relation is

$$E^2 = p^2 + m^2. \tag{2.15}$$

Applying the correspondence principle to this relation results in the Klein-Gordon equation, in the absence of external fields,

$$E^2 - p^2 = m^2 \ \to \left[-\partial_0^2 + \nabla^2 - m^2\right] \psi = 0. \tag{2.16}$$

Using Eq.(2.13), it simplifies to

$$\left[p^\mu p_\mu - m^2\right] \psi = 0. \tag{2.17}$$

If one wishes to include interactions to this equation, the standard minimal coupling procedure is applied, using the 4-potential $A_\mu = (\phi, \mathbf{A})$, via

$$p_\mu \to p_\mu - eA_\mu. \tag{2.18}$$

Being second order in space and time, this containing only scalars, thus the equation is manifestly Lorentz invariant. The natural next step is to construct the probability density and confirm that it obeys the requirements of a proper quantum mechanical equation. The related probability density is given by

$$\rho = \frac{i}{2m} \left(\psi^* \partial_0 \psi - \psi \partial_0 \psi^*\right). \tag{2.19}$$

This poses a serious problem as the integral of this density is no longer positive or even definite. In this framework, the wave function and its time derivative are initial conditions we must provide, so ρ can take arbitrary positive or negative values. This issue has been addressed independently by Dirac, Feshbach, and Villars, which will be covered in the following sections.

Dirac Equation

Dirac sought to rectify the issue of a non-positive definite probability density by deriving a proper relativistic equation for electrons that was linearly symmetric in space and time via addition of variables α_i, β for $i = 1, 2, 3$ [1]. The derivation again starts with looking at the relativistic dispersion equation,

$$E^2 - p^2 - m^2 = 0, \tag{2.20}$$

where the goal is an equation of the form

$$E - \alpha_1 p_1 - \alpha_2 p_2 - \alpha_3 p_3 - \beta m = 0. \tag{2.21}$$

Eq.(2.20) can be split into two parts with the use our the new variables α_i, β as

$$(p_0 - \alpha_1 p_1 - \alpha_2 p_2 - \alpha_3 p_3 - \beta m)(p_0 + \alpha_1 p_1 + \alpha_2 p_2 + \alpha_3 p_3 + \beta m)\psi = 0, \tag{2.22}$$

wherein the substitution $E \to p_0$ has been performed. Presently, all that can be said about the objects α_i, β is they are independent of momentum p_0, p_1, p_2, p_3 and they commute with coordinate variables $x_0 = t, x_1 = x, x_2 = y, x_3 = z$. Expanding Eq.(2.22), we find

$$\left(p_0^2 - \sum \alpha_1^2 p_1^2 - \sum (\alpha_1\alpha_2 + \alpha_2\alpha_1)p_1 p_2 - \beta^2 m^2 - \sum (\alpha_1\beta + \beta\alpha_1)p_1\right)\psi = 0, \tag{2.23}$$

where the sum is taken over cyclic permutations of the suffixes $1, 2, 3$. Using the anticommutator notation $\{x, y\} = xy + yx$, Eq.(2.23) becomes

$$\left(p_0^2 - \sum \alpha_1^2 p_1^2 - \sum \{\alpha_1, \alpha_2\}p_1 p_2 - \beta^2 m^2 - \sum \{\alpha_1, \beta\}p_1\right)\psi = 0. \tag{2.24}$$

Since the goal is to derive Eq.(2.20), the following structure for the objects α_i, β is required:

$$\alpha_i^2, \beta^2 = 0, \qquad \{\alpha_i, \beta\} = 0, \qquad \{\alpha_i, \alpha_j\} = 0 \quad (i \neq j). \tag{2.25}$$

We can readily see these relations cannot be satisfied by numbers. These objects must be taken as matrices to satisfy the above relations. We can make use of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.26}$$

since they obey the same structure as the α_i's. However, since four matrices are required and the identity does not satisfy the relations, the three Pauli matrices alone do not suffice. To remedy this, new matrices are formed as $\Sigma_i = \mathbb{1}_2 \otimes \sigma_i$, using the tensor product $\otimes$, giving

$$\Sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \Sigma_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \qquad \Sigma_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{2.27}$$

Interchanging the second and third rows and columns gives three more independent matrices,

$$\rho_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \qquad \rho_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \qquad \rho_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

These new Σ_i and ρ_i matrices obey the same structure defined by Eq.(2.25), with the additional property of $[\Sigma_i, \rho_j] = 0$ by construction, where $[\,,]$ is the usual commutator. Constructing the new α_i, β as

$$\beta = \rho_3, \qquad \alpha_1 = \rho_1\Sigma_1, \qquad \alpha_2 = \rho_1\Sigma_2, \qquad \alpha_3 = \rho_1\Sigma_3, \tag{2.28}$$

the structure of Eq.(2.25) is preserved. These α_i matrices take the form

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}. \tag{2.29}$$

Then, Eq.(2.21) is satisfied with these matrices giving

$$[p_0 - \boldsymbol{\alpha} \cdot \mathbf{p} - \beta m]\, \psi = 0, \tag{2.30}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and $\mathbf{p} = (p_1, p_2, p_3)$. Applying the correspondence principle gives

$$[i\partial_t - \boldsymbol{\alpha} \cdot (-i\,\nabla) - \beta m]\, \psi = 0. \tag{2.31}$$

Multiplying by β from the left and making the substitutions

$$(t, x, y, z) \to (0, 1, 2, 3), \qquad \beta \to \gamma^0, \qquad \beta\alpha_i \to \gamma^i, \tag{2.32}$$

generates the γ^μ matrices in the Dirac representation

$$\gamma^0 = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}. \tag{2.33}$$

With these matrices, we have the well known form of the Dirac equation,

$$[i\gamma^\mu \partial_\mu - m]\, \psi = 0, \tag{2.34}$$

where $\mu = 0, 1, 2, 3$. These new γ^μ matrices have the structure

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}\mathbb{1}_4, \tag{2.35}$$

which is associated to the Clifford algebra $\mathrm{Cl}_{1,3}(\mathbb{C})$. This algebra represents the structure of the space-time manifold on which the Dirac equation is defined [2]. Subtracting both sides of Eq.(2.35) by $\gamma^\mu\gamma^\nu$ gives us the important relation,

$$\gamma^\mu\gamma^\nu = \eta^{\mu\nu}\mathbb{1}_4 + \frac{1}{2}[\gamma^\mu, \gamma^\nu]. \tag{2.36}$$

It can be shown that Eq.(2.34) is Lorentz covariant [1], however not manifestly. This is expected as the equation is entirely first order, yet it was derived from the invariant length of the 4-momentum vector. Due to its first order symmetry in space and time, the probability density is

$$\rho = \psi^\dagger\psi, \tag{2.37}$$

of which the integral is definite. This allows the probabilistic interpretation, where the positive and negative solutions are associated to particles and antiparticles, respectively.

Feynman–Gell-Mann Equation

Feynman and Gell-Mann demonstrated that it is possible to rewrite the Dirac equation using two components in an equation which is second order in space and time [3]. To show this, we need to define γ^5, which, in the Dirac representation, is given by

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 \end{pmatrix}. \tag{2.38}$$

Using this operator, we can construct the projection operators as $P_\pm = \frac{1}{2}(1 \pm \gamma^5)$, which splits the ψ into components as

$$P_\pm\psi = \psi_\pm. \tag{2.39}$$

It is also clear that these operators have the following properties:

$$P_+ + P_- = \mathbb{1}_4, \qquad P_\pm^2 = \mathbb{1}_4, \qquad [P_-, P_+] = 0, \qquad P_+\gamma^\mu = \gamma^\mu P_-. \tag{2.40}$$

The final property is not obvious, it makes use of the Clifford structure of the γ^μ matrices. Looking at Eq.(2.34), it is seen that $i\gamma^\mu\partial_\mu\psi = m\psi$. Therefore, we can equate

$$\psi_- = \frac{1}{m}P_-(i\gamma^\mu\partial_\mu)\psi = \frac{i}{m}\gamma^\mu\partial_\mu\psi_+. \tag{2.41}$$

Then, from $P_+ + P_- = \mathbb{1}_4$, we find

$$\psi = \psi_+ + \psi_- = \psi_+ + \frac{i}{m}\gamma^\mu\partial_\mu\psi_+ = \frac{1}{m}(i\gamma^\mu\partial_\mu + m)\psi_+. \tag{2.42}$$

We can introduce interaction by using the minimal coupling. Plugging Eq.(2.42) in for the wave function of Eq.(2.34) with $D_\mu \equiv \partial_\mu + ieA_\mu$, we get

$$\left[i\gamma^\mu D_\mu + m\right]\left[i\gamma^\nu D_\nu - m\right]\psi_+ = [\gamma^\mu\gamma^\nu D_\mu D_\nu + m^2]\psi_+ = 0. \tag{2.43}$$

Looking at the first term, we can make use of Eq.(2.36) to show

$$\begin{aligned}\gamma^\mu\gamma^\nu D_\nu D_\mu &= \eta^{\mu\nu}D_\mu D_\nu + \frac{1}{2}[\gamma^\mu, \gamma^\nu]D_\mu D_\nu \\ &= D^\mu D_\mu + \frac{1}{2}[\gamma^\mu, \gamma^\nu]D_\mu D_\nu,\end{aligned} \tag{2.44}$$

where the final line makes use of the symmetry property of the metric $\eta^{\mu\nu} = \eta^{\nu\mu}$. The

$[\gamma^\nu, \gamma^\nu]D_\mu D_\nu$ term can be expanded, where for every permutation of μ, ν we have

$$\begin{aligned}
[\gamma^\nu, \gamma^\nu]D_\mu D_\nu &= \frac{1}{2}(\gamma^\mu\gamma^\nu D_\mu D_\nu - \gamma^\nu\gamma^\mu D_\nu D_\mu + \gamma^\nu\gamma^\mu D_\nu D_\mu - \gamma^\mu\gamma^\nu D_\nu D_\mu) \\
&= \frac{1}{2}(\gamma^\mu\gamma^\nu[D_\mu, D_\nu] + \gamma^\nu\gamma^\mu[D_\nu, D_\mu]) \\
&= \frac{1}{2}[\gamma^\mu, \gamma^\nu][D_\mu, D_\nu] \\
&= \gamma^\mu\gamma^\nu[D_\mu, D_\nu],
\end{aligned} \tag{2.45}$$

which gives

$$\gamma^\mu\gamma^\nu\left([\partial_\mu, \partial_\nu] + ie\left([\partial_\mu, A_\nu] + [A_\mu, \partial_\nu]\right) - e^2[A_\mu, A_\nu]\right). \tag{2.46}$$

We can immediately see two terms drop out as $[A_\mu, A_\nu] = 0$ and, by Clairaut's theorem, we have $[\partial_\mu, \partial_\nu]\psi = 0$ as well. This leaves

$$ie\gamma^\mu\gamma^\nu\left([\partial_\mu, A_\nu] + [A_\mu, \partial_\nu]\right). \tag{2.47}$$

Expanding the commutators gives

$$\begin{aligned}
[\partial_\mu, A_\nu] + [A_\mu, \partial_\nu] &= \partial_\mu A_\nu - A_\nu\partial_\mu + A_\mu\partial_\nu - \partial_\nu A_\mu \\
&= \partial_\mu A_\nu - \partial_\nu A_\mu + A_\mu\partial_\nu - A_\nu\partial_\mu.
\end{aligned} \tag{2.48}$$

Acting on ψ_+ then produces

$$\begin{aligned}
\partial_\mu(A_\nu\psi_+) - \partial_\nu(A_\mu\psi_+) + A_\mu\partial_\nu\psi_+ - A_\nu\partial_\mu\psi_+ &= \partial_\mu A_\nu\psi_+ + A_\nu\partial_\mu\psi_+ - \partial_\nu A_\mu\psi_+ - A_\mu\partial_\nu\psi_+ \\
&\quad + A_\mu\partial_\nu\psi_+ - A_\nu\partial_\mu\psi_+ \\
&= (\partial_\mu A_\nu - \partial_\nu A_\mu)\psi_+.
\end{aligned} \tag{2.49}$$

The resulting term $\partial_\mu A_\nu - \partial_\nu A_\mu$ is the Maxwell electromagnetic field tensor $F_{\mu\nu}$, which, in its

covariant form, is given by

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{pmatrix}. \tag{2.50}$$

We can therefore rewrite Eq.(2.43) as

$$\left[D^\mu D_\mu + \frac{1}{2} ie\gamma^\mu\gamma^\nu F_{\mu\nu} + m^2 \right] \psi_+ = 0. \tag{2.51}$$

This can be further simplified using the relations

$$\begin{aligned} i\Sigma_i &= -\gamma_j\gamma_k = \gamma_k\gamma_j, \\ \alpha_i &= -\gamma_i\gamma_0 = \gamma_0\gamma_i, \end{aligned} \tag{2.52}$$

where we take the subscripts $i, j = 1, 2, 3$. The Σ_i relation holds for all cyclic permutations of indices. Upon evaluating the independent elements, we get

$$\begin{aligned} \gamma^2\gamma^3 F_{23} &= i\Sigma_1 B_1, \\ \gamma^3\gamma^1 F_{31} &= i\Sigma_2 B_2, \\ \gamma^1\gamma^2 F_{12} &= i\Sigma_3 B_3, \\ \gamma^0\gamma^1 F_{01} &= \alpha_1 E_1, \\ \gamma^0\gamma^2 F_{02} &= \alpha_2 E_2, \\ \gamma^0\gamma^3 F_{03} &= \alpha_3 E_3. \end{aligned} \tag{2.53}$$

Every term is double counted due to the Clifford structure of the γ^μ and the antisymmetry of $F^{\mu\nu}$.

