Relativistic Spin-0 Feshbach–Villars Equations for Polynomial Potentials

Abstract We propose a solution method for studying relativistic spin-0 particles. We adopt the Feshbach–Villars formalism of the Klein–Gordon equation and express the formalism in an integral equation form. The integral equation is represented in the Coulomb–Sturmian basis. The corresponding Green’s operator with Coulomb and linear confinement potential can be calculated as a matrix continued fraction. We consider Coulomb plus short range vector potential for bound and resonant states and linear confining scalar potentials for bound states. The continued fraction is naturally divergent at resonant state energies, but we made it convergent by an appropriate analytic continuation.

1 Introduction

The Klein–Gordon equation is the basic relativistic quantum mechanical equation of spin-0 particles. However, it contradicts some of the postulates of quantum mechanics. In quantum mechanics, it is postulated that the system is completely determined by the wave function and the time evolution of the wave function is determined by the time-dependent Schrödinger equation. The Klein–Gordon equation is second order in time derivative. Therefore, to determine the system uniquely we need its time derivative as well.

In order to give a proper interpretation Feshbach and Villars rewrote the Klein–Gordon equation in Hamiltonian form [1]. In the Feshbach–Villars (FV0) formalism we split the Klein–Gordon wave function into two components, and for the components vector we arrive at a Schrödinger-like equation with a first order time derivative. The equations look like usual coupled differential equations, but the components are coupled by the kinetic energy operator, which makes them difficult to solve. A few demonstrations of their use are in Refs. [2–8].

In a recent work we have proposed a solution method for the Feshbach–Villars equations [9]. The method amounts to rewriting the eigenvalue problem into an integral equation form and representing the equation on a discrete Hilbert space basis. The Green’s operator has been calculated by a matrix continued fraction. However, the continued fraction in Ref. [9] converges only for bound state energies.

The aim of this work is to further develop the solution method of spin-zero FV0 equations to include resonant states and confining potentials. In Sect. 2, we outline the FV0 formalism. Then, in Sect. 3 we recapitulate the
solution method of Ref. [9]. In Sect. 4 we perform the analytic continuation and in Sect. 5 we examine the case of linear confining potential. Finally we summarize our findings and draw some conclusions.

2 Feshbach–Villars Equations for Spin-Zero Particles

The Klein–Gordon equation for a free spin-0 particle is given by

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \Psi = \left( c^2 p^2 + m^2 c^4 \right) \Psi. \quad (1)$$

We can introduce interaction by minimal coupling $p_\mu \rightarrow p_\mu - q/c A_\mu$, where $p_\mu$ and $A_\mu$ are the four-momentum and the four-potential, respectively. This interaction transforms like a four-vector with respect to the Lorentz transformation. We can also introduce a scalar interaction $S$ by the substitution $m \rightarrow m + S/c^2$, which is basically a position dependent effective mass. So, if we take $A = 0$ and denote the fourth component of the vector potential by $V$, we have

$$(i\hbar \partial/\partial t - V)^2 \Psi = \left[ c^2 p^2 + (m + S/c^2)^2 c^4 \right] \Psi. \quad (2)$$

In the FV0 formalism the wave function is split into two components

$$\Psi = \phi + \chi, \quad (3)$$

and for the components we can readily derive the coupled equations

$$i\hbar \frac{\partial}{\partial t} \phi = \left( \frac{p^2}{2m} + U \right) (\phi + \chi) + (mc^2 + V)\phi, \quad (5)$$

$$i\hbar \frac{\partial}{\partial t} \chi = -\left( \frac{p^2}{2m} + U \right) (\phi + \chi) - (mc^2 - V)\chi, \quad (6)$$

where $U = S + S^2/2mc^2$.

