Matrix continued fraction solution of spin-0 and spin-1/2 Feshbach-Villars equation

Bita Motamedi & Antonio Garcia Vallejo & Zoltán Papp

Department of Physics & Astronomy
California State University Long Beach

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Outline

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- Schrödinger

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- Dirac (spin 1/2 particles)

$$i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0$$

Postulates of QM

- 2nd postulate of QM: At any given time the quantum state is described by $\psi(t)$.
- 5th postulate of QM: The time evolution is described by

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$$-\hbar^2 \frac{\partial^2}{\partial t^2}\psi = (c^2 p^2 + m^2 c^4)\psi$$

- The Klein-Gordon equation, one of the basics eq. of relativistic QM, is not a quantum mechanical equation.

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Klein-Gordon equation in Hamiltonian form

$$(i\hbar\partial/\partial t - V)^2\psi = (c^2p^2 + (m + S/c^2)^2c^4)\psi$$

$\psi = \phi + \chi$ $\quad (i\hbar\frac{\partial}{\partial t} - V)\psi = (m + S/c^2)c^2(\phi - \chi)$ $\quad \Psi = \begin{pmatrix}\phi \\ \chi\end{pmatrix}$

$$i\hbar\frac{\partial}{\partial t}\Psi = H_{FV0}\Psi$$

$$H_{FV}^{(0)} = \begin{pmatrix}1 & 1 \\ -1 & -1\end{pmatrix}\left(\frac{p^2}{2m} + U\right) + \begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix}mc^2 + \begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix}V$$

Feshbach-Villars (1958)
$U = S + S^2/2mc^2$

Feshbach-Villars equation

$$\phi = \frac{1}{2}\left[\left(1 - \frac{1}{mc^2}V\right)\psi + \frac{E}{mc^2}\psi\right]$$

$$\chi = \frac{1}{2}\left[\left(1 + \frac{1}{mc^2}V\right)\psi - \frac{E}{mc^2}\psi\right]$$

$V = 0,\ E > mc^2,\ E \simeq mc^2$

$$\phi = \frac{1}{2}\left[\psi + \frac{E}{mc^2}\psi\right] \qquad \chi = \frac{1}{2}\left[\psi - \frac{E}{mc^2}\psi\right]$$

$\phi \rightarrow \psi \quad \chi \rightarrow 0$

FV0

$V = 0,\ E = mc^2/\sqrt{1 - v^2/c^2}$

$$\frac{|\chi|}{|\phi|} = \frac{1 - \sqrt{1 - v^2/c^2}}{1 + \sqrt{1 - v^2/c^2}}$$

as $v \to c$ $\quad |\chi|/|\phi| \to 1$

- if $E > 0,\ \ \phi > \chi$ $\quad \chi$ is "shadow" antiparticle component
- if $E < 0,\ \ \phi < \chi$ $\quad \phi$ is "shadow" particle component

Feshbach-Villars for spin-1/2

- $(\gamma_0 P_0 + \gamma_1 P_1 + \gamma_2 P_2 + \gamma_3 P_3 - imc)\,\psi = 0$
- $(i\hbar\partial/\partial t - V_0)^2\,\psi = [\mathbf{p}^2 c^2 + (m + S/c^2)^2 c^4 + c\sigma(\mathbf{p}V_0)]\psi$

$$H_{FV}^{(1/2)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \left(\frac{p^2}{2m} + U + \frac{\sigma \cdot (pV)}{c} \right) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + V \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Hamiltonian formalism

- non-relativistic

$$H = \frac{p^2}{2m} + V$$

- relativistic spin-0

$$H_{FV}^{(0)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \left(\frac{p^2}{2m} + U \right) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} V$$

- relativistic spin-1/2

$$H_{FV}^{(1/2)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \left(\frac{p^2}{2m} + U + \frac{\sigma \cdot (pV)}{c} \right) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + V \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Eigenvalue problem

$$E \begin{pmatrix} |\phi\rangle \\ |\chi\rangle \end{pmatrix} = H_{FV}^{(0)} \begin{pmatrix} |\phi\rangle \\ |\chi\rangle \end{pmatrix}$$

$$H_{FV}^{(0)} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \frac{p^2}{2m} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} V$$

- $H_{FV}^{(0)}$ is not hermitian
- yet it has real eigenvalues
- very bad equation: asymptotic coupling by the kinetic energy
- we have to put the asymptotic coupling into the Green's op.

