NUMERICAL SOLUTION OF THE SPINLESS SALPETER EQUATION BY A SEMIANALYTICAL MATRIX METHOD (A Mathematica 4.0 Routine)

Wolfgang LUCHA

Institut für Hochenergiephysik, Österreichische Akademie der Wissenschaften, Nikolsdorfergasse 18, A-1050 Wien, Austria

Franz F. SCHÖBERL

Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria

Abstract

In quantum theory, the “spinless Salpeter equation,” the relativistic generalization of the nonrelativistic Schrödinger equation, is used to describe both bound states of scalar particles and the spin-averaged spectra of bound states of fermions. A numerical procedure solves the spinless Salpeter equation by approximating this eigenvalue equation by a matrix eigenvalue problem with explicitly known matrices.

PACS numbers: 03.65.Ge, 03.65.Pm, 11.10.St

* E-mail: wolfgang.lucha@oeaw.ac.at
† E-mail: franz.schoeberl@univie.ac.at
1 Introduction

The appropriate framework for the description of bound states within a relativistic quantum field theory is, beyond doubt, the famous Bethe–Salpeter equation [1]. Its actual application, however, faces several well-known problems of both conceptual as well as practical nature. For this reason, one usually considers some (three-dimensional) reduction of this formalism. In particular, assuming a static interaction between the bound-state constituents, neglecting all spin degrees of freedom, and considering exclusively positive-energy solutions, one ends up with what is called the “spinless Salpeter equation.” For some brief accounts of the reduction of the Bethe–Salpeter equation to the spinless Salpeter equation, see, for instance, Refs. [2, 3]. This eigenvalue equation generalizes the Schrödinger equation of the nonrelativistic quantum theory towards relativistic kinematics. It thus accomplishes the description of bound states of spinless constituents (scalar bosons) as well as of the spin-averaged spectra of bound states of fermions, like, e. g., in elementary particle physics the description of hadrons as bound states of quarks [4] within the (intuitive) framework of potential models for the strong interactions.

Here we present a very efficient method, based on Ref. [5], for solving the spinless Salpeter equation in configuration space, where the interaction potentials are usually formulated. The efficiency of this method stems from the fact that it does not require numerical integrations; rather, the aim of this method is to employ analytical results wherever these are available.

The outline of this paper is as follows. In Sect. 2 the configuration-space representation of the spinless Salpeter equation is briefly recalled. The resulting integro-differential equation is then approximated, in Sect. 3, by a (finite-dimensional) matrix eigenvalue problem. The only nontrivial ingredient of this matrix equation, viz., the piece emerging from the kinetic energy, is calculated in Sect. 4. This procedure for the determination of both energy eigenvalues and corresponding wave functions of bound states described by a spinless Salpeter equation with an, in principle, arbitrary interaction potential is eventually condensed, in Sect. 5 to a simple Mathematica routine. (This routine may be obtained, of course, by contacting the authors.)

2 The Spinless Salpeter Equation in Configuration Space

For notational and conceptual simplicity, we consider only the case of equal masses \( m \) of the bound-state constituents; the generalization to the case of unequal masses is straightforward.

The semirelativistic Hamiltonian \( H \) governing the dynamics of two relativistically moving spinless particles of equal masses \( m \), which interact via some arbitrary coordinate-dependent static potential \( V = V(\mathbf{x}) \) reads, in the center-of-momentum frame of these two particles,

\[
H = 2T + V,
\]

where \( T \) denotes the “square-root” operator of the relativistic expression for the free (kinetic) energy of some particle of mass \( m \) and momentum \( \mathbf{p} \),

\[
T = T(\mathbf{p}) \equiv \sqrt{\mathbf{p}^2 + m^2}.
\]

The spinless Salpeter equation is nothing else but the eigenvalue equation for the operator \( H \),

\[
H|\chi_k\rangle = E_k|\chi_k\rangle, \quad k = 0, 1, 2, \ldots,
\]

for the complete set of Hilbert-space eigenvectors \( |\chi_k\rangle \) with corresponding energy eigenvalues

\[
E_k \equiv \frac{\langle \chi_k|H|\chi_k\rangle}{\langle \chi_k|\chi_k\rangle}, \quad k = 0, 1, 2, \ldots.
\]