If we introduce the two-component wave function

$$|\psi\rangle = \begin{pmatrix} \phi \\ \chi \end{pmatrix}, \quad (7)$$

we can define the Hamiltonian

$$H_{FV0} = (\tau_3 + i\tau_2) \frac{p^2}{2m} + \tau_3 mc^2 + (\tau_3 + i\tau_2)U + V, \quad (8)$$

where $\tau_i$ denote the Pauli matrices

$$\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (9)$$

Now we can write (5) and (6) into a form analogous to the time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H_{FV0} |\psi\rangle, \quad (10)$$

or, for stationary states we have

$$H_{FV0} |\psi\rangle = E |\psi\rangle. \quad (11)$$

The Hamiltonian $H_{FV0}$ of Eq. (8) is Hermitian in the generalized sense

$$H_{FV0} = \tau_3 H_{FV0}^\dagger \tau_3, \quad (12)$$
and it has real eigenvalues [1, 10]. The wave function is normalized according to
\[ \langle \psi | \tau_3 | \psi \rangle = \pm 1, \quad (13) \]
where the plus or minus sign corresponds to particle or antiparticle.

This Hamiltonian looks like a usual coupled-channel Hamiltonian. However, in a usual coupled-channel Hamiltonian the channels are coupled by a short-range potential. Here the coupling is due to the kinetic energy operator, which is not a short range operator and cannot be neglected even at asymptotic distances. This may be the reason why the FV0 equations are not used frequently in practical calculations. If we want to solve the FV0 equations in a proper way we should not approximate the kinetic energy operator even in the coupling terms.

3 Solution Method

In order to solve the equations we need to write the Hamiltonian as
\[ H_{FV0} = H_{FV0}^{(l)} + H_{FV0}^{(s)}, \quad (14) \]
where \( H_{FV0}^{(l)} \) is the asymptotically relevant long range, and \( H_{FV0}^{(s)} \) is the asymptotically irrelevant short range part. If we make a similar separation of the potentials,
\[ V = V^{(l)} + V^{(s)} \quad \text{and} \quad U = U^{(l)} + U^{(s)}, \quad (15) \]
we can write
\[ H_{FV0}^{(l)} = (\tau_3 + i \tau_2) \frac{p^2}{2m} + \tau_3 m c^2 + (\tau_3 + i \tau_2) U^{(l)} + V^{(l)} \quad (16) \]
and
\[ H_{FV0}^{(s)} = (\tau_3 + i \tau_2) U^{(s)} + V^{(s)}. \quad (17) \]
Then we can cast the eigenvalue problem of Eq. (11), for bound and resonant states, into a Lippmann–Schwinger form
\[ |\psi\rangle = G_{FV0}^{(l)}(E) H_{FV0}^{(s)} |\psi\rangle, \quad (18) \]
where \( G_{FV0}^{(l)}(E) = (E - H_{FV0}^{(l)})^{-1} \) is the Green’s operator of the long-range FV0 Hamiltonian.

A natural way of solving this integral equation is to approximate \( H_{FV0}^{(s)} \) on a finite subset of a discrete basis. This results in a finite-rank expansion of the short range term. Several expansion schemes have been proposed. Recently we have found a simple, straightforward, yet very efficient approximation scheme [11]. We need to represent the short-range potential in a larger basis, invert the potential matrix, truncate to a smaller basis, and then invert it back. This way we achieve a low-rank representation of the potential operator that contains the relevant information from the larger basis. With this approach, even a low-rank representation gives very good results, while higher-rank representations provide extremely accurate results. If we represent the short-range interaction by an \( N \times N \) basis, then for solving Eq. (18) we need only an \( N \times N \) representation of \( G_{FV0}^{(l)} \).