Lippmann-Schwinger equation

- $H = H_0 + H'$
- $|\psi\rangle = G_0(E)H'|\psi\rangle$ $\qquad G(E) = (E - H_0)^{-1}$
- $H' \approx \sum^N |i\rangle\langle i|H'|j\rangle\langle j|$
- $G_0 = |i\rangle\langle i|G_0(E)|j\rangle\langle j|$
- $\underline{\psi} = \underline{G}_0(E)\underline{H}'\underline{\psi}$
- if $J = E - H_0$ is tridiagonal then G_0 is given in terms of continued fraction

$$\underline{G} = (\underline{J} - \delta_{iN}\delta_{jN}J_{N,N+1}C_{N+1}J_{N+1,N})^{-1} \tag{1}$$

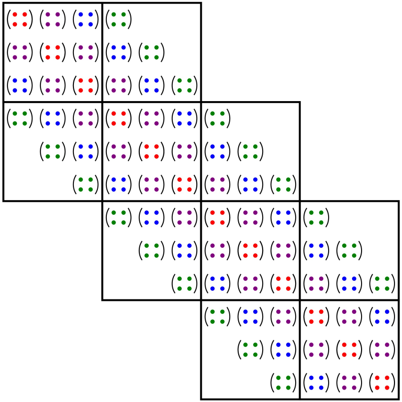
$$C_{N+1} = (J_{N+1,N+1} - J_{N+1,N+2}C_{N+2}J_{N+2,N+1})^{-1} \tag{2}$$

Coulomb-Sturmian basis

- $S_n(r) = \langle r|n\rangle = \left(\frac{\Gamma(n+1)}{\Gamma(n+2l+2)}\right)^{1/2} e^{-br}(2br)^{l+1} L_n^{2l+1}(2br)$
-
- $\langle n|E - p^2/(2m) - Z/r|n'\rangle$ tridiagonal
- $\langle n|(E - p^2/(2m) - Z/r)^{-1}|n'\rangle$ continued fraction
-
- $\langle n|r|n'\rangle$ 5-diagonal
- $\langle n|r^2|n'\rangle$ 7-diagonal

FV0 Green's operator for Coulomb plus confining potentials

$$J = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} E - \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \left(\frac{p^2}{2m} + a_1 r \right) - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{Z}{r}$$



block - tridiagonal

FV0 Green's operator for Coulomb plus confining potentials

$$G(E) = \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} E - \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \left(\frac{p^2}{2m} + a_1 r \right) - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 - \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{Z}{r} \right)^{-1}$$

$$\underline{G} = \left(\underline{J} - \delta_{iN}\delta_{jN} \underline{J}_{N,N+1} \underline{C}_{N+1} \underline{J}_{N+1,N} \right)^{-1}$$

$$\underline{C}_{N+1} = (\underline{J}_{N+1,N+1} - \underline{J}_{N+1,N+2} \underline{C}_{N+2} \underline{J}_{N+2,N+1})^{-1}$$

continued fraction with block matrices $\longrightarrow$ matrix continued fraction

FV1/2 case

$$G(E) =$$
$$\left(\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}E - \begin{pmatrix}1 & 1\\-1 & -1\end{pmatrix}\left(\frac{p^2}{2m} + \frac{\sigma\hbar Z}{c}\frac{1}{r^2}\right) - \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}mc^2 - \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\frac{Z}{r}\right)^{-1}$$

$$l \to -1/2 + \sqrt{1/4 + (j+1/2)^2 \pm \sqrt{(j+1/2)^2 - Z^2\alpha^2}}$$

perfect agreements with Klein-Gordon and Dirac results !!!

Outline

Feshbach-Villars formalism

- relativistic quantum mechanical equation
- multi-component wave function
- linear time & quadratic spatial derivative
- non-hermitian Hamiltonian

  $\bar{\Omega} = \tau_3 \Omega^{\dagger} \tau_3$ FV adjoint

  $\bar{\Omega} = \Omega$ FV hermitian $\rightarrow$ real eigenvalues
- explicit particle - antiparticle components
- interesting formalism, worth studying