This allows Eq.(2.51) to be rewritten as

$$\left[D^\mu D_\mu + m^2 + ie\left(\boldsymbol{\alpha}\cdot\mathbf{E} + i\,\boldsymbol{\Sigma}\cdot\mathbf{B}\right)\right]\psi_+ = 0, \tag{2.54}$$

Using the definition of the wave function in Eq.(2.39), we can further simplify the above equation. A Dirac spinor in the Dirac representation is given by $\psi = (\phi_a, \phi_b, \phi_c, \phi_d)^T$. From $\psi_+ = P_+\psi$, we see

$$\psi_+ = \begin{pmatrix} \phi_a + \phi_c \\ \phi_b + \phi_d \\ \phi_c + \phi_a \\ \phi_d + \phi_b \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix}. \tag{2.55}$$

From this result, it is clear that

$$\phi_1 = \phi_3 \quad \text{and} \quad \phi_2 = \phi_4, \tag{2.56}$$

and the equation is thus invariant under permutation of the equivalent pairs. We can make use of the structure of the α_i and Σ_i matrices and Eq.(2.56) to write Eq.(2.54) as two equations:

$$\begin{aligned} [D_0^2 - D_1^2 - D_2^2 - D_3^2 + m^2]\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} + ie\,\boldsymbol{\sigma}\cdot\mathbf{E}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} - \boldsymbol{\sigma}\cdot\mathbf{B}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} = 0, \\ [D_0^2 - D_1^2 - D_2^2 - D_3^2 + m^2]\begin{pmatrix}\phi_3\\ \phi_4\end{pmatrix} + ie\,\boldsymbol{\sigma}\cdot\mathbf{E}\begin{pmatrix}\phi_3\\ \phi_4\end{pmatrix} - \boldsymbol{\sigma}\cdot\mathbf{B}\begin{pmatrix}\phi_3\\ \phi_4\end{pmatrix} = 0. \end{aligned} \tag{2.57}$$

We can therefore take just one of them with no loss of generality. The entire energy spectrum follows from either of them. In order to most closely match the nonrelativistic limit, we shall Wick rotate our sytem to express the equation in Euclidean space, rather than Minkowski space, meaning our metric signature transforms as $(+,-,-,-) \to (+,+,+,+)$. This is done by going to complex time, implying we take the zeroth component of every object and multiply it by i.

Using the notation $\phi = (\phi_1, \phi_2)^T$, we can Wick rotate the upper equation of Eq.(2.57) to give

$$[D_0^2 + D_1^2 + D_2^2 + D_3^2 - m^2 - \boldsymbol{\sigma} \cdot (ie\mathbf{E} - \mathbf{B})]\phi = 0. \tag{2.58}$$

This equation is in, what is often called, the nonrelativistic representation. In the work of this thesis, it will be solved numerically to evaluate the energy spectrum of a short range potential.

Chiral Decoupling

Eq.(2.54) can also be decoupled in the Weyl representation. To achieve this, we will again make use of the γ^5 matrix. We can transform to the Weyl representation using the unitary transformation matrix

$$U = \frac{1}{\sqrt{2}}(1 + \gamma^5\gamma^0) = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1}_2 & -\mathbb{1}_2 \\ \mathbb{1}_2 & \mathbb{1}_2 \end{pmatrix}. \tag{2.59}$$

An operator $\hat{O}$ is transformed as $\hat{O}_W = U^\dagger \hat{O} U$ and a vector as $\psi_W = U\psi$, where the subscript is added to avoid confusion with other representations. We can transform Eq.(2.54) to the Weyl representation as

$$\begin{aligned} &U^\dagger \left[\mathbb{1}_4(D^\mu D_\mu + m^2) + ie\,(\boldsymbol{\alpha} \cdot \mathbf{E} + i\,\boldsymbol{\Sigma} \cdot \mathbf{B})\right] U U^\dagger \psi \\ &= \left[\mathbb{1}_4(D^\mu D_\mu + m^2) + ie\,U^\dagger(\boldsymbol{\alpha} \cdot \mathbf{E} + i\,\boldsymbol{\Sigma} \cdot \mathbf{B})U\right] \psi_W = 0. \end{aligned} \tag{2.60}$$

The object $D^\mu D_\mu$ is a scalar, therefore we can pass our transformation operators right to the coupling terms. Evaluating them individually, we first start with $U(\boldsymbol{\Sigma} \cdot \mathbf{B})U^\dagger$. The B_i terms are invariant under this transformation, so we can focus specifically on how each $U^\dagger \Sigma_i U$ transforms:

$$U^\dagger \Sigma_i U = \Sigma_i. \tag{2.61}$$

This allows us to represent the object $\mathbf{\Sigma} \cdot \mathbf{B}$ in the Weyl basis as

$$U^\dagger(\mathbf{\Sigma} \cdot \mathbf{B})U = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \boldsymbol{\sigma} \cdot \mathbf{B}. \tag{2.62}$$

We also transform our α_i matrices and find

$$\begin{aligned} U^\dagger \alpha_1 U &= \begin{pmatrix} \sigma_1 & 0 \\ 0 & -\sigma_1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \sigma_1, \\ U^\dagger \alpha_2 U &= \begin{pmatrix} \sigma_2 & 0 \\ 0 & -\sigma_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \sigma_2, \\ U^\dagger \alpha_3 U &= \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \sigma_3. \end{aligned} \tag{2.63}$$

From this, it follows that $\boldsymbol{\alpha} \cdot \mathbf{E}$ is given in the Weyl representation as

$$U^\dagger(\boldsymbol{\alpha} \cdot \mathbf{E})U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \boldsymbol{\sigma} \cdot \mathbf{E}. \tag{2.64}$$

Finally, the Feynman–Gell-Mann equation in the Weyl representation reads

$$\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \mathbb{1}_2 (D^\mu D_\mu + m^2) + ie \left(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \boldsymbol{\sigma} \cdot \mathbf{E} + i \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \boldsymbol{\sigma} \cdot \mathbf{B} \right) \right] \psi_W. \tag{2.65}$$

Taking the wave function as two component Weyl spinors,

$$\psi_W = \begin{pmatrix} \phi_L \\ \phi_R \end{pmatrix}, \tag{2.66}$$

we can use these to rewrite Eq.(2.65) as two separate equations:

$$\begin{aligned}\left[D^{\mu}D_{\mu}+m^{2}+ie\boldsymbol{\sigma}\cdot(i\mathbf{B}+\mathbf{E})\right]\phi_{L}&=0\\ \left[D^{\mu}D_{\mu}+m^{2}+ie\boldsymbol{\sigma}\cdot(i\mathbf{B}-\mathbf{E})\right]\phi_{R}&=0.\end{aligned}\tag{2.67}$$

Unlike in Eq.(2.58), we cannot take one or the other and solve the entire system, as they are not individually parity invariant. This is because the wave functions are now expressed in Weyl spinors. These objects are representatives of elements in Spin(1,3), a double covering of the proper Lorentz group SO(1,3), and parity is contained only in the complete Lorentz group O(1,3). Thus, either individual equation for ϕ_L or ϕ_R is insufficient to properly describe a quantum electrodynamic system. Under parity, the Weyl spinors swap, and the equations transform into each other to maintain invariance. This is best observed in a spinor representation [4]. Given the first order equation, Eq.(2.34), acting on a Dirac spinor, which contains linear combinations of Weyl spinors, it remains invariant under parity and therefore *acts* like a representative of Pin(1,3). Pin(1,3) is a double covering of O(1,3), the complete Lorentz group, thereby transforming accordingly under parity. This means one should take both equations in Eq.(2.67) if a "proper" relativistic quantum electrodynamic description of nature is desired. This desire is precisely what is addressed in the following section where a Hamiltonian form of Eq.(2.67) is derived in an 8-component representation.

Feshbach-Villars Formalism

Feshbach and Villars introduced a linearization procedure capable of casting the second order spin-0 equations into a Hamiltonian form, meaning first order in time [5]. The procedure was extended to the Feynman-Gell-Mann equation for spin-$1/2$ particles later by Robson [6, 7]. This method is applied to Eq.(2.67), as it remains decoupled in the Weyl representation. The method derived here follows the work of Staudte [4]. The linearization procedure introduces new

wave functions given by

$$\begin{aligned} \varphi &= \left(1 + \frac{iD_0}{m}\right)\psi, \\ \chi &= \left(1 - \frac{iD_0}{m}\right)\psi. \end{aligned} \tag{2.68}$$

The new functions satisfy the equations:

$$\psi = \varphi + \chi \qquad \frac{iD_0}{m}\psi = \varphi - \chi. \tag{2.69}$$

Substituting one into the other gives

$$D_0(\varphi + \chi) = -im(\varphi - \chi)\cdot \tag{2.70}$$

From Eq.(2.67), repeated below,

$$\left[D^\mu D_\mu + m^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right]\phi_L = 0 \tag{2.71a}$$

$$\left[D^\mu D_\mu + m^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} - \mathbf{E})\right]\phi_R = 0, \tag{2.71b}$$

we take either of the Weyl spinor wave functions ϕ_L or ϕ_R as ψ in Eq.(2.68). First with ϕ_L, let φ_L, χ_L be defined by Eq.(2.68) as

$$\begin{aligned} \varphi_L &= \left(1 + \frac{iD_0}{m}\right)\phi_L \\ \chi_L &= \left(1 - \frac{iD_0}{m}\right)\phi_L. \end{aligned} \tag{2.72}$$

Using Eq.(2.70), we have

$$D_0(\varphi_L + \chi_L) = -im(\varphi_L - \chi_L). \tag{2.73}$$

Since $D^\mu D_\mu = D_0^2 - \mathbf{D}^2$, Eq.(2.71a) can be rearranged as

$$\mathbb{1}_2 D_0^2\phi_L = \left[\mathbb{1}_2(\mathbf{D}^2 - m^2) + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right]\phi_L, \tag{2.74}$$

where identity operators have been added for clarity. Using Eq.(2.73) and Eq.(2.69), we see that

$$D_0^2\phi_L = D_0 D_0(\varphi_L + \chi_L) = -imD_0(\varphi_L - \chi_L). \tag{2.75}$$

This is then substituted into Eq.(2.74), along with $\phi_L = \varphi_L + \chi_L$, to give

$$\mathbb{1}_2 D_0(\varphi_L - \chi_L) = \frac{i}{m}\left[\mathbb{1}_2(\mathbf{D}^2 - m^2) + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right](\varphi_L + \chi_L). \tag{2.76}$$

Next, add the left side of Eq.(2.73) to the left side of Eq.(2.76) and the same for the right sides, so that we can write both D_0 and m in terms of φ_L only:

$$\begin{aligned}
\mathbb{1}_2 D_0(\varphi_L - \chi_L) + \mathbb{1}_2 D_0(\varphi_L + \chi_L) &= \frac{i}{m}\left(\mathbb{1}_2\mathbf{D}^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right)(\varphi_L + \chi_L) - \mathbb{1}_2 im(\varphi_L + \chi_L) \\
&\quad - \mathbb{1}_2 im(\varphi_L - \chi_L) \\
2\mathbb{1}_2 D_0\varphi_L &= \frac{i}{m}\left(\mathbb{1}_2\mathbf{D}^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right)(\varphi_L + \chi_L) - 2\mathbb{1}_2 im\varphi_L \\
\mathbb{1}_2 iD_0\varphi_L &= -\frac{1}{2m}\left(\mathbb{1}_2\mathbf{D}^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right)(\varphi_L + \chi_L) + \mathbb{1}_2 m\phi_L.
\end{aligned} \tag{2.77}$$

We can make the substitution $D_0 = \partial_0 + ieA_0$ to put it in a Hamiltonian form,

$$\mathbb{1}_2 i\partial_0\varphi_L = \frac{1}{2m}\left(-\mathbb{1}_2\mathbf{D}^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right)(\varphi_L + \chi_L) + \mathbb{1}_2 m\varphi_L + \mathbb{1}_2 eA_0\varphi_L. \tag{2.78}$$

Then, subtracting the left and right side of Eq.(2.73) from the left and right side respectively of Eq.(2.76) gives

$$\mathbb{1}_2 i\partial_0\chi_L = -\frac{1}{2m}\left(-\mathbb{1}_2\mathbf{D}^2 + ie\,\boldsymbol{\sigma}\cdot(i\mathbf{B} + \mathbf{E})\right)(\varphi_L + \chi_L) - \mathbb{1}_2 m\chi_L + \mathbb{1}_2 eA_0\chi_L. \tag{2.79}$$

We can combine these two equations into a 4-component Hamiltonian $\hat{H}_L$ using the wave function $\Psi_L = \frac{1}{\sqrt{2}}(\varphi_L, \chi_L)^T$:

$$\mathbb{1}_4 i\partial_0 \Psi_L = \left[\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \otimes \frac{1}{2m} \left(-\mathbb{1}_2 \mathbf{D}^2 + ie\boldsymbol{\sigma} \cdot (i\mathbf{B} + \mathbf{E}) \right) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \mathbb{1}_2 m + \mathbb{1}_4 eA_0 \right] \Psi_L. \tag{2.80}$$

If we make use of the Pauli matrices, we can see

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_3, \qquad \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} = \sigma_3 + i\sigma_2. \tag{2.81}$$

Here, the Pauli matrices that act on the component space, rather than spin space, will be relabelled to τ to avoid confusion with the Pauli matrices in the spin coupled terms. Defining a new squared momentum variable $\boldsymbol{\pi}_L^2 = (-\mathbb{1}_2 \mathbf{D}^2 + ie\boldsymbol{\sigma} \cdot (i\mathbf{B} + \mathbf{E}))$, we can simplify Eq.(2.80) to

$$\mathbb{1}_4 i\partial_0 \Psi_L = \left[(\tau_3 + i\tau_2) \otimes \frac{\boldsymbol{\pi}_L^2}{2m} + \tau_3 \otimes \mathbb{1}_2 m + \mathbb{1}_4 eA_0 \right] \Psi_L. \tag{2.82}$$

Repeating the process for Eq.(2.71b) amounts only to defining a $\boldsymbol{\pi}_R^2 = (-\mathbb{1}_2 \mathbf{D}^2 + ie\boldsymbol{\sigma} \cdot (i\mathbf{B} - \mathbf{E}))$, then the rest of the equation for $\hat{H}_R$ is identical:

$$\mathbb{1}_4 i\partial_0 \Psi_R = \left[(\tau_3 + i\tau_2) \otimes \frac{\boldsymbol{\pi}_R^2}{2m} + \tau_3 \otimes \mathbb{1}_2 m + \mathbb{1}_4 eA_0 \right] \Psi_R. \tag{2.83}$$

Combining both of these equations into one 8-component representation with $\Psi = (\Psi_L, \Psi_R)^T$ gives

$$\mathbb{1}_8 i\partial_0 \Psi = \begin{pmatrix} (\tau_3 + i\tau_2) \otimes \frac{\boldsymbol{\pi}_L^2}{2m} + \tau_3 \otimes \mathbb{1}_2 m + \mathbb{1}_4 eA_0 & 0 \\ 0 & (\tau_3 + i\tau_2) \otimes \frac{\boldsymbol{\pi}_R^2}{2m} + \tau_3 \otimes \mathbb{1}_2 m + \mathbb{1}_4 eA_0 \end{pmatrix} \Psi, \tag{2.84}$$

or equivalently,

$$\begin{pmatrix} \mathbb{1}_4 i\partial_0 - \hat{H}_L & 0 \\ 0 & \mathbb{1}_4 i\partial_0 - \hat{H}_R \end{pmatrix} \begin{pmatrix} \Psi_L \\ \Psi_R \end{pmatrix} = (\mathbb{1}_8 i\partial_0 - \hat{H}_{FV1/2})\Psi = 0. \tag{2.85}$$

If we define an operator $\tau_4 = \tau_3 \otimes \gamma^0_W$, the Hamiltonian $\hat{H}_{FV1/2}$ is τ_4-Hermitian, meaning we have $\hat{H}_{FV1/2} = \tau_4 \hat{H}^\dagger_{FV1/2} \tau_4$. The inner product is also defined with τ_4 as

$$\langle \Psi | \Psi \rangle = \int \Psi^\dagger \tau_4 \Psi = \pm 1. \tag{2.86}$$

This need not be positive definite as it is square integrable for stationary states and $\langle \Psi | \Psi \rangle = \pm 1$ can be chosen for particle or antiparticle solutions.