The Green’s operator \( G \) satisfies the operator equation
\[ JG = GJ = 1, \quad (19) \]
where \( J = (E - H) \). The evaluation of the Green’s operator basically amounts to inverting an infinite matrix, which is, in general, rather complicated. A notable exception is when the basis is such that \( J \) appears as an infinite tridiagonal matrix [12,13]. In this case
\[ G = (J - \delta_{iN} \delta_{jN} J_{N,N+1} C_{N+1} J_{N+1,N})^{-1}, \quad (20) \]
where the underline denotes $N \times N$ matrices and $C$ is a continued fraction. Basically, $G$ is almost the inverse of $J$, only the right-lower corner of $J$ is modified by a continued fraction. The continued fraction is constructed from the higher-index elements of $J$ and is defined by the recursion relation

$$C_{N+1} = (J_{N+1,N+1} - J_{N+1,N+2}C_{N+2}J_{N+2,N+1})^{-1}. \quad (21)$$

The validity of this approach has been established for infinite tridiagonal $J$ matrices [12]. The derivation is based on the intimate relation between three-term recursion relations and continued fractions. So, if $J$ is a band matrix, such as penta-diagonal or septa-diagonal, the method is not applicable. However, all band matrices can be considered as tridiagonal matrices of block matrices. Therefore the above procedure is applicable [14]. The only difference is that $J_{i,j}$ is not a number any more, but rather an $m \times m$ block matrix and $C$ therefore is a matrix continued fraction.

In matrix representation Eq. (18) becomes a homogeneous algebraic equation

$$\left[ (G_{FV0}^{(l)}(E))^{-1} - H_{FV0}^{(s)} \right] \psi = 0, \quad (22)$$

which is solvable if the determinant of the expression in the bracket vanishes.

3.1 The Basis

As a basis, we adopted the Coulomb–Sturmian (CS) functions

$$\langle r| n \rangle = \left( \frac{n!}{(n + 2l + 1)!} \right)^{1/2} e^{-br} \frac{(2br)^{l+1}}{(p^2 + b^2)^{l+2}} L_n^{2l+1} (2br), \quad (23)$$

where $l$ is the angular momentum, $L$ is the Laguerre polynomial, and $b$ is a parameter.

They also have a nice form in momentum representation

$$\langle p| n \rangle = \frac{2^{l+3/2}l!(n + l + 1)\sqrt{n!}}{\sqrt{\pi(n + 2l + 1)!}} \frac{b(2bp)^{l+1}}{(p^2 + b^2)^{l+2}} \times G_n^{l+1} \left( \frac{p^2 - b^2}{p^2 + b^2} \right); \quad (24)$$

where $G$ is the Gegenbauer polynomial.

The CS functions satisfy Sturm–Liouville type differential equations

$$\left( -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{2b(n + l + 1)}{r} + b^2 \right) \langle r| n \rangle = 0. \quad (25)$$

Consequently with $\langle r| n' \rangle = \langle r| n \rangle/r$ we have the orthogonality $\langle n| n' \rangle = \delta_{nn'}$ and the completeness relation

$$1 = \lim_{N \to \infty} \sum_{n=0}^{N} |n\rangle \langle n| = \lim_{N \to \infty} \sum_{n=0}^{N} |n'\rangle \langle n|. \quad (26)$$

3.2 Matrix Elements

The simple form of the CS basis allows the exact and analytic calculation of the matrix elements

$$\langle n| 1/r| n' \rangle = \delta_{nn'}, \quad (27)$$

$$\langle n| n' \rangle = \langle n'| n \rangle = \begin{cases} \frac{(n + l + 1)/b}{\sqrt{n'(n' + 2l + 1)/(2b)}} & n = n', \\ 0 & n' = n + 1, \\ \sqrt{n'(n' + 2l + 1)/b} & n' > n + 1, \end{cases} \quad (28)$$

$$\langle n| p^2| n' \rangle = \langle n'| p^2| n \rangle = \begin{cases} (n + l + 1) b & n = n', \\ \sqrt{n'(n' + 2l + 1)} b/2 & n' = n + 1, \\ 0 & n' > n + 1, \end{cases} \quad (29)$$
\[ \langle n|r|n' \rangle = \langle n'|r|n \rangle = \begin{cases} 
(6n^2 + 2(l + 1)(6n + 2l + 3))/(4b^2) & n' = n, \\
-(2n' + 2l + 1)\sqrt{n'(n' + 2l + 1)/(2b^2)} & n' = n + 1, \\
\sqrt{n'(n' - 1)(n' + 2l)/(4b^2)} & n' = n + 2, \\
0 & n' > n + 2, 
\end{cases} \tag{30}
\]