However, in contrast to, e. g., the (nonrelativistic) Schrödinger equation, the semirelativistic Hamiltonian \( H \) is a nonlocal operator, i.e., either the relativistic kinetic-energy operator \( T \) in configuration space or, in general, the interaction-potential operator \( V \) in momentum space is nonlocal.
In configuration space, the action of the kinetic-energy operator $\hat{E}$ on some element $\psi$ of $L_2(R^3)$, the Hilbert space of square-integrable functions on the three-dimensional Euclidian space $R^3$, is defined by
\[
(T\psi)(x) = \frac{1}{(2\pi)^3} \int d^3p \int d^3y \sqrt{p^2 + m^2} \exp[i \mathbf{p} \cdot (x - y)] \psi(y) .
\]

With this definition, an integral representation of the spinless Salpeter equation can be found \[3, 4\]. We focus our interest, for the moment, to spherically symmetric interaction potentials $V(x) = V(r)$, depending only on the radial coordinate $r \equiv |x|$. For a nonvanishing mass of the bound-state constituents, that is, $m > 0$, upon rescaling the radial variable $r$ according to $x := m r$ and introducing the scaled counterpart $\tilde{w}(x)$ of the reduced radial wave function $w(r)$ by defining $w(r) := m^{\ell+1} \tilde{w}(x)$, any dependence of the eigenvalue equation \[3\] on the mass $m$ of the two bound-state constituents may be absorbed into a scaled (and therefore dimensionless) energy eigenvalue $\tilde{E}$ and interaction potential $\tilde{V}(x)$:
\[
\tilde{E} := \frac{E}{m} , \quad \tilde{V}(x) := \frac{V(r)}{m} .
\]

The spinless Salpeter equation \[3\] is then equivalent to the integro-differential equation \[3, 5\]
\[
\left[\tilde{E} - \tilde{V}(x)\right] x^{\ell+1} \tilde{w}(x) = \frac{2}{\pi} \int_0^\infty \mathrm{d}y G_\ell(x, y) y^{\ell+1} \left[ 1 - \frac{\mathrm{d}^2}{\mathrm{d}y^2} - \frac{2(\ell + 1)}{y} \frac{\mathrm{d}}{\mathrm{d}y} \right] \tilde{w}(y) ,
\]
where the kernel $G_\ell(x, y)$ is defined by
\[
G_\ell(x, y) := 2^\ell x^{\ell+1} \left( \frac{1}{z} \frac{\partial}{\partial z} \right)^\ell \frac{1}{z} \left[ (s - z)^{\ell/2} K_\ell \left( \sqrt{s - z} \right) - (s + z)^{\ell/2} K_\ell \left( \sqrt{s + z} \right) \right] ,
\]
with the abbreviations $s \equiv x^2 + y^2$ and $z \equiv 2 x y$. Here, $K_\ell$ is the modified Bessel function of the second kind of order $\ell$ \[5\].

### 3 Conversion into an Equivalent Matrix Eigenvalue Problem

In order to rephrase the eigenvalue equation \[3\] in the form of an (easier-to-handle) algebraic problem, we expand every function on the positive real line $R^+$ we encounter into a complete orthonormal system $\{f_n(x), n = 0, 1, 2, \ldots\}$ of basis functions for the Hilbert space $L_2(R^+)$. The solutions $\tilde{w}(x)$ of Eq. \[4\], in particular, are then obtained in the form
\[
\tilde{w}(x) = \sum_{n=0}^N c_n f_n(x)
\]
with some set of real coefficients $c_n$. This treatment would be exact for $N = \infty$ and represents an approximation for $N < \infty$ of, however, increasing accuracy with increasing matrix size $N$. By application of this procedure, we are able to recast the spinless Salpeter equation \[3\] into the form of a matrix eigenvalue equation for the vector $c \equiv \{c_n\}$ of the expansion coefficients:
\[
\tilde{E} c = \left( P^{(\ell)} \right)^{-1} \left( T^{(\ell)} \right)^T + V^{(\ell)} c .
\]
\[5\]
Here, the elements of the \( P^{(\ell)} \) and \( V^{(\ell)} \) are defined by

\[
P_{nm}^{(\ell)} := \int_0^\infty dx x^{\ell+1} f_n(x) f_m(x) = P_{mn}^{(\ell)} , \quad m, n = 0, 1, \ldots, N ,
\]

\[
V_{nm}^{(\ell)} := \int_0^\infty dx x^{\ell+1} \tilde{V}(x) f_n(x) f_m(x) = V_{mn}^{(\ell)} , \quad m, n = 0, 1, \ldots, N .
\]

The matrices \( T^{(\ell)} \) represent the action of the kinetic term on the vector of basis functions \( f_n \).