The Hamiltonian $\hat{H}_{FV1/2}$ is also built out of irreducible representations of the proper Lorentz group SO(1,3), $\hat{H}_L$ and $\hat{H}_R$ exchange under spacial inversion, and Ψ_L and Ψ_R transform into one and other, thus maintaining parity invariance. It is multi-component, displaying explicitly the particle-antiparticle features of nature. All together, this makes the Feshbach–Villars spin-$1/2$ equation the natural second order relativistic wave equation. In this thesis, this equation is solved with a short range potential to calculate resonant states, as well as linear and quadratic confinement potentials to model quark confinement.

For spin-0 particles, the procedure is applied to the Klein-Gordon equation, which is identified as either Eq.(2.71a) or Eq.(2.71b), with no $\boldsymbol{\sigma}$ term and the index L/R dropped from the wave function. The same process gives an identical equation to either $\hat{H}_L$ or $\hat{H}_R$, where $\boldsymbol{\pi}^2_{L/R}$ is replaced by the usual minimally coupled squared momentum operator $\boldsymbol{\pi}^2 = (\mathbf{p} - e\mathbf{A})^2$. This provides us the Feshbach-Villars equation for spin-0 particles,

$$\hat{H}_{FV0} = (\tau_3 + i\tau_2)\frac{\boldsymbol{\pi}^2}{2m} + \tau_3 m + \mathbb{1}_2 e A_0. \tag{2.87}$$

In the same fashion as the FV$1/2$ equation, this Hamiltonian is τ_3-Hermitian.

Scalar Interaction

We can introduce confinement interaction by modifying the mass term as $m \to m + S/c^2$. For Klein-Gordon equation, this gives

$$\begin{aligned} E^2 &= p^2 + (m + S/c^2)^2 \\ &= p^2 + m^2 + 2mS/c^2 + S^2/c^4 \\ &= p^2 + 2mU + m^2, \end{aligned} \tag{2.88}$$

where $U = S + S^2/2mc^2$. We can therefore include a scalar interaction into our final Feshbach-Villars equation for spin-0 through the substitution given by

$$\frac{\boldsymbol{\pi}^2}{2m} \to \frac{\boldsymbol{\pi}^2}{2m} + U. \tag{2.89}$$

In the spin-$1/2$ case, the situation is the same so we can make the substitution

$$\frac{\boldsymbol{\pi}^2_{L/M}}{2m} \to \frac{\boldsymbol{\pi}^2_{L/M}}{2m} + U. \tag{2.90}$$

This amounts to adding

$$\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} U \tag{2.91}$$

to $\hat{H}_{FV0}$ for the spin-0 case and

$$\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \otimes \mathbb{1}_2 U \tag{2.92}$$

to $\hat{H}_L$ and $\hat{H}_R$ for spin-$1/2$.

CHAPTER 3

COULOMB-STURMIAN BASIS

The Coulomb-Sturmian basis functions, with angular momentum l and real parameter b, are defined as

$$\langle r \mid nl\rangle = \frac{\sqrt{\Gamma(n+1)}}{\sqrt{\Gamma(n+2l+2)}} \exp(-br)(2br)^{l+1} L_n^{2l+1}(2br), \tag{3.93}$$

where L_n^{2l+1} are the associated Laguerre polynomials. This basis has a biorthogonal pairing with $\langle r|\widetilde{nl}\rangle = \langle r|nl\rangle/r$, which generates the completeness relation

$$\lim_{N\to\infty} \sum_{n=0}^{N} |nl\rangle\langle\widetilde{n'l}| = \mathbb{1}. \tag{3.94}$$

This is also understood as orthogonality with respect to a r^{-1} weighting function, meaning this basis is well suited for representing Coulomb systems. When the inner product is taken without the weighting function, we get the symmetric tridiagonal structure,

$$\begin{aligned}&\langle n,l;b|m,l;b\rangle = \\ &\quad \frac{1}{2b}\left[\delta_{nm}(2n+2l+2) - \delta_{nm-1}\sqrt{(n+1)(n+2l+2)} - \delta_{nm+1}\sqrt{n(2l+n+1)}\right].\end{aligned} \tag{3.95}$$

Approximation of Potentials

A short range potential $v_l^{(s)}$ can be approximated on a finite subset of this basis as

$$v_l^{(s)} \approx \sum_{nm}^{N} \widetilde{|nl;b\rangle}\tilde{v}_{l,nm}^{(s)}\widetilde{\langle ml;b|}, \tag{3.96}$$

where $\tilde{v}_{l,nm}^{(s)} = \langle nl;b|\tilde{v}_l^{(s)}|ml;b\rangle$. The matrix $\tilde{v}_{l,nm}^{(s)}$ is calculated following [8]. Taking the basis to $N' > N$, the operator is inverted and truncated from N' to N, then inverted again. This has been shown to produce more accurate approximations of potentials than alternative methods [8].

Continued Fraction Representation

Consider a Hamiltonian H and an operator J, defined as $J(z) = z - H$ for complex z, such that an infinite tridiagonal symmetric (Jacobi) structure is generated when represented on a discrete Hilbert space basis $\{|i\rangle\}$. This operator has an associated Green's operator, $G(z)$, given by the resolvent equation

$$J(z)G(z) = \mathbb{1}. \tag{3.97}$$

In the basis representation, the above equation becomes

$$\begin{pmatrix} J_{0,0} & J_{0,1} & 0 & 0 & \dots \\ J_{1,0} & J_{1,1} & J_{1,2} & 0 & \dots \\ 0 & J_{2,1} & J_{2,2} & J_{2,3} & \dots \\ 0 & 0 & J_{3,2} & J_{3,3} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \times \begin{pmatrix} G_{0,0} & G_{0,1} & G_{0,2} & G_{0,3} & \dots \\ G_{1,0} & G_{1,1} & G_{1,2} & G_{1,3} & \dots \\ G_{2,0} & G_{2,1} & G_{2,2} & G_{2,3} & \dots \\ G_{3,0} & G_{3,1} & G_{3,2} & G_{3,3} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{3.98}$$

Letting any $N \times N$ truncation of an operator J be denoted as $J^{(N)}$, we multiply $J^{(N\times\infty)}$ by $G^{(\infty\times N)}$ to generate the identity operator, $\mathbb{1}^{(N)}$. Given the tridiagonal structure of the Jacobi matrix, this equation reduces to a three term recurrence relation

$$J_{n,n-1}G_{n-1,m} + J_{n,n}G_{n,m} + J_{n,n+1}G_{n+1,m} = \delta_{n,m}, \tag{3.99}$$

where $n, m = 0, 1, \dots, N$. If $n < N$ is taken, this relation makes use of only elements found in $G^{(N)}$. When $n = N$, the relation requires $G_{N+1,m}$, which is outside of the truncated subspace. Using Eq.(3.99), we can evaluate the matrix element by solving

$$J_{N,N-1}G_{N-1,m} + J_{N,N}G_{N,m} + J_{N,N+1}G_{N+1,m} = \delta_{N,m}. \tag{3.100}$$

If we reorganize as

$$J_{N,N-1}G_{N-1,m} + \left[J_{N,N} + J_{N,N+1}\frac{G_{N+1,m}}{G_{N,m}}\right] G_{N,m} = \delta_{N,m}, \tag{3.101}$$

we see all the elements outside of the truncated subspace now contribute to just a single term. In order to eliminate the $G_{N+1,m}/G_{N,m}$ term, we again start with Eq.(3.99) as

$$J_{N+1,N}G_{N,m} + J_{N+1,N+1}G_{N+1,m} + J_{N+1,N+2}G_{N+2,m} = 0, \tag{3.102}$$

then rearrange such that we have

$$\left(-\frac{1}{J_{N+1,N}}\frac{G_{N+1,m}}{G_{N,m}}\right)^{-1} = J_{N+1,N+1} - J_{N+1,N+2} \times \left(-\frac{1}{J_{N+2,N+1}}\frac{G_{N+2,m}}{G_{N+1,m}}\right) J_{N+2,N+1}. \tag{3.103}$$

If we define the term

$$C_{N+1} = -\frac{1}{J_{N+1,N}}\frac{G_{N+1,m}}{G_{N,m}}, \tag{3.104}$$

it allows us to rewrite Eq.(3.103) as

$$C_{N+1}^{-1} = J_{N+1,N+1} - J_{N+1,N+2}\frac{J_{N+2,N+1}}{C_{N+2}^{-1}}. \tag{3.105}$$

Repeated action of this relation produces a continued fraction. Given the symmetry of the Jacobi matrix, $J_{N+1,N+2} = J_{N+2,N+1}$. Therefore, the continued fraction can be written as

$$C_{N+1}^{-1} = J_{N+1,N+1} - \cfrac{J_{N+1,N+2}^2}{J_{N+2,N+2} - \cfrac{J_{N+2,N+3}^2}{J_{N+3,N+3} - \cfrac{J_{N+3,N+4}^2}{\ddots}}}. \tag{3.106}$$

The Green's elements have also been eliminated from the relation, giving us a continued fraction constructed entirely of elements of our Jacobi matrix lying outside of the truncated subspace. Furthermore, there is no m dependence in this relation so the correction term to $J^{(N)}$ is the same for all m. We can therefore write Eq.(3.101) as

$$\left(J^{(N)} - \delta_{i,N}\delta_{j,N}J_{N,N+1}^2 C_{N+1}\right) G^{(N)} = \mathbb{1}^{(N)}. \tag{3.107}$$

This modified Jacobi matrix is the inverse of $G^{(N)}$:

$$(G^{(N)})^{-1} = J^{(N)} - \delta_{i,N}\delta_{j,N}J^2_{N,N+1}C_{N+1}. \tag{3.108}$$

From Eq.(3.107), all C_N may be derived if C_{N+1} is known. If there is term H' to our Hamiltonian, it can be represented on the finite basis as $H'^{(N)}$ and subtracted from Eq.(3.108), while the tail remains the same:

$$(G^{(N)})^{-1} = J^{(N)} - \delta_{i,N}\delta_{j,N}J^2_{N,N+1}C_{N+1} - H'_{i,j}{}^{(N)}. \tag{3.109}$$

When H' is not asymptotically relevant, it can always be approximated on a finite basis. For the short range potential considered in this thesis, this will always be the case and they can therefore be approximated using Eq.(3.96).