and
\[ \langle n|r^2|n' \rangle = \langle n'|r^2|n \rangle = \\
\begin{cases} 
(10n - 2l + 4)(n + 2l + 3) + 9(n - 1)(n + 2l + 2) + n(n - 1)(n - 2))/8b^3 & n' = n, \\
-(4n' + 2l)(n' + 2l + 2) + (n' - 1)(n' - 2)\sqrt{n'(n' + 2l + 1)/8b^3} & n' = n + 1, \\
(2n' + 2l)\sqrt{n'(n' - 1)(n' + 2l + 1)/(8b^3)} & n' = n + 2, \\
-\sqrt{n'(n' - 2)(n' + 2l + 1)(n' + 2l)/(n' - 1)/8b^3} & n' = n + 3, \\
0 & n' > n + 3. 
\end{cases} \tag{31}
\]

### 4 Coulomb Plus Short Range Potential

We assume here that the fourth component of the vector potential is Coulomb-like
\[ V = Z/r + v_4^{(s)}. \tag{32} \]
Consequently we have
\[ H_{FV0}^{(s)} = v_4^{(s)}, \tag{33} \]
whose CS matrix elements can easily be determined.

The real difficulty lies in the evaluation of the CS matrix representation of $G_{FV0}^{(l)}$. From Eq. (8) we have
\[ J = E - H_{FV0}^{(l)} = E - \left( (\tau_3 + i\tau_2)\frac{p^2}{2m} + \tau_3mc^2 + \frac{Z}{r} \right). \tag{34} \]

We have learned before that in the CS basis the constants $E$ and $mc^2$, the $p^2$ and the $1/r$ terms are either tridiagonal or diagonal $\infty \times \infty$ matrices. On the other hand, due to the matrix structure of the FV0 equations, a $2 \times 2$ matrix structure becomes superimposed on the tridiagonal structure. Therefore, $J$ is a block tridiagonal matrix with $2 \times 2$ blocks. As a result Eq. (20) is applicable and $C_{N+1}$ becomes a matrix continued fraction with $2 \times 2$ blocks.

This method has been used in Ref. [9] for calculating bound states. The matrix continued fraction was evaluated iteratively. Assuming that $C_{N'} = 0$ for $N' >> N$, the continued fraction in Eq. (21) was evaluated backwards. However, this procedure converges only for bound state energies.

#### 4.1 Analytic Continuation of the Coulomb Green’s Matrix

In order to extend the method for resonant states we need to perform analytic continuation of the matrix continued fraction. For this purpose we need to estimate the tail of the continued fraction. We can see from Eqs. (27–29) that $J_{N'+1,N'+1} \simeq JN'$ with
\[ J = \begin{pmatrix} 
\frac{E}{b} & -mc^2 & -\frac{h^2b}{2m} \\
\frac{-mc^2}{2m} & \frac{E}{b} & \frac{-h^2b}{2m} \\
\frac{-\frac{h^2b}{2m}}{2m} & \frac{\frac{-h^2b}{2m}}{2m} & \frac{E}{2b} 
\end{pmatrix}, \tag{35} \]
and $J_{N',N'+1} \simeq J'N'$ with
\[ J' = \begin{pmatrix} 
\frac{E}{2b} & -mc^2 & -\frac{h^2b}{4m} \\
\frac{-mc^2}{4m} & \frac{E}{2b} & \frac{-\frac{h^2b}{4m}}{4m} \\
\frac{-\frac{h^2b}{4m}}{4m} & \frac{\frac{-\frac{h^2b}{4m}}{4m}}{4m} & \frac{E}{2b} 
\end{pmatrix}. \tag{36} \]
as \( N' \to \infty \). Then from Eq. \( (21) \) it also follows that \( C_{N'+1} \simeq C/N' \). So, as \( N' \to \infty \) we find
\[
C = (J - J'CJ')^{-1}.
\] (37)