The main advantage of our procedure is the fact that the “kinetic-energy matrices” \( T^{(\ell)} \) have to be calculated only once (for a chosen matrix size \( N \)!) The elements \( T_{nm}^{(\ell)} \) of these matrices, however, have to be calculated separately for every value of the orbital angular momentum \( \ell \).

The solution of the matrix equation (5) then gives the energy eigenvalues \( E_k, k = 0, 1, \ldots, N \), as well as the reduced radial wave functions

\[
w_k(r) = m^{\ell+1} \sum_{n=0}^N c_n^{(k)} f_n(m r) , \quad k = 0, 1, \ldots, N .
\] (6)

Our choice of the basis functions \( f_n(x) \) is primarily dictated by our demand to allow for an analytical treatment of the spinless Salpeter equation (3) to the utmost (reasonable) extent:

\[
f_n(x) := \sqrt{2} \exp(-x) L_n(2x) , \quad n = 0, 1, 2, \ldots,
\]

where \( L_n(x) \) are the Laguerre polynomials \([7]\)

\[
L_n(x) = \sum_{t=0}^n (-1)^t \binom{n}{t} x^t t! .
\]

Trivially, these basis functions satisfy the orthonormalization condition

\[
\int_0^\infty dx f_n(x) f_m(x) = \delta_{nm} .
\]

For this choice of basis functions it is straightforward to write down the explicit expression for the matrix elements \( P_{nm}^{(\ell)} \):

\[
P_{nm}^{(\ell)} = \frac{1}{2^{\ell+1}} \sum_{p=0}^n \sum_{q=0}^m (-1)^{p+q} \binom{n}{p} \binom{m}{q} \frac{(p+q+\ell+1)!}{p! q!} .
\]

This easy availability of the explicit expressions for the power matrices \( P^{(\ell)} \) strongly suggests to consider, as a special case, a class of interaction potentials of (generalized) power-law form:

\[
V(r) = \sum_{n \in \mathbb{Z}} a_n r^n ,
\] (7)

where the two sets of (otherwise arbitrary) integers \( n \) and real constants \( a_n \) (playing the rôle of coupling strengths) are only constrained by the necessary boundedness from below of the Hamiltonian \( H \) defined in Eq. (2): \( n \geq -1 \) if \( a_n < 0 \). For this class of interaction potentials, the potential matrices \( V^{(\ell)} \) simply become linear combinations of the power matrices \( P^{(\ell)} \):

\[
V^{(\ell)} = \sum_{n \in \mathbb{Z}} \frac{a_n}{m^{n+1}} P^{(\ell+n)} .
\]

It goes without saying that the procedure described here works in the same way also, at least, for all power-law potentials involving additional exponential (damping) factors, that is, for all interaction potentials of the form

\[
V(r) = \sum_{n \in \mathbb{Z}} a_n r^n \exp(-b_n r) , \quad b_n \geq 0 .
\]
4 The Kinetic-Energy Matrix

Clearly, the main task in our game is the calculation of the kinetic-energy matrix $T^{(\ell)}$. This enterprise is somewhat involved but, as already mentioned, has to be undertaken only once. In general, the elements of the kinetic-energy matrix $T^{(\ell)}$ are given by some expression of the form

$$T^{(\ell)}_{nm} = \frac{2}{\pi} \sum_{k=0}^{N} D(\ell; n, k) c(\ell; k, m) , \quad m, n = 0, 1, \ldots, N .$$

Here, the factors $D(\ell; n, k)$ represent the action of the differential operator on the right-hand side of the integro-differential equation on the chosen basis functions $f_n(x)$. For our choice of basis functions, these factors read explicitly

$$D(\ell; n, k) \equiv 2 \sqrt{2} \frac{(-1)^k}{k!} 2^k \left[ (k + \ell + 1) \binom{n}{k} + (k + 2\ell + 2) \binom{n}{k+1} \right] .$$