Lippmann–Schwinger Equation for Coulomb Scattering

We will need some machinery from Coulomb scattering theory to define the method by which we solve for bound and resonant states which may be probed in a typical scattering experiment. For this, we define our Hamiltonian to be the Coulomb Hamiltonian in angular momentum channel l, $\hat{H}_l^C$, plus some short range potential v_l,

$$\hat{H}_l = \hat{H}_l^C + v_l^{(s)}. \tag{3.110}$$

We know that the initial (in) and final (out) state of the system, associated with $t = -\infty$ and $t = \infty$ respectively, belong to the Hilbert space $\mathcal{H}_C$ associated to $\hat{H}_l^C$. These states are never free states due to the non-negligibly infinite effect of the Coulomb potential. Similarly, the states at $t = 0$ belong to the Hilbert space $\mathcal{H}$ associated to $\hat{H}_l$. The in and out states can be written as

$$\left|\psi_l^{in}\right\rangle = \left|\psi_l^{-}\right\rangle \quad \text{and} \quad \left|\psi_l^{out}\right\rangle = \left|\psi_l^{+}\right\rangle. \tag{3.111}$$

We also take the momentum representation, where any $\left|\psi_l^{\pm}\right\rangle$ is an element of the continuum of initial and final momentum states in angular momentum channel l, defined as

$$|p\rangle = \int |p\rangle \left\langle p\middle|\psi_l^{\pm}\right\rangle \mathrm{d}p. \tag{3.112}$$

Similarly, scattering states $|\phi_l\rangle \in \mathcal{H}$ of our interacting Hamiltonian, $\hat{H}_l$, are represented as

$$|p_{\pm}\rangle = \int |p\rangle \langle p|\phi_l\rangle \, \mathrm{d}p. \tag{3.113}$$

In this representation, we recall the Lippmann-Schwinger equation for scattering states,

$$|p_{\pm}\rangle = |p\rangle + \hat{G}\hat{V} \, |p_{\pm}\rangle \, . \tag{3.114}$$

Here, we use the Coulomb Green's operator defined as $G_l^C(z) = z - \hat{H}_l^C$, and take our potential operator to be the short range potential $v_l^{(s)}$. This means that scattering states of this system obey the relation

$$|p_{\pm}\rangle = |p\rangle + G_l^C(z) v_l^{(s)} \, |p_{\pm}\rangle \, . \tag{3.115}$$

Rearranging this, we find

$$(\mathbb{1} - G_l^C(z) v_l^{(s)}) \, |p_{\pm}\rangle = |p\rangle \, . \tag{3.116}$$

The scattering states $|p_{\pm}\rangle$ are elements of $\mathcal{H}$, which has a combination of discrete and continuum states representing bound and scatterings states respectively. We know that scattering states are states which can be time evolved into the continuum states at $t = \pm\infty$, while the time evolution of bound states goes to 0 as $t \to \pm\infty$. Taking the discrete states $|\phi_n\rangle$ as the basis, for bound or resonant energies E, we find

$$\lim_{z \to E} (\mathbb{1} - G_l^C(z) v_l^{(s)}) \, |\phi_n\rangle \to 0. \tag{3.117}$$

This means that when $z = E$, we have

$$(\mathbb{1} - G_l^C(z)v_l^{(s)})\,|\phi_n\rangle = ((G_l^C)^{-1}(z) - v_l^{(s)})\,|\phi_n\rangle = 0. \tag{3.118}$$

This is the homogenous Lippmann–Schwinger equation. It is also expressed as

$$G_l^C(z)v_l^{(s)}\,|\phi_n\rangle = |\phi_n\rangle\,. \tag{3.119}$$

This reduces the problem to an algebraic determinant problem, where we wish to evaluate the roots of the Fredhold determinant, i.e.,

$$|(G_l^C)^{-1}(z) - v_l^{(s)}| = 0. \tag{3.120}$$

We can now take the Coulomb-Sturmian basis to evaluate this relation. Writing a basis element as $|i\rangle$, which is assumed to be in angular momentum channel l, we start with the homogenous Lippmann–Schwinger equation,

$$|\psi_l\rangle = G_l^C(z)v_l^{(s)}\,|\psi_l\rangle\,. \tag{3.121}$$

Then, we insert a finite completeness around the short range potential operator to represent it in the same way as Eq.(3.96),

$$|\psi_l\rangle = \sum_{i,j}^{N} G_l^C(z)\,|j\rangle\,\langle j|\,v_l^{(s)}\,|i\rangle\,\langle i|\psi_l\rangle\,, \tag{3.122}$$

where the truncated basis matrix elements $\langle j|\,v_l^{(s)}\,|i\rangle$ are calculated by the method used in [8]. So, Eq.(3.122) is the wavefunction with which we will evaluate Eq.(3.120). Acting from the left with $\langle k|$ gives

$$\sum_{k}^{N}\langle k|\psi_l\rangle = \sum_{i,j,k}^{N}\langle k|\,G_l^C(z)\,|j\rangle\,\langle j|\,v_l^{(s)}\,|i\rangle\,\langle i|\psi_l\rangle\,, \tag{3.123}$$

which is how the Coulomb-Sturmian coefficients of $|\psi\rangle$ are determined. This results in a matrix equation

$$\underline{\psi}_l = \underline{G}_l^C(z)\underline{v}_l^{(s)}\underline{\psi}_l, \tag{3.124}$$

where $\underline{G}_l^C(z) = \langle i|\, G_l^C(z)\, |j\rangle$ as Eq.(3.119) imposes a δ_{ik} on the relation. With this, we again return to the Fredhold determinant,

$$|\underline{G}_l^C(z)^{-1} - \underline{v}_l^{(s)}| = 0, \tag{3.125}$$

which is given on a finite basis on functions defined by Eq.(3.122). Due to Eq.(3.108), the only approximation in this procedure is in the short range potential as the finite basis representation of the inverse Green's operator is analytic due to the continued fraction term in the final $G^{-1}_{N,N}$ matrix element. As given in Eq.(3.109), this short range potential can be included to yield Eq.(3.125), the roots of which provide the bound and resonant energy spectrum of any Coulomb plus short range Hamiltonian.

CHAPTER 4

SOLUTION PROCEDURES

Here, the methods for solving each equation are presented. They can all be summarized as *working the equations into an effective radial Schrödinger form so that the method we provide for the standard Schrödinger equation is valid in each case.*

Schrödinger Solution

Consider a Coulomb Hamiltonian with an additional spherically symmetric short range potential $v^{(s)}$ in angular momentum channel l:

$$\hat{H} = \hat{H}_l^0 + \frac{Ze^2}{r} + v_l^{(s)} = \hat{H}_C + v_l^{(s)}. \tag{4.126}$$

Here, $\hat{H}_l^0$ is the non-relativistic kinetic energy operator, Z is charge number, and e is the unit charge. If we assume some sufficient basis $|\psi_l\rangle$ in angular momentum channel l, then the Hamiltonian gives us the eigenvalue equation

$$(\hat{H}_l^0 + \frac{Z}{r} + v_l^{(s)})|\psi_l\rangle = E|\psi_l\rangle. \tag{4.127}$$

For the purpose of this work, a reasonable Hamiltonian constructed out of the complete set of commuting observables for a Coulomb system is

$$\hat{H}_C = -\frac{\hbar}{2m}\left(\partial_r^2 - \frac{l(l+1)}{r^2}\right) + \frac{Ze^2}{r}, \tag{4.128}$$

where we follow the procedure established in the previous chapter and include the short range potential operator $v_l^{(s)}$ in the final step as an approximate truncated operator $\tilde{v}_l^{(s)(N)}$. Evaluating

the matrix $J(z) = z - \hat{H}_C$ on the Coulomb-Sturmian basis, we find matrix elements

$$J = \begin{cases} \frac{k^2-b^2}{2m/\hbar^2 b}(n+l+1) - Ze^2 & \text{for } n = m, \\ -\frac{k^2+b^2}{4m/\hbar^2 b}\sqrt{(n+1)(n+2l+2)} & \text{for } m = n+1, \\ -\frac{k^2+b^2}{4m/\hbar^2 b}\sqrt{n(n+2l+1)} & \text{for } m = n-1, \\ 0 & \text{otherwise,} \end{cases} \tag{4.129}$$

where $k = \sqrt{2m/\hbar^2 z}$. J is therefore the symmetric tridiagonal structure required of the continued fraction representation. Using these elements, we can evaluate Eq.(3.106)

$$C_N^{-1} = \frac{k^2-b^2}{2m/\hbar^2 b}(N+l+1) - Ze^2 - \cfrac{\left(\frac{k^2+b^2}{4m/\hbar^2 b}\right)^2 (N+1)(N+2l+2)}{\frac{k^2-2}{2m/\hbar^2 b}(N+l+2) - Ze^2 - \cfrac{\left(\frac{k^2+b^2}{4m/\hbar^2 b}\right)^2 (N+2)(N+2l+3)}{\frac{k^2-b^2}{2m/\hbar^2 b}(N+l+3) - Ze^2 - \ddots}}. \tag{4.130}$$

This is a T-fraction class, which p.308 of Ref[9] shows can be mapped to the ratio of two ${}_2F_1$ hypergeometric functions

$$T(a,b;c;y) = c + (b-a+1)y - \cfrac{(c-a+1)(b+1)y}{c+1+(b-a+2)y - \cfrac{(c-a+2)(b+2)y}{c+2+(b-a+3)y - \ddots}} = c\frac{{}_2F_1(a,b;c;y)}{{}_2F_1(a,b+1;c+1;y)}, \tag{4.131}$$

with complex parameters a, b, c and complex variable y. This is a valid map so long as $|y| < 1$ is satisfied. The mapping results in

$$c\frac{{}_2F_1(a,b;c;y)}{{}_2F_1(a,b+1;c+1;y)} = \delta C_N^{-1}, \tag{4.132}$$

with a scale parameter δ. Using the relations from p.324 of Ref[9] and the $|y| < 1$ convergence condition, a, b, c, y and δ are found by solving

$$y = \delta^2 \left(\frac{k^2 + b^2}{4m/\hbar^2 b} \right)^2, \tag{4.133}$$

$$1 + y = \delta \left(\frac{k^2 - b^2}{2m/\hbar^2 b} \right)^2, \tag{4.134}$$

$$b + 1 = N + 1, \tag{4.135}$$

$$c - a + 1 = N + 2l + 2, \tag{4.136}$$

$$c + (b - a + 1)y = \delta \left(\left(\frac{k^2 - b^2}{2m/\hbar^2 b} \right)^2 (N + l + 1) - Ze^2 \right). \tag{4.137}$$

Using Eq.(4.133), Eq.(4.134), and the convergence condition, we find that

$$\delta = -\frac{4m/\hbar^2 b}{(b - ik)^2} \tag{4.138}$$

and

$$y = \left(\frac{b + ik}{b - ik} \right)^2. \tag{4.139}$$

Defining $\gamma = Zm/\hbar^2 k$, we have solutions for the other parameters:

$$a = -l + i\gamma, \quad b = N, \quad c = N + l + 1 + i\gamma \tag{4.140}$$

The resulting ${}_2F_1$ functions are related by the relation

$${}_2F_1(l+1+i\gamma, N+2l+1; N+l+1+i\gamma; y) = {}_2F_1(-l+i\gamma, N; N+l+1+i\gamma; y)(1-y)^{2l+1}, \tag{4.141}$$

so for C_N, we find

$$C_N = -\frac{4m/\hbar^2 b}{(b-ik)^2\,(N+l+1+i\gamma)} \times \frac{{}_2F_1\left(-l+i\gamma, N+1; N+l+2+i\gamma; \left(\frac{b+ik}{b-ik}\right)^2\right)}{{}_2F_1\left(-l+i\gamma, N; N+l+1+i\gamma; \left(\frac{b+ik}{b-ik}\right)^2\right)}. \quad (4.142)$$

Using this equation with $N \to N+1$, we can evaluate J and thus $(G_l^C)^{-1}(z)$ on a finite basis of any degree without approximation using Eq.(3.108). Upon approximating the potential $\tilde{v}_l^{(s)(N)}$, the Fredholm determinant given by Eq.(3.125) is calculated. Roots of the determinant correspond to the complete bound and resonant energy spectrum of this Hamiltonian.

Klein-Gordon Solution

Consider the Klein-Gordon equation:

$$(E-V)^2 = (p^2c^2 + m^2c^4)\psi. \quad (4.143)$$

Diving by $2mc^2$ and expanding we obtain

$$\left[\frac{1}{2m}p^2 + \frac{mc^2}{2} - \frac{1}{2mc^2}(E^2 - 2EV - V^2)\right]\psi = 0. \quad (4.144)$$

From here, the equation is reorganized as

$$\left[\frac{1}{2m}p^2 - \frac{1}{2mc^2}\left(E^2 - m^2c^4\right) + V\left(\frac{E}{mc^2} - \frac{V}{2mc^2}\right)\right]\psi = 0. \quad (4.145)$$

We can now define effective energy ε and effective potential $\tilde{V}$ by

$$\varepsilon = \frac{1}{2mc^2}(E^2 - m^2c^4) \quad (4.146)$$

and

$$\tilde{V} = V\left(\frac{E}{mc^2} - \frac{V}{2mc^2}\right), \quad (4.147)$$

which allow the Klein-Gordon equation to be written in a simpler form:

$$\tilde{H}\psi = \left[\frac{p^2}{2m} + \tilde{V}\right]\psi = \varepsilon\psi. \tag{4.148}$$

We must keep in mind that this is a relativistic energy, so the rest energy must be removed as $E' = E - mc^2$. The effective variables then change as

$$\varepsilon = E'\left(1 + \frac{E'}{2mc^2}\right) \tag{4.149}$$

and

$$\tilde{V} = V\left(1 + \frac{E'}{mc^2} - \frac{V}{2mc^2}\right). \tag{4.150}$$

In order to move further, we assume the potential is again in the form of a Coulomb plus short range potential

$$V = \frac{Ze^2}{r} + v_l^{(s)}(r). \tag{4.151}$$

Since this is spherically symmetric, our effective Hamiltonian commutes with $\hat{L}^2$ and $\hat{L}_z$, giving the complete set of commuting observables $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$. In light of this, we can make use of the Laplacian

$$\nabla^2 = \partial_r^2 - \frac{\hat{L}^2}{\hbar^2 r^2}, \tag{4.152}$$

to rewrite the Hamiltonian in terms of the complete set as

$$\tilde{H} = -\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2 l(l+1)}{2mr^2} + \left(\frac{Ze^2}{r} + v_l^{(s)}\right)\left(1 + \frac{E'}{mc^2} - \frac{1}{2mc^2}\left(\frac{Ze^2}{r} + v_l^{(s)}\right)\right). \tag{4.153}$$

Further simplification is achieved by creating new effective variables:

$$Z' = Z\left(1 + \frac{E'}{2mc^2}\right) \qquad w_l^{(s)} = v_l^{(s)}\left(1 + \frac{E'}{mc^2} - \frac{1}{2mc^2}\left(\frac{Ze^2}{r} + v_l^{(s)}\right)\right). \tag{4.154}$$

With these variables, the Hamiltonian becomes

$$\tilde{H} = -\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{l(l+1) - Z^2\alpha^2}{r^2} + \frac{Z'e^2}{r} + w_l^{(s)}, \tag{4.155}$$

with the fine structure constant $\alpha = e^2/\hbar c$. Looking at the term proportional to r^{-2}, we can analytically continue our integer quantum number l to an effective angular momentum variable u by solving $l(l+1) - Z^2\alpha^2 = u(u+1)$, where we find

$$u = \frac{1}{2} - \sqrt{\left(l + \frac{1}{2}\right)^2 - Z^2\alpha^2}. \tag{4.156}$$

This allows us to cast the Klein-Gordon equation in a Schrödinger form,

$$\tilde{H} = -\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{u(u+1)}{r^2} + \frac{Z'e^2}{r} + w_l^{(s)}, \tag{4.157}$$

such that the solution method outlined for the Schrödinger equation is then applicable to numerically evaluate the energy spectrum of a Coulomb plus short range potential.