With a little manipulation we obtain
\[
CJ' = (J - J'CJ')^{-1}J' = (J^{-1}J - CJ')^{-1},
\] (38)
or with \( X = C J' \) and \( B = J'^{-1}J \) we arrive at the quadratic matrix equation
\[
X^2 - BX - 1 = 0.
\] (39)

The solution of a quadratic matrix equation of the form \( AX^2 + BX + C \), in general, cannot be given in a closed form unless \( A = 1 \), \( B \) commutes with \( C \), and the square root of \( B^2 - 4C \) exists. In this case the solution is given by
\[
X_{\pm} = -B/2 \pm \sqrt{B^2 - 4C}/2.
\] (40)

Obviously our Eq. \( (39) \) meets this condition, and so the equation can be solved and \( C \) can be calculated, although the final formula is a little lengthy to present here. Nevertheless a closed form expression has been obtained for the tail. Starting with \( C_{N'+1} \simeq C/N' \) the matrix continued fraction becomes convergent for the whole complex energy plane and thus the method became amenable for calculating resonant states.

4.2 Numerical Illustration

Here we adopt units such that \( m = h = e = 1 \) and \( c = 137.036 \). As a numerical illustration we consider the potential
\[
V(r) = 92/r - 240\exp(-r)/r + 320\exp(-4r)/r.
\] (41)

This potential, for an \( l = 0 \) partial wave, has one bound state and a very narrow resonant state. We used the parameter \( b = 8 \). The non-relativistic energies are \(-5.9293680 \) and \( 15.6091791 - 0.0000015i \), respectively, while the relativistic ones are \(-5.9335096 \) and \( 15.5994090 - 0.0000004i \). We see that the method can calculate resonant states in a very accurate way such that it is able to pinpoint the fine relativistic effects.

5 Confinement Potential

In this section we consider confinement potentials. We assume that the confinement potential is scalar and the vector potential is Coulomb-like
\[
U = \alpha_1 r + \alpha_2 r^2 + v_0^{(s)} \quad \text{and} \quad V = Z/r + v_4^{(s)}.
\] (42)

For the short range part of the Hamiltonian we find
\[
H_{FV0}^{(s)} = (\tau_3 + i \tau_2)v_0^{(s)} + v_4^{(s)},
\] (43)
and for the long range part we obtain
\[
H_{FV0}^{(l)} = (\tau_3 + i \tau_2) \left( \frac{p^2}{2m} + \alpha_1 r + \alpha_2 r^2 \right) + \tau_3 mc^2 + \frac{Z}{r}.
\] (44)

We have seen before that the representation of the constant \( E \) and the \( p^2 \) are tridiagonal infinite matrices, but the confining \( r \) term is penta-diagonal and the \( r^2 \) term is septa-diagonal. Consequently, the \( \tau_i \) matrices of the FV0 equation get superimposed on a septa-diagonal structure. As a result, we obtain an infinite tridiagonal matrix with \( 6 \times 6 \) blocks and the procedure of Eqs. \( (20) \) and \( (21) \) for the Green’s operator is applicable with \( 6 \times 6 \) blocks. We can also see that in the \( N' \to \infty \) limit the \( r \) term behaves like \( N'^2 \) and the \( r^2 \) term like \( N'^3 \). Therefore, the confining terms dominate over the energy and kinetic energy terms. Hence, as \( N' \to \infty \), \( C_{N'+1} \simeq 1/N'^2 \) or \( C_{N'+1} \simeq 1/N'^3 \). In either case, the evaluation of the matrix continued fraction can be initiated with \( C_{N'+1} = 0 \).
Table 1 Non-relativistic and relativistic FV0 results for states with Coulomb ($Z = -1$) plus linear ($\alpha_1 = 1$) and quadratic ($\alpha_2 = 1/2$) confinement potentials

|                  | Sch: $\alpha_1 = 1$ | FV0: $\alpha_1 = 1$ | Sch: $\alpha_2 = 1/2$ | FV0: $\alpha_2 = 1/2$ |
|------------------|----------------------|----------------------|----------------------|----------------------|
| 0.57792135       | 0.57774937           | 0.17966848           | 0.15989685           |
| 2.45016289       | 2.44983403           | 2.50000000           | 2.37624749           |
| 3.75690569       | 3.75635589           | 4.63195241           | 4.33778167           |
| 4.85567124       | 4.85486537           | 6.71259573           | 6.18557261           |
| 5.83602989       | 5.83494151           | 8.76951960           | 7.93366119           |
| 6.73662100       | 6.73522824           | 10.8129243           | 9.56883321           |

5.1 Numerical Illustration

We assume here that the Hamiltonian is in the form of Eq. (44) and there is no short range term. Table 1 shows the non-relativistic and relativistic results for the few lowest bound states of the system with $Z = -1$ and $\alpha_1 = 1$, as well as $Z = -1$ and $\alpha_2 = 1/2$. The former case is called the Cornell potential, and it is typically used in describing quarks confined in hadrons, while the later one is a Coulomb plus harmonic oscillator potential. We can see in Table 1 that the method can pinpoint the fine relativistic effects.

6 Summary and Conclusions

There are a great deal of methods addressing problems in non-relativistic quantum mechanics, but much fewer methods are available for relativistic systems. In this work we addressed relativistic problems through the Feshbach–Villars formalism. In this formalism we dealt with Schrödinger-like Hamilton eigenvalue problems. This formalism features a multicomponent wave function with kinetic energy coupling the components. In this approach we cast the FV0 equations into an integral equation, which is represented in a discrete basis. The corresponding Green’s operator is calculated for two important long-range potentials, the Coulomb and confining potentials. The multicomponent character with the kinetic energy and long range terms as asymptotic couplings were successfully treated with the help of the matrix continued fractions. By calculating the tail we managed to extend the methods for complex energies as well.

References

1. H. Feshbach, F. Villars, Rev. Mod. Phys. 30, 24 (1958)
2. M.G. Fuda, Phys. Rev. C 21(4), 1480 (1980)
3. J.L. Friar, Z. Phys. A At. Nucl. 297(2), 147 (1980)
4. M.G. Fuda, Phys. Rev. C 24(2), 614 (1981)
5. M. Merad, L. Chetouani, A. Bounames, Phys. Lett. A 267(4), 225 (2000)
6. K. Khounfais, T. Boudjedaa, L. Chetouani, Czech J. Phys. 54(7), 697 (2004)
7. A. Bounames, L. Chetouani, Phys. Lett. A 279(3–4), 139 (2001)
8. M. Horbatsch, D.V. Shapoval, Phys. Rev. A 51(3), 1804 (1995)
9. N.C. Brown, Z. Papp, R. Woodhouse, Few-Body Syst. 57(2), 103 (2016)
10. A. Wachter, Relativistic Quantum Mechanics (Springer, Berlin, 2010)
11. N.C. Brown, S.E. Grefe, Z. Papp, Phys. Rev. C 88(4), 047001 (2013)
12. B. Konya, G. Levai, Z. Papp, J. Math. Phys. 38, 4832 (1997)
13. F. Demir, Z.T. Hlousek, Z. Papp, Phys. Rev. A 74, 041701 (2006)
14. E. Kelbert, A. Hyder, F. Demir, Z.T. Hlousek, Z. Papp, J. Phys. A Math. Theor. 40(27), 7721 (2007)

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