Feynman–Gell-Mann Solution

Now, we apply the solution technique to the Feynman–Gell-Mann equation, where we are considering a Coulomb plus short range potential with no magnetic field. By comparing to the Klein-Gordon equation in Eq.(2.17), we see it differs only by the $-ie\boldsymbol{\sigma}\cdot\mathbf{E}$ term. Expanding the equation and substituting in $e\mathbf{E} = -\nabla V$, we have

$$\left[\nabla^2 + \frac{1}{\hbar^2c^2}(E-V)^2 - \frac{m^2c^2}{\hbar^2} + \frac{i}{\hbar c}\nabla V\cdot\boldsymbol{\sigma}\right]. \tag{4.158}$$

We again assume the spherically symmetric potential of Eq.(4.151) to allow the construction of a Hamiltonian using the complete set of commuting observables $\{\hat{H}, \hat{L}^2, \hat{L}_z\}$. The associated Laplacian is again given by Eq.(4.152). Separating off the rest energy and introducing

the same effective variables ε, Z', and $w_l^{(s)}$, defined in Eq.(4.149) and Eq.(4.154), allows the equation to be written similarly to Eq.(4.155), with $l_\pm = j \mp 1/2$ and two extra terms to account for the spin interaction:

$$\tilde{H}\Psi^{(\pm)} = \left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{l_\pm(l_\pm+1) - Z^2\alpha^2}{r^2} + \frac{Z'}{r} + w_l^{(s)} - \frac{\hbar^2}{2m}\frac{iZ\alpha}{r^2}\left(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma}\right) - \frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)\left(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma}\right)\right]\Psi = \varepsilon\Psi. \tag{4.159}$$

Or, after grouping similar terms, we find

$$\tilde{H}\Psi^{(\pm)} = \left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{l_\pm(l_\pm+1) - Z^2\alpha^2 + iZ\alpha\left(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma}\right)}{r^2} + \frac{Z'}{r} + w_l^{(s)} + w_l^{'(s)}\right]\Psi = \varepsilon\Psi, \tag{4.160}$$

where $w_l^{'(s)}$ is given by

$$w_l^{'(s)} = -\frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)\left(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma}\right), \tag{4.161}$$

due to the spherical symmetry.

In order to determine the wave function, we need to determine how the $\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma}$ operator acts on the angular basis. In spherically symmetric potentials, we have a product state of radial and angular functions,

$$\Psi_j = \frac{1}{r}\psi_j^{(\pm)}(r)\Phi_{jm}^{(\pm)}(\theta,\varphi). \tag{4.162}$$

The angular functions, also known as the spinor spherical harmonics, are constructed using the usual Clebsch-Gordon coupling of the spherical harmonics $Y_{l_\pm,m_l}(\theta,\varphi)$ and spinor functions χ_{m_s}:

$$\Phi_{jm}^{(\pm)} = \sum_{m_l,m_s}\langle l_\pm, 1/2; m_l, m_s|j,m\rangle\, Y_{l_\pm,m_l}(\theta,\varphi)\chi_{m_s}. \tag{4.163}$$

This wavefunction has a manifest rotational symmetry, given the spherical potential, but we must see also check its transformation under parity $\hat{\Pi}$. In the spherical coordinate system, parity is applied as $\theta \to \pi - \theta$ and $\varphi \to \varphi + \pi$. Spherical harmonics therefore transform as $\hat{\Pi}Y_{lm} = (-1)^l Y_{(lm)}$, implying that our product state also transforms as $\hat{\Pi}\Phi_{jm}^{(\pm)} = (-1)^{l_\pm}\Phi_{jm}^{(\pm)}$.

This means states $\Phi^{(+)}_{jm}$ and $\Phi^{(-)}_{jm}$ have opposite parity. We can now examine the $\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}$ operator in spherical coordinates as

$$\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma} = \sigma_1 \sin\theta\cos\varphi + \sigma_2 \sin\theta \sin\varphi + \sigma_3 \cos\theta = \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}. \tag{4.164}$$

Applying parity in the same way as before shows us this operator is odd under parity, i.e. $\hat{\Pi}(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\hat{\Pi} = -\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}$. We also find

$$\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} \begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.165}$$

i.e. $(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})^2 = \mathbb{1}_2$. An easy calculation for $[\hat{\mathbf{J}}, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}]$, where we take $\hat{J}_z = \hat{L}_z + \hat{S}_z$, $\hat{L}_z = -i\hbar\partial_\varphi$

and $\hat{S}_z = \frac{\hbar}{2}\sigma_3$, gives

$$\begin{aligned}
[\hat{L}_z, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}]\psi = [-i\hbar\partial_\varphi, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}]\,\psi &= -i\hbar\partial_\varphi(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\psi + \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}(m_l\hbar)\psi - \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}(m_l\hbar)\psi \\
&= -i\hbar\partial_\varphi(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\psi \\
&= -i\hbar\partial_\varphi(\sigma_1 \sin\theta\cos\varphi + \sigma_2 \sin\theta\sin\varphi + \sigma_3\cos\theta) \\
&= -i\hbar(-\sigma_1 \sin\theta\sin\varphi + \sigma_2 \sin\theta\cos\varphi),
\end{aligned}$$

$$\begin{aligned}
[\hat{S}_z, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] = \frac{\hbar}{2}\,[\sigma_3, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] &= \frac{\hbar}{2}(\sigma_3\sigma_1 \sin\theta\cos\varphi + \sigma_3\sigma_2 \sin\theta\sin\varphi + \sigma_3\sigma_3\cos\theta \\
&\qquad - \sigma_1\sigma_3 \sin\theta\cos\varphi - \sigma_2\sigma_3 \sin\theta\sin\varphi - \sigma_3\sigma_3\cos\theta) \\
&= \frac{\hbar}{2}([\sigma_3, \sigma_1] \sin\theta\cos\varphi + [\sigma_3, \sigma_2] \sin\theta\sin\varphi) \\
&= i\hbar(\sigma_2 \sin\theta\cos\varphi - \sigma_1 \sin\theta\sin\varphi),
\end{aligned}$$

$$\therefore \qquad [\hat{J}_z, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] = [\hat{L}_z, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] + [\hat{S}_z, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] = 0. \tag{4.166}$$

The other components of $\hat{\mathbf{J}}$ follow from rotational invariance [10]. Since $[\hat{\mathbf{J}}, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] = 0$, then $[\hat{\mathbf{J}}^2, \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}] = 0$, and these operators have simultaneous eigenstates. This means $\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}$ operating on the wave function remains within the subspace spanned by $|\Phi_{jm}^{(\pm)}\rangle$. The odd parity of this operator, together with the fact that $(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})^2 = \mathbb{1}_2$, results in the matrix elements

$$\left\langle \Phi_{jm}^{(\pm)} \right| \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma} \left| \Phi_{jm}^{(\pm)} \right\rangle = 0 \qquad \text{and} \qquad \left\langle \Phi_{jm}^{(\pm)} \right| \hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma} \left| \Phi_{jm}^{(\mp)} \right\rangle = 1, \tag{4.167}$$

giving the operator $\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}$ a representation on this basis by

$$(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})_{\Phi_{jm}^{(\pm)}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.168}$$

So, our Hamiltonian has the structure

$$\hat{H} = \begin{pmatrix} -\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{l_+(l_++1)-Z^2\alpha^2}{r^2} + \frac{Z'}{r} + w_l^{(s)} & \frac{\hbar^2}{2m}\frac{iZ\alpha}{r^2} + w_l^{'(s)} \\ \frac{\hbar^2}{2m}\frac{iZ\alpha}{r^2} + w_l^{'(s)} & -\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{l_-(l_-+1)-Z^2\alpha^2}{r^2} + \frac{Z'}{r} + w_l^{(s)} \end{pmatrix}. \tag{4.169}$$

We can diagonalize our system and absorb the off diagonal angular momentum term,

$$\frac{\hbar^2}{2m}\frac{iZ\alpha}{r^2}, \tag{4.170}$$

which amounts to an analytic continuation of the angular momentum number $l_\pm(l_\pm+1) \to u_\pm(u_\pm+1)$. The effect this has on $w_l^{'(s)}$, however, will have to be calculated explicitly in the new basis. We can find our new basis by diagonalizing the angular momentum term,

$$\frac{\hbar^2}{2m}\frac{1}{r^2}\begin{pmatrix} (j-\frac{1}{2})(j+\frac{1}{2}) - Z^2\alpha^2 & iZ\alpha \\ iZ\alpha & (j+\frac{1}{2})(j+\frac{3}{2}) - Z^2\alpha^2 \end{pmatrix}\begin{pmatrix} \Phi_{jm}^{(+)} \\ \Phi_{jm}^{(-)} \end{pmatrix}, \tag{4.171}$$

where we have replaced $l_\pm \to j \mp 1/2$. The eigenvectors of this system are given by

$$|F_{jm}^{(\pm)}\rangle = i\left(\frac{j+\frac{1}{2}\pm s}{Z\alpha}\right)|\Phi_{jm}^{(+)}\rangle + |\Phi_{jm}^{(-)}\rangle, \tag{4.172}$$

where $s = \sqrt{\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2}$. We will need to manipulate these a little as they do not behave properly under basic limit evaluations. Our equation must certainly hold for a chargeless particle, meaning $Z \to 0$, yet that makes this transformation singular. Furthermore, keeping in mind $\alpha \sim 1/c$, taking the nonrelativistic limit by $c \to \infty$ is again singular. We can remedy this through

some basic algebraic steps, as we only need to make sure the proportion of $\Phi_{jm}^{(+)} : \Phi_{jm}^{(-)}$ remains the same to have an equivalent basis, up to normalization. What we desire, upon taking either limit $Z \to 0$ or $c \to \infty$, is that we get $F_{jm}^{(\pm)} \to \Phi_{jm}^{(\pm)}$. To this end, we first treat $F_{jm}^{(+)}$ then $F_{jm}^{(-)}$ separately. Up to normalization, we find

$$\begin{aligned} |F_{jm}^{(+)}\rangle &= i\left(\frac{j+\frac{1}{2}+s}{Z\alpha}\right)|\Phi_{jm}^{(+)}\rangle + |\Phi_{jm}^{(-)}\rangle \\ &\sim -i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left(i\left(\frac{j+\frac{1}{2}+s}{Z\alpha}\right)|\Phi_{jm}^{(+)}\rangle + |\Phi_{jm}^{(-)}\rangle\right) \\ &= \frac{\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}}{Z\alpha}|\Phi_{jm}^{(+)}\rangle - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi_{jm}^{(-)}\rangle. \end{aligned} \tag{4.173}$$

If we remember $s = \sqrt{\left(j+\frac{1}{2}\right)^2 - Z^2\alpha^2}$, we can see the coefficient of $\Phi_{jm}^{(+)}$ is actually $\frac{\sqrt{Z^2\alpha^2}}{Z\alpha} = 1$. Thus we find

$$|F_{jm}^{(+)}\rangle \sim \left(|\Phi_{jm}^{(+)}\rangle - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi_{jm}^{(-)}\rangle\right). \tag{4.174}$$

This has the proper limit behavior as taking either $Z \to 0$ or $c \to \infty$ makes the coefficient on $\Phi_{jm}^{(-)}$ go to 0 and we get $F_{jm}^{(+)} \to \Phi_{jm}^{(+)}$. If we follow the same process for $F_{jm}^{(-)}$, we have

$$|F_{jm}^{(-)}\rangle \sim \left(|\Phi_{jm}^{(-)}\rangle + i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi_{jm}^{(+)}\rangle\right). \tag{4.175}$$

Given we only require equivalence up to normalization, we can replace the proportional symbols $(\sim)$ with equivalence symbols $(=)$. We can now express the complete transformation compactly as

$$|F_{jm}^{(\pm)}\rangle = |\Phi_{jm}^{(\pm)}\rangle \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi_{jm}^{(\mp)}\rangle. \tag{4.176}$$

These states are not orthogonal, as the matrix in Eq.(4.171) was not Hermitian. Under the inner

product definition of our Hilbert space, as defined in Eq.(2.1) however, we find

$$\langle F_{jm}^{(\mp)}|F_{jm}^{(\pm)}\rangle = \mp 2i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}. \tag{4.177}$$

The linear operator $\langle F_{jm}^{(\pm)}|$ carries a different sign on the superposed state $|\Phi_{jm}^{(\mp)}\rangle$ than the eigenvectors of the diagonalized system, therefore use of it would be invalid. This is due to the conjugation affecting the coefficients as well. We can fix this issue by defining a biorthogonal partner $\langle \tilde{F}_{jm}^{(\pm)}|$ to satisfy the orthonormality requirement of our angular basis. This is valid as it is still built out of a linear combination of the original $\langle \Phi_{jm}^{(\pm)}|$ which diagonalize the system. More formally justified, the elements of the dual space $\mathscr{H}^*$ are defined through the inner product, meaning the elements we are interested in are those for which acting on $|\Phi_{jm}^{(\pm)}\rangle$ maps the vector to 0 or 1. We can therefore build the initial $\langle \tilde{F}_{jm}^{(\pm)'}|$ by constructing them out of the eigenvectors, where only the states $|\Phi_{jm}^{(\pm)}\rangle$ are conjugate transposed and the coefficients are left the same. This is given by

$$\langle \tilde{F}_{jm}^{(\pm)'}| = \langle \Phi_{jm}^{(\pm)}| \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\langle \Phi_{jm}^{(\mp)}|, \tag{4.178}$$

which satisfies $\langle \tilde{F}_{jm}^{(\pm)'}|F_{jm}^{(\mp)}\rangle = 0$ by construction. We then can absorb the normalization into $\langle \tilde{F}_{jm}^{(\pm)'}|$ to give the final biorthogonal partner $\langle \tilde{F}_{jm}^{(\pm)}|$, defined through the inner product. Taking the norm, we find

$$\langle \tilde{F}_{jm}^{(\pm)'}|F_{jm}^{(\pm)}\rangle = 1 - \frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s} = \frac{2s}{j+\frac{1}{2}+s}. \tag{4.179}$$

We can now define our new biorthogonal partner as the dual space elements given by

$$\langle \tilde{F}_{jm}^{(\pm)}| = \frac{j+\frac{1}{2}+s}{2s}\left(\langle \Phi_{jm}^{(\pm)}| \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\langle \Phi_{jm}^{(\mp)}|\right). \tag{4.180}$$

It is evident that this new linear functional satisfies the requirements

$$\langle \tilde{F}_{jm}^{(\mp)}|F_{jm}^{(\pm)}\rangle = 0 \qquad \text{and} \qquad \langle \tilde{F}_{jm}^{(\pm)}|F_{jm}^{(\pm)}\rangle = 1. \tag{4.181}$$

Now that we have an orthonormal basis which diagonalizes the system, we can determine the associated eigenvalues of our angular momentum operator. The action on this basis is given by

$$\left(\frac{\hat{L}^2}{\hbar^2} - Z^2\alpha^2 + iZ\alpha(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\right) \begin{pmatrix} F_{jm}^{(+)} \\ \\ F_{jm}^{(-)} \end{pmatrix}. \tag{4.182}$$

We can make the substitutions $-Z^2\alpha^2 = s^2 - \left(j + \frac{1}{2}\right)^2$ and $Z\alpha = \sqrt{\left(j + \frac{1}{2}\right)^2 - s^2}$ to be consistent with the basis coupling terms and find

$$\begin{aligned} &\left(\frac{\hat{L}^2}{\hbar^2} + s^2 - \left(j + \frac{1}{2}\right)^2 + i\sqrt{\left(j + \frac{1}{2}\right)^2 - s^2}\ (\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\right) \begin{pmatrix} F_{jm}^{(+)} \\ \\ F_{jm}^{(-)} \end{pmatrix} \\ &= \left(\frac{\hat{L}^2}{\hbar^2} + s^2 - \left(j + \frac{1}{2}\right)^2 + i\sqrt{\left(j + \frac{1}{2}\right)^2 - s^2}\ (\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\right) \begin{pmatrix} \Phi_{jm}^{(+)} - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\Phi_{jm}^{(-)} \\ \\ i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\Phi_{jm}^{(+)} + \Phi_{jm}^{(-)} \end{pmatrix}. \end{aligned} \tag{4.183}$$

Remembering that $\hat{L}^2|\Phi_{jm}^{(\pm)}\rangle = \hbar^2 l_\pm(l_\pm + 1) = \hbar^2(j \mp 1/2)(j \mp 1/2 + 1)$ and $(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})|\Phi_{jm}^{(\pm)}\rangle = |\Phi_{jm}^{(\mp)}\rangle$, we can evaluate the action on each $F_{jm}^{(\pm)}$ individually. Starting with $F_{jm}^{(+)}$,

we find

$$
\begin{aligned}
&\left(\left(j-\frac{1}{2}\right)\left(j+\frac{1}{2}\right)+s^2-\left(j+\frac{1}{2}\right)^2\right)|\Phi^{(+)}_{jm}\rangle+i\sqrt{\left(j+\frac{1}{2}\right)^2-s^2}\;|\Phi^{(-)}_{jm}\rangle\\
&\qquad-i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left[\left(\left(j+\frac{1}{2}\right)\left(j+\frac{3}{2}\right)+s^2-\left(j+\frac{1}{2}\right)^2\right)|\Phi^{(-)}_{jm}\rangle\right.\\
&\qquad\left.+i\sqrt{\left(j+\frac{1}{2}\right)^2-s^2}\;|\Phi^{(+)}_{jm}\rangle\right]\\
&=\left[\left(j-\frac{1}{2}\right)\left(j+\frac{1}{2}\right)+s^2-\left(j+\frac{1}{2}\right)^2+\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\sqrt{\left(j+\frac{1}{2}\right)^2-s^2}\;\right]|\Phi^{(+)}_{jm}\rangle\\
&\qquad-i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left[\left(j+\frac{1}{2}\right)\left(j+\frac{3}{2}\right)+s^2-\left(j+\frac{1}{2}\right)^2\right.\\
&\qquad\left.-\sqrt{\frac{j+\frac{1}{2}+s}{j+\frac{1}{2}-s}}\sqrt{\left(j+\frac{1}{2}\right)^2-s^2}\;|\Phi^{(-)}_{jm}\rangle\right]\\
&=\left[j^2-\frac{1}{4}+s^2-\left(j+\frac{1}{2}\right)^2+j+\frac{1}{2}-s\right]|\Phi^{(+)}_{jm}\rangle\\
&\qquad-i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left[j^2+2j+\frac{3}{4}+s^2-\left(j+\frac{1}{2}\right)^2-j-\frac{1}{2}-s\right]|\Phi^{(-)}_{jm}\rangle\\
&=[s(s-1)]\,|\Phi^{(+)}_{jm}\rangle-i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\,[s(s-1)]\,|\Phi^{(-)}_{jm}\rangle.
\end{aligned}
\tag{4.184}
$$

Finally, we have

$$
\left(\frac{\hat{L}^2}{\hbar^2}+s^2-\left(j+\frac{1}{2}\right)^2+i\sqrt{\left(j+\frac{1}{2}\right)^2-s^2}\;(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})\right)|F^{(+)}_{jm}\rangle=s(s-1)|F^{(+)}_{jm}\rangle. \tag{4.185}
$$

If we repeat for $F^{(-)}_{jm}$, we obtain

$$
\left(\frac{\hat{L}^2}{\hbar^2}+s^2-\left(j+\frac{1}{2}\right)^2+i\sqrt{\left(j+\frac{1}{2}\right)^2-s^2}\;(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})\right)|F^{(-)}_{jm}\rangle=s(s+1)|F^{(-)}_{jm}\rangle. \tag{4.186}
$$

Equating $s(s \mp 1) = u_\pm(u_\pm + 1)$ gives $u_\pm = s - \frac{1}{2} \mp \frac{1}{2}$. So, Eq.(4.183) becomes

$$\begin{pmatrix} u_+(u_+ + 1) & 0 \\ 0 & u_-(u_- + 1) \end{pmatrix} \begin{pmatrix} F_{jm}^{(+)} \\ F_{jm}^{(-)} \end{pmatrix}. \tag{4.187}$$

This allows the Hamiltonian to be rewritten as

$$\tilde{H}\Psi^{(\pm)} = \left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{u_\pm(u_\pm + 1)}{r^2} + \frac{Z'}{r} + w_l^{(s)} + w_l^{'(s)} \right] \Psi = \varepsilon\Psi. \tag{4.188}$$

To figure out how $w_l^{'(s)}$ acts, we need only consider the $(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})$ term, as the rest of the operator only affects the radial part of the wave function. This operator will not be diagonal, so we will need to evaluate the individual matrix elements $\langle F^{(\pm)}|(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})|F^{(\pm)}\rangle$ and $\langle F^{(\mp)}|(\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})|F^{(\pm)}\rangle$. From Eq.(4.167), it follows

$$\begin{aligned} (\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})|F^{(\pm)}\rangle &= (\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma}) \left(|\Phi_{jm}^{(\pm)}\rangle \mp i\sqrt{\frac{j + \frac{1}{2} - s}{j + \frac{1}{2} + s}}|\Phi_{jm}^{(\mp)}\rangle \right) \\ &= |\Phi_{jm}^{(\mp)}\rangle \mp i\sqrt{\frac{j + \frac{1}{2} - s}{j + \frac{1}{2} + s}}|\Phi_{jm}^{(\pm)}\rangle. \end{aligned} \tag{4.189}$$

We can then find the off diagonal couplings by applying $\langle F^{(\pm)}|$ from the left. Varying the $\pm$ of

$\langle \tilde{F}^{(\pm)}_{jm}|$ and $|F^{(\pm)}_{jm}\rangle$ independently, we use Eq.(4.180) to evaluate the matrix elements as

$$\begin{aligned}
&\langle \tilde{F}^{(\pm)}_{jm}|(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})|F^{(\pm)}_{jm}\rangle = \\
&\quad \frac{j+\frac{1}{2}+s}{2s}\left(\langle\Phi^{(\pm)}_{jm}| \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\langle\Phi^{(\mp)}_{jm}|\right)\left(|\Phi^{(\mp)}_{jm}\rangle \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi^{(\pm)}_{jm}\rangle\right) \\
&\quad = \frac{j+\frac{1}{2}+s}{2s}\begin{pmatrix} -2i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}} & 1+\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s} \\ 1+\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s} & 2i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}} \end{pmatrix} \\
&\quad = \frac{1}{s}\begin{pmatrix} -iZ\alpha & j+\frac{1}{2} \\ j+\frac{1}{2} & iZ\alpha \end{pmatrix}.
\end{aligned} \tag{4.190}$$

This matrix also behaves well under the limit conditions as taking either $Z \to 0$ or $c \to \infty$ returns us to Eq.(4.165). Using this relation, we can now define $\underline{w_l}'^{(s)} = -\frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)\langle\tilde{F}^{(\pm)}_{jm}|(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})|F^{(\pm)}_{jm}\rangle$, where again the $\pm$ on either side of the inner product is varied independently to give the coupling matrix elements as well. Operating on Eq.(4.188) from the left by $\langle F^{(\pm)}_{jm}|$ produces a Hamiltonian that acts only on the radial wave function,

$$\tilde{H}\psi^{(\pm)}_j(r) = \left[-\frac{\hbar^2}{2m}\partial_r^2 + \frac{\hbar^2}{2m}\frac{u_\pm(u_\pm+1)}{r^2} + \frac{Z'}{r} + w_l^{(s)} + \underline{w_l}'^{(s)}\right]\psi^{(\pm)}_j(r) = \varepsilon\psi^{(\pm)}_j(r). \tag{4.191}$$

While this is not diagonal, the method presented in the previous chapter allows for the short range potential operators $w_l^{(s)}$ and $\underline{w_l}'^{(s)}$ to be approximated such that the energy spectrum of Eq.(4.191) may be found numerically.

Feshbach–Villars Spin-$1/2$ Solution

The solution to the Feshbach–Villars spin-$1/2$ equation will proceed like to the previous section. We can begin by working from Eq.(2.84), for which the Hamiltonian is repeated below with the relevant constants placed back in:

$$\begin{pmatrix} (\tau_3 + i\tau_2) \otimes \frac{\boldsymbol{\pi}_L^2}{2m} + \tau_3 \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4 eA_0 & 0 \\ 0 & (\tau_3 + i\tau_2) \otimes \frac{\boldsymbol{\pi}_R^2}{2m} + \tau_3 \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4 eA_0 \end{pmatrix} \Psi. \tag{4.192}$$

As the decoupled systems differ only by a sign in the $\boldsymbol{\pi}$ operator, we can work with a compact notation,

$$\hat{H}_{FV1/2} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \otimes \frac{\hbar^2}{2m} \left(-\mathbb{1}_2 \nabla^2 \pm \frac{ie}{\hbar c} (\boldsymbol{\sigma} \cdot \mathbf{E}) \right) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4 eA_0. \tag{4.193}$$

By using the relations $e\mathbf{E} = -\nabla V$ and $eA_0 = V$, we find

$$\hat{H}_{FV1/2} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \otimes \frac{\hbar^2}{2m} \left(-\mathbb{1}_2 \nabla^2 \mp \frac{i}{\hbar c} (\boldsymbol{\sigma} \cdot \nabla V) \right) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4 V. \tag{4.194}$$

If we again assume a spherical potential of the form

$$V = \frac{Ze^2}{r} + v_l^{(s)}(r), \tag{4.195}$$

with associated Laplacian,

$$\nabla^2 = \partial_r^2 - \frac{\hat{L}^2}{\hbar^2 r^2}, \tag{4.196}$$

Eq.(4.194) becomes

$$\begin{aligned}\hat{H}_{FV1/2} = &\begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \otimes \frac{\hbar^2}{2m}\left(-\mathbb{1}_2\partial_r^2 + \mathbb{1}_2\frac{\hat{L}^2}{\hbar^2 r^2} \pm \frac{iZ\alpha}{r^2}(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r)\right) + \begin{pmatrix} 1 & 0 \\ \\ 0 & -1 \end{pmatrix} \otimes \mathbb{1}_2 mc^2 \\ &+ \mathbb{1}_4\frac{Ze^2}{r} \mp \begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \otimes \frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r) + \mathbb{1}_4 v_l^{(s)}(r).\end{aligned} \tag{4.197}$$

This results in

$$\hat{H}_L = \begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \otimes \frac{\hbar^2}{2m}\left(-\mathbb{1}_2\partial_r^2 + \mathbb{1}_2\frac{\hat{L}^2}{\hbar^2 r^2}\right) + \begin{pmatrix} 1 & 0 \\ \\ 0 & -1 \end{pmatrix} \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4\frac{Ze^2}{r}$$
$$- \begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \otimes \left(-\frac{iZ\alpha}{r^2}(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r) + \frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r)\right) + \mathbb{1}_4 v_l^{(s)}(r),$$

$$\hat{H}_R = \begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \otimes \frac{\hbar^2}{2m}\left(-\mathbb{1}_2\partial_r^2 + \mathbb{1}_2\frac{\hat{L}^2}{\hbar^2 r^2}\right) + \begin{pmatrix} 1 & 0 \\ \\ 0 & -1 \end{pmatrix} \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4\frac{Ze^2}{r}$$
$$+ \begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \otimes \left(-\frac{iZ\alpha}{r^2}(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r) + \frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r)\right) + \mathbb{1}_4 v_l^{(s)}(r), \tag{4.198}$$

such that the whole 8-component Hamiltonian is given by

$$\hat{H}_{FV1/2} = \hat{H}_L \oplus \hat{H}_R, \tag{4.199}$$

where $\oplus$ is a direct sum. For the spin-0 case, the equation is identical to either $\hat{H}_L$ or $\hat{H}_R$ with the spin coupling terms related to $\boldsymbol{\sigma}$ removed. Therefore, the equation to be solved is

$$\hat{H}_{FV0} = \begin{pmatrix} 1 & 1 \\ \\ -1 & -1 \end{pmatrix} \frac{\hbar^2}{2m}\left(-\partial_r^2 + \frac{\hat{L}^2}{\hbar^2 r^2}\right) + \begin{pmatrix} 1 & 0 \\ \\ 0 & -1 \end{pmatrix} mc^2 + \mathbb{1}_2 \frac{Ze^2}{r} + \mathbb{1}_2 v_l^{(s)}(r). \quad (4.200)$$

The diagonalization of Eq.(4.198) follows the same procedure as the previous section, yet we must continue carefully as the two 4-component Hamiltonians $\hat{H}_L$ and $\hat{H}_R$, comprising $\hat{H}_{FV1/2}$, act on a chirally decoupled 8-component wavefunction. This is due to the fact that the 4-component wavefunction for $\Psi_{L,R}$ is constructed out of the Weyl spinor $\phi_{L,R}$. This allows for invariance under spacial inversion as the left and right handed spinors swap to match the equations, which transform into each other as well. Since this equation is decoupled in the Weyl representation, we can diagonalize $\hat{H}_L$ and $\hat{H}_R$ individually. We first treat $\hat{H}_L$, as it corresponds to the $+ie\boldsymbol{\sigma}\cdot\mathbf{E}$ choice made in the previous section. This results in an angular momentum operator similar to Eq.(4.171):

$$\mathbb{1}_2 \frac{\hat{L}^2}{\hbar^2} + iZ\alpha(\boldsymbol{\sigma}\cdot\hat{\mathbf{e}}_r). \quad (4.201)$$

Given this operator differs from Eq.(4.171) by a diagonal term $\mathbb{1}_2 Z^2\alpha^2$, the eigenvectors of the system will be the same. This means that again, we have

$$|F_{jm}^{(\pm),L}\rangle = |\Phi_{jm}^{(\pm)}\rangle \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi_{jm}^{(\mp)}\rangle, \quad (4.202)$$

where the superscript has been added to avoid confusion with the other diagonalizing basis for $\hat{H}_R$. This basis again requires the biorthogonal partner

$$\langle\tilde{F}_{jm}^{(\pm),L}| = \frac{j+\frac{1}{2}+s}{2s}\left(\langle\Phi_{jm}^{(\pm)}| \mp i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\langle\Phi_{jm}^{(\mp)}|\right). \quad (4.203)$$

The form of Eq.(4.201) also implies that the eigenvalues will differ by the same term, $\mathbb{1}_2 Z^2\alpha^2$. We can derive the associated eigenvalues from acting on the $|F_{jm}^{(\pm),L}\rangle$ basis to demonstrate this point. Following the same procedure as in the previous section, the action of this operator on the $|F_{jm}^{(+)}\rangle$ state is given by

$$
\begin{aligned}
&\left(\frac{\hat{L}^2}{\hbar^2} + i\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}\ (\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})\right)|F_{jm}^{(+),L}\rangle \\
&\left(\frac{\hat{L}^2}{\hbar^2} + i\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}\ (\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})\right)\left(|\Phi_{jm}^{(+)}\rangle - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}|\Phi_{jm}^{(-)}\rangle\right) \\
&= \left(j-\frac{1}{2}\right)\left(j+\frac{1}{2}\right)|\Phi_{jm}^{(+)}\rangle + i\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}\ |\Phi_{jm}^{(-)}\rangle \\
&\qquad\qquad - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left(\left(j+\frac{1}{2}\right)\left(j+\frac{3}{2}\right)|\Phi_{jm}^{(-)}\rangle + i\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}\ |\Phi_{jm}^{(+)}\rangle\right) \\
&= \left(\left(j-\frac{1}{2}\right)\left(j+\frac{1}{2}\right) + j + \frac{1}{2} - s\right)|\Phi_{jm}^{(+)}\rangle \\
&\qquad\qquad - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left(\left(j+\frac{1}{2}\right)\left(j+\frac{3}{2}\right) - \left(j+\frac{1}{2}+s\right)\right)|\Phi_{jm}^{(-)}\rangle \\
&= \left(\left(j+\frac{1}{2}\right)^2 - s\right)|\Phi_{jm}^{(+)}\rangle - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left(\left(j+\frac{1}{2}\right)^2 - s\right)|\Phi_{jm}^{(-)}\rangle \\
&= \left(s(s-1) + Z^2\alpha^2\right)|\Phi_{jm}^{(+)}\rangle - i\sqrt{\frac{j+\frac{1}{2}-s}{j+\frac{1}{2}+s}}\left(s(s-1)+Z^2\alpha^2\right)|\Phi_{jm}^{(-)}\rangle \\
&= \left(s(s-1) + Z^2\alpha^2\right)|F_{jm}^{(+),L}\rangle,
\end{aligned}
\tag{4.204}
$$

where, as before, $s = \sqrt{(j+\frac{1}{2})^2 - Z^2\alpha^2}$. If we follow this procedure for $|F_{jm}^{(-),L}\rangle$, we find

$$
\left(\frac{\hat{L}^2}{\hbar^2} + i\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}\ (\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})\right)|F_{jm}^{(-),L}\rangle = \left(s(s+1) + Z^2\alpha^2\right)|F_{jm}^{(-),L}\rangle. \tag{4.205}
$$

Equating $s(s \mp 1) + Z^2\alpha^2 = u_\pm^{(L)}(u_\pm^{(L)} + 1)$ then gives

$$u_\pm^{(L)} = \sqrt{\left(j + \frac{1}{2}\right)^2 + \frac{1}{4} \mp s} - \frac{1}{2}. \tag{4.206}$$

The diagonalization of $\hat{H}_R$ is nearly identical to Eq.(4.171) and follows the same procedure as $\hat{H}_L$. The term we want to treat is given by

$$\frac{\hbar^2}{2m}\frac{1}{r^2}\begin{pmatrix} (j+\frac{1}{2})(j+\frac{3}{2}) & -iZ\alpha \\ -iZ\alpha & (j-\frac{1}{2})(j+\frac{1}{2}) \end{pmatrix}\begin{pmatrix} \Phi_{jm}^{(-)} \\ \Phi_{jm}^{(+)} \end{pmatrix}. \tag{4.207}$$

The eigenvectors of this system are found to be the same as before, except swapped. This means we have

$$|F_{jm}^{(\mp)}\rangle = i\left(\frac{j+\frac{1}{2} \pm s}{Z\alpha}\right)|\Phi_{jm}^{(\mp)}\rangle + |\Phi_{jm}^{(\pm)}\rangle. \tag{4.208}$$

Repeating the steps of Eq.(4.173), we find eigenvectors,

$$|F_{jm}^{(\mp),R}\rangle = |\Phi_{jm}^{(\mp)}\rangle \mp i\sqrt{\frac{j+\frac{1}{2}+s}{j+\frac{1}{2}-s}}|\Phi_{jm}^{(\pm)}\rangle. \tag{4.209}$$

These clearly do not have the proper limit behavior, but we we can continue along and hope the resulting radial only equation does. Following the same procedure as the previous section for the biorthogonal partner, we find

$$\langle\tilde{F}_{jm}^{(\mp),R}| = -\frac{j+\frac{1}{2}-s}{2s}\left(\langle\Phi_{jm}^{(\mp)}| \mp i\sqrt{\frac{j+\frac{1}{2}+s}{j+\frac{1}{2}-s}}\langle\Phi_{jm}^{(\pm)}|\right). \tag{4.210}$$

To find the eigenvalues in this basis we act on the states and obtain

$$\left(\frac{\hat{L}^2}{\hbar^2} - i\sqrt{\left(j+\frac{1}{2}\right)^2 - s^2}\ (\hat{\mathbf{e}}_r \cdot \boldsymbol{\sigma})\right)|F_{jm}^{(\mp)}\rangle = \left(s(s \mp 1) + Z^2\alpha^2\right). \tag{4.211}$$

This is the same as for $\hat{H}_L$, therefore $u_{\mp}^{(R)}(u_{\mp}^{(R)}+1) = u_{\pm}^{(L)}(u_{\pm}^{(L)}+1) = s(s\mp 1) + Z^2\alpha^2$ we get

$$u_{\mp}^{(R)} = \sqrt{\left(j+\frac{1}{2}\right)^2 + \frac{1}{4} \mp s} - \frac{1}{2}. \tag{4.212}$$

We now must calculate the matrix elements of $w_l^{'(s)}$ in this basis, given again by the relation

$$\underline{w_l}^{'(s)}_{L/R} = -\frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)\langle \tilde{F}_{jm}^{(\pm),L/R}|(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})|F_{jm}^{(\pm),L/R}\rangle. \tag{4.213}$$

For $\hat{H}_L$, this is the same case as the Feynman–Gell-Mann equation, so we again have

$$\underline{w_l}^{'(s)}_{L} = -\frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)\frac{1}{s}\begin{pmatrix} -iZ\alpha & j+\frac{1}{2} \\ j+\frac{1}{2} & iZ\alpha \end{pmatrix}. \tag{4.214}$$

For $\hat{H}_R$, we need to use our new basis and evaluate $\langle \tilde{F}_{jm}^{(\mp),R}|(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})|F_{jm}^{(\mp),R}\rangle$:

$$\langle \tilde{F}_{jm}^{(\mp),R}|(\hat{\mathbf{e}}_r\cdot\boldsymbol{\sigma})|F_{jm}^{(\mp),R}\rangle = \frac{1}{s}\begin{pmatrix} iZ\alpha & j+\frac{1}{2} \\ j+\frac{1}{2} & -iZ\alpha \end{pmatrix}. \tag{4.215}$$

This gives us the representation of $w_l^{'(s)}$ in this basis as

$$\underline{w_l}^{'(s)}_{R} = -\frac{i\hbar}{2mc}\partial_r v_l^{(s)}(r)\frac{1}{s}\begin{pmatrix} iZ\alpha & j+\frac{1}{2} \\ j+\frac{1}{2} & -iZ\alpha \end{pmatrix}. \tag{4.216}$$

Since the new angular momentum variable $u_{\pm}^{(L)} = u_{\mp}^{(R)}$, we can relabel both to $u_{\pm}$ and introduce $\tilde{\boldsymbol{\pi}}$ as

$$\begin{aligned}\tilde{\boldsymbol{\pi}}^2 &= \hbar^2 \left(-\mathbb{1}_2 \partial_r^2 + \frac{1}{r^2} \begin{pmatrix} s(s-1) + Z^2\alpha^2 & 0 \\ 0 & s(s+1) + Z^2\alpha^2 \end{pmatrix} \right) \\ &= \hbar^2 \left(-\mathbb{1}_2 \partial_r^2 + \frac{1}{r^2} \begin{pmatrix} u_+(u_+ + 1) & 0 \\ 0 & u_-(u_- + 1) \end{pmatrix} \right).\end{aligned} \tag{4.217}$$

Putting this all together, we find $\hat{H}_{FV1/2} = \hat{H}_L \oplus \hat{H}_R$ is now given by

$$\begin{aligned}\hat{H}_L &= (\tau_3 + i\tau_2) \otimes \frac{\tilde{\boldsymbol{\pi}}^2}{2m} + \tau_3 \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4 \frac{Ze^2}{r} + (\tau_3 + i\tau_2) \otimes \underline{w}_L^{\prime(s)} + \mathbb{1}_4 v_l^{(s)}(r), \\ \hat{H}_R &= (\tau_3 + i\tau_2) \otimes \frac{\tilde{\boldsymbol{\pi}}^2}{2m} + \tau_3 \otimes \mathbb{1}_2 mc^2 + \mathbb{1}_4 \frac{Ze^2}{r} + (\tau_3 + i\tau_2) \otimes \underline{w}_R^{\prime(s)} + \mathbb{1}_4 v_l^{(s)}(r),\end{aligned} \tag{4.218}$$

which act only on the radial wave functions. We can see that this resulting radial equation does maintain the proper limit behavior for $c \to \infty$ and $Z \to 0$.

Scalar Interaction

As given by Eq.(2.92), we can modify our Hamiltonian to include a scalar interaction via addition of the term

$$\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \otimes \mathbb{1}_2 U. \tag{4.219}$$

For modelling quark confinement, we will take the case that U is given by a linear and quadratic term,

$$U = \alpha_1 r + \alpha_2 r^2. \tag{4.220}$$

Clearly, these are not short range terms and thusly contribute to the asymptotic motion of the inverse Green's operator. We therefore must analytically evaluate these operators in the Coulomb-Sturmian basis. From Ref[11], for r and r^2, we have

$$\langle n, l_\pm; b|r|m, l_\pm; b\rangle = \langle m, l_\pm; b|r|n, l_\pm; b\rangle = \begin{cases} \left(6n^2 + 2(l_\pm+1)(6n+2l_\pm+3)\right)/\left(4b^2\right) & m = n, \\ -\left(2m+2l_\pm+1\right)\sqrt{m\left(m+2l_\pm+1\right)}/\left(2b^2\right) & m = n+1, \\ \sqrt{m\left(m-1\right)\left(m+2l_\pm\left(m+2l_\pm+1\right)\right)}/4b^2 & m = n+2, \\ 0 & m > n+2, \end{cases} \tag{4.221}$$

and

$$\left\langle n, l_\pm; b\left|r^2\right|m, l_\pm; b\right\rangle = \left\langle m, l_\pm; b\left|r^2\right|n, l_\pm; b\right\rangle = \begin{cases} \frac{[(((10n+2l_\pm+4)(n+2l_\pm+3)+9n(n-1))(n+2l_\pm+2)+n(n-1)(n-2))]}{(8b^3)} & m = n, \\ \frac{-[(4m+2l_\pm(m+2l_\pm+2)+(m-1)(m-2)]\sqrt{m(m+2l_\pm+1)}3}{(8b^3)} & m = n+1, \\ \frac{(2m+2l_\pm\sqrt{m(m-1)(m+2l_\pm+1)(m+2l_\pm)}3}{(8b^3)} & m = n+2, \\ \frac{-\sqrt{m(m-1)(m-2)(m+2l_\pm+1)(m+2l_\pm(m+2l_\pm-1)}}{(8b^3)} & m = n+3, \\ 0 & m > n+3. \end{cases} \tag{4.222}$$

The above relations are given for the spin-$1/2$ case, but for spin-0, we simply substitute $l_\pm \to l$ and drop the tensor product with unity from Eq.(4.219) and use Eq.(2.91), then the rest is identical. It should be noted that in the spin-$1/2$ case, the $\pm$ are always kept the same on either side of the inner product as there is no angular momentum coupling through U.

Truncated Matrix Continued Fraction Tail

The continued fraction in the solution method becomes a matrix continued fraction due to the multi-component structure of the Feshbach-Villars formalism and the nature of the

confinement interaction. It converges for bound states, however for complex resonant state energies, it fails to converge. This is due to the non square integrability of the scattering and resonant state wave functions. Resonant state energies all have small negative complex contributions, therefore we must analytically continue across the branch cut to provide convergence to these states. The best way of achieving this is to calculate an optimal final term C_∞, then calculate all previous terms back to C_{N+1} in Eq.(3.109). At first, this will be applied to the spin-0 case where we only have l, as in the analytically continued Klein-Gordon. It will then be seen that in the infinite limit of the spin-1/2 case, N dominates and makes the C_∞ element irrespective of $l_\pm$, meaning we can derive C_∞ for spin-0, then construct the spin-1/2 truncation term as $\mathbb{1}_2 \otimes C_\infty$. To calculate C_∞ for spin-0, we start with Eq.(3.105), given as

$$C_{N+1} = (J_{N+1,N+1} - J_{N+1,N+2} C_{N+2} J_{N+2,N+1})^{-1}. \tag{4.223}$$

Multiplying both sides by $J_{N+1,N+2}$ gives

$$C_{N+1} \cdot J_{N+1,N+2} = \left(J^{-1}_{N+1,N+2} J_{N+1,N+1} - C_{N+2} J_{N+2,N+1}\right)^{-1}. \tag{4.224}$$

As we can see in Eq.(3.95), matrix elements are proportional to N, which means in the large N limit, $N+1 \approx N$ and $C_N \approx C_{N+1}$ Taking the limit of $N \to \infty$ thus gives

$$C_{N+1} J_{N+1,N+2} \approx C_{N+2} J_{N+2,N+1} \to C_\infty J'_\infty \tag{4.225}$$

and

$$J^{-1}_{N+1,N+2} J_{N+1,N+1} \to (J'_\infty)^{-1} J_\infty. \tag{4.226}$$

This lets us write Eq.(4.224) as

$$C_\infty J'_\infty = \left((J'_\infty)^{-1} J_\infty - C_\infty J'_\infty\right)^{-1}. \tag{4.227}$$

If we introduce variables $X = C_\infty J'_\infty$ and $B = (J'_\infty)^{-1} J_\infty$, we clearly see this is a quadratic matrix equation:

$$\begin{aligned} X &= (B - X)^{-1} \\ \mathbb{1} &= X(B - X) \\ 0 &= X^2 - BX + \mathbb{1}. \end{aligned} \tag{4.228}$$

A general quadratic matrix equation is

$$AX^2 - BX + C = 0. \tag{4.229}$$

This equation, while not in general solvable in closed form, has solutions if $A = \mathbb{1}$, $[B, C] = 0$, and $B^2 - 4C$ has a square root [12]. The solution for a quadratic matrix equation satisfying these conditions is

$$X = -\frac{1}{2}B \pm \frac{1}{2}(B^2 - 4C)^{\frac{1}{2}}. \tag{4.230}$$

As Eq.(4.227) satisfies these conditions, we can solve for $C_\infty J'_\infty$ as

$$C_\infty J'_\infty = -\frac{1}{2}(J'_\infty)^{-1} J_\infty \pm \frac{1}{2}\left(((J'_\infty)^{-1} J_\infty)^2 - 4\mathbb{1}\right)^{\frac{1}{2}}. \tag{4.231}$$

To determine these matrices, we need to evaluate J_∞ and $J_\infty^{'}$ in matrix continued fraction representation. We can construct our required truncation terms as

$$J_\infty = \begin{pmatrix} \frac{E}{b} - \frac{\hbar^2 b}{2b} - \frac{mc^2}{b} & -\frac{\hbar^2 b}{2m} \\ \frac{\hbar^2 b}{2m} & \frac{E}{b} + \frac{\hbar^2 b}{2b} + \frac{mc^2}{b} \end{pmatrix} N,$$
$$J_\infty^{'} = \begin{pmatrix} -\frac{E}{b} - \frac{\hbar^2 b}{2b} + \frac{mc^2}{b} & -\frac{\hbar^2 b}{2m} \\ \frac{\hbar^2 b}{2m} & -\frac{E}{b} + \frac{\hbar^2 b}{2b} - \frac{mc^2}{b} \end{pmatrix} N. \tag{4.232}$$

From Eq.(4.223) we can see that $C_\infty \sim 1/N$. This means that the term we defined as $X = C_\infty J^{'}{}_\infty$ is independent of N. If we define $S_0 = E^2 + b^2\hbar^2c^2 - mc^2$, we can construct $B = (J_\infty^{'})^{-1} J_\infty$ as

$$B = \frac{1}{S_0} \begin{pmatrix} -(E^2 - \frac{E^2 b^2 \hbar^2}{m} - mc^2) & \frac{(E+mc^2)b^2\hbar^2}{m} \\ -\frac{(E-mc^2)b^2\hbar^2}{m} & -(E^2 + \frac{E^2 b^2 \hbar^2}{m} - mc^2) \end{pmatrix}. \tag{4.233}$$

Now taking the $+$ equation from Eq.(4.230) to match the nonrelativistic limit as E approaches mc^2 and introducing $Q_0 = ib\hbar c \frac{\sqrt{E^2 - m^2c^4}}{mc^2}$, we can solve for X:

$$X = \frac{1}{S_0} \begin{pmatrix} -(E^2 - \frac{E^2 b^2 \hbar^2}{m} - mc^2) + (E+mc^2)Q_0 & \frac{(E+mc^2)b^2\hbar^2}{m} + (E+mc^2)Q_0 \\ -\frac{(E-mc^2)b^2\hbar^2}{m} - (E-mc^2)Q_0 & -(E^2 + \frac{E^2 b^2 \hbar^2}{m} - mc^2) - (E-mc^2)Q_0 \end{pmatrix}. \tag{4.234}$$

From $X = C_\infty J^{'}{}_\infty$, we can now solve for the truncation term C_∞ as

$$C_\infty = X(J^{'}_\infty)^{-1}, \tag{4.235}$$

which will now be labelled C^0_∞. If we look at Eq.(4.129), there is an l dependence which becomes $l_\pm$ in the case of spin-$1/2$, however in the limit of $N \to \infty$ we applied, the N term clearly dominates the angular momentum terms. This makes the matrix element irrespective of $l_\pm$, meaning we can construct our desired truncation term through a simple tensor product with unity, giving

$$C^{1/2}_\infty = \mathbb{1}_2 \otimes C^0_\infty, \tag{4.236}$$

which is used to truncate the matrix continued fraction associated to either $\hat{H}_L$ or $\hat{H}_R$ of $\hat{H}_{FV_{1/2}}$.

CHAPTER 5

NUMERICAL RESULTS

In this section, the results will be given for bound states of a nicely behaved gaussian potential using each presented method. Following, we will evaluate the bound and resonant states of a short range potential modelling proton scattering with a Uranium nucleus. Finally, the results for a confinement potential modelling quark-antiquark interaction will be given using Schrödinger, Feshbach-Villars spin-0, and Feshbach-Villars spin-$1/2$ equations. First, however, the use of the continued fraction method must be justified as there are certainly less mathematically complex methods available.

Justification of the Continued Fraction Method

As the continued fraction method is built of an analytic solution to the Coulomb Green's operator, it will manifestly provide more accurate results than a simple Runge-Kutta solution, which starts to break down around very small r as the r^{-2} terms diverge heavily. This also means that higher angular momentums pose an issue for Runge-Kutte as well due to the stronger effect of the centrifugal barrier term $l(l+1)/r^2$. Obviously, approximation is worse than analytic results, but we can show that even at $l = 1, 2$, a Runge-Kutta method performs less than ideally. We take atomic units where $m = 1$, $\hbar = 1$, $e^2 = 1$, and $\alpha = e^2/\hbar c = 1/137.036$, as well as our radial parameter to be $b = 8$.

TABLE 1. Hydrogen Energies

	Schrödinger RK4	Schrödinger CF	Analytic
l=0	-0.50000000001	-0.05	-0.05
l=1	-0.05539088219	-0.05555555555	-0.05555555555
l=2	-0.02715565947	-0.02	-0.02

While the ground states evaluates nicely due to the r^{-2} term being eliminated at $l = 0$,

clearly Table 1 shows the continued fraction method continues to provide the exact result at higher energies and angular momentum states.

Gaussian Potential

We take a Gaussian potential of the form

$$v_l^{(s)}(r) = -50e^{-0.5r^2}, \tag{5.237}$$

with $Z = 1$. The results for this potential are given below.

TABLE 2. Bound States in Potential Eq.(5.1) ($Z = 1$, $l = 0$, $j = 0.5$)

Sch	K–G	FV0	F–G	FV1/2
-1.6630629	-1.6712101	-1.6700158	-1.6700788	-1.6702394
-7.3901658	-7.4004257	-7.3991315	-7.3985183	-7.3990722
-15.511899	-15.520684	-15.518899	-15.518143	-15.519033
-25.540693	-25.546693	-25.544319	-25.543542	-25.544203
-37.137653	-37.141618	-37.138463	-37.137789	-37.137940

TABLE 3. Bound States in Potential Eq.(5.1) ($Z = 1$, $l = 1$, $j = 1.5$)

Sch	K–G	FV0	F–G	FV1/2
-4.2398001	-4.2496608	-4.2488239	-4.2486322	-4.2487215
-11.345874	-11.355504	-11.354341	-11.354013	-11.354065
-20.581329	-20.588319	-20.586761	-20.586396	-20.586236
-31.605272	-31.609259	-31.607224	-31.606874	-31.606366

Yukawa Potential

The Schrödinger and Feshbach-Villars equations will be used to numerically evaluate bound and resonant states of a short range potential. A Yukawa type potential is used which is representative of a typical nucleon-nucleon interaction. To this end, we will use

$$v_l^{(s)}(r) = -\frac{240\, e^{-r}}{r} + \frac{320\, e^{-4r}}{r}, \tag{5.238}$$

with $Z = 92$, which models proton scattering with a Uranium nucleus. This system has one bound and one resonant state at $l = 0$. The results for this potential are given in Table 4 and Table 5.

TABLE 4. Bound Energies of Potential Eq.(5.2) ($Z = 92$)

Sch	FV0	FV1/2
-5.929368	-5.933465	-5.928157

TABLE 5. Resonant Energies of Potential Eq.(5.2) ($Z = 92$)

Sch	FV0	FV1/2
15.60918 -0.0000015**i**	15.59950 -0.00000000002**i**	15.60266 -0.000000000006**i**

Confinement Potential

For the scalar interaction, we use U of the form

$$U = \alpha_1 r + \alpha_2 r^2, \tag{5.239}$$

and take $Z = -1$ in the vector potential. Evaluating either linear or quadratic confinement, corresponding to the cases

$$\alpha_1 = 1,\ \alpha_2 = 0 \qquad \text{or} \qquad \alpha_1 = 0,\ \alpha_2 = 1/2.$$

This gives, for the linear confinement case,

$$V = -\frac{1}{r} + r, \tag{5.240}$$

and, for the quadratic confinement case,

$$V = -\frac{1}{r} + \frac{r^2}{2}. \tag{5.241}$$

The results for the Schrödinger, Feshbach–Villars spin-0, and spin-$1/2$ are given in Table 6 and Table 7.

TABLE 6. Bound Energies in Coulomb plus Linear Confinement Potential

Schr (l=0)	FV0 (l=0)	FV1/2	Schr (l=1)	FV0 (l=1)	FV1/2
0.577924	0.577749	0.577806	1.974214	1.974013	1.974004
2.450164	2.449834	2.449862	3.335497	3.335086	3.335080
3.756907	3.756356	3.756377	4.468114	4.467458	4.467453
4.855672	4.854865	4.854883	5.472592	5.471664	5.471660
5.836031	5.834942	5.834958	6.391709	6.390484	6.390481
6.736622	6.735228	6.735242	7.248384	7.246845	7.246841

TABLE 7. Bound Energies in Coulomb plus Quadratic Confinement Potential

Schr (l=0)	FV0 (l=0)	FV1/2	Schr (l=1)	FV0 (l=1)	FV1/2
0.179668	0.179538	0.179595	1.709018	1.708842	1.708831
2.500002	2.499612	2.499652	3.801930	3.801378	3.801368
4.631955	4.631087	4.631123	5.860357	5.859219	5.859209
6.712598	6.711039	6.711074	7.902318	7.900380	7.900371
8.769522	8.767059	8.767092	9.934707	9.931758	9.931749
10.81293	10.80935	10.80938	11.96088	11.95671	11.95670

CHAPTER 6

CONCLUSION

In this work, we presented a method which solves the relativistic Feshbach–Villars spin-$1/2$ equations. The Feshbach–Villars equations have the advantage over the Klein–Gordon and Feynman–Gell-Mann equations in that they are true relativistic quantum mechanical equations, meaning they have a first order time derivative, which allows for a probabilistic interpretation. The Klein–Gordon and Feynman–Gell-Mann equations must be transformed into an effective Schrödinger form and thus have no definite probability density. The Feshbach–Villars spin-$1/2$ equation is built out of irreducible representations of the Proper Lorentz Group SO(1,3) and transforms properly under parity. Furthermore, being multi-component, the Feshbach–Villars equations explicitly display the particle-antiparticle nature of the relativistic system. All together, this makes the Feshbach–Villars equations the natural relativistic quantum mechanical equations for spin-0 and spin-$1/2$ particles.

In order to solve the Feshbach–Villars equations, the multi-component eigenvalue problems were expressed in a Lippmann–Schwinger form. We approximated the short range part of the potential on a discrete Hilbert space basis, in particular, in the Coulomb–Sturmian basis. We evaluated the corresponding Green's operator as a matrix continued fraction. This method provides a unified description of bound, resonant, and scattering states of a Coulomb plus short range potential Hamiltonian.

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