The factors $c(\ell; k, m)$ are the expansion coefficients, in terms of the basis functions $f_n(x)$, of a particular integral over the kernel $G_\ell(x, y)$:

$$c(\ell; k, m) = \int_{0}^{\infty} dx \ f_m(x) \int_{0}^{\infty} dy \ G_\ell(x, y) y^{\ell+k} \exp(-y) .$$

For increasing orbital angular momentum $\ell$, the kernels $G_\ell(x, y)$, $\ell = 0, 1, 2, \ldots$, become very rapidly rather complicated expressions. This circumstance forces us to calculate these factors $c(\ell; k, m)$ separately for every single value of the orbital angular momentum $\ell = 0, 1, 2, \ldots$ we are interested in. Here, we confine ourselves to the discussion of the cases $\ell = 0$ and $\ell = 1$.

We find, for states with orbital angular momentum $\ell = 0$ (the so-called “S waves”),

$$c(0; k, m) = 2 \sqrt{2} k! \sum_{p=0}^{[k/2]} \sum_{q=0}^{p} \sum_{r=0}^{m} (-1)^{q+r} \binom{k+1}{2p+1} \binom{p}{q} \binom{m}{r} \times \frac{2^r (r+1) (2k - 2q + r + 1)!}{(2k - 2q + 1)!! (2k - 2q + 2r + 3)!!} ,$$

and, for states with orbital angular momentum $\ell = 1$ (the so-called “P waves”),

$$c(1; k, m) = 2 \sqrt{2} k! \sum_{p=0}^{[k/2]+1} \sum_{q=0}^{p+1} \sum_{r=0}^{m} (-1)^{q+r} \binom{k+2}{2p+1} \binom{p}{q-1} \frac{1}{(2k - 2q + 5)!!} \binom{m}{r} 2^r (2k - 2q + r + 4)! \frac{(2k - 2q + 2r + 5)!!}{(2k - 2q + 2r + 3)!!} ,$$

where

$$\left[ \frac{k}{2} \right] \equiv \begin{cases} \frac{k}{2} & \text{for } k \text{ even} , \\ \frac{k-1}{2} & \text{for } k \text{ odd} , \end{cases}$$

and

$$(2n+1)!! \equiv 1 \times 3 \times \cdots \times (2n-1) \times (2n+1) , \quad n = 0, 1, 2, \ldots .$$

The calculation of the factors $c(\ell; k, m)$ for $\ell > 1$ is straightforward but somewhat involved because of the increasing complexity of the kernels $G_\ell(x, y)$. 
5 The Mathematica 4.0 Notebook Salpeter.

The „semianalytical matrix method” developed here for the solution of the spinless Salpeter equation has been implemented in a Mathematica 4.0 routine called Salpeter.nb (which may be obtained by contacting the authors). The routine Salpeter.nb requires as input, for two particles of mass $m$ experiencing some interaction potential $V(r)$ and for a chosen matrix size $d = N + 1$, only this potential $V(r)$ expressed in terms of the single terms $a_n r^n$ in Eq. (7), these terms written in the form $v_{pot}[asubn,n,m,d]$. For instance, for the “funnel” potential $V(r) = -a^{-1} r + a_1 r$, type

$v[m_,d_]:=v_{pot}[-asubminus1,-1,m,d]+v_{pot}[asub1,1,m,d]$.

Upon entering the command $etot[ell,m,d]$, this routine then computes, for orbital angular momentum $\ell$, particle mass $m$, and matrix size $d = N + 1$, the bound-state energy eigenvalues $E_k$, $k = 0, 1, \ldots, N$, together with the eigenvectors $c^{(k)}$, $k = 0, 1, \ldots, N$, from Eq. (8) and the corresponding radial eigenfunctions $R_k(r) \equiv r^\ell w_k(r)$, $k = 0, 1, \ldots, N$, according to Eq. (6).

We illustrate the power of the „semianalytical matrix method” by applying it to the case of a harmonic-oscillator potential $V(r) = a r^2$, $a > 0$, for the following reason: In momentum space, the operator $r^2$ is represented by the Laplacian w. r. t. the momentum $p$, $r^2 \rightarrow -\Delta p$, while the kinetic energy $T$, nonlocal in configuration space, is represented by a multiplication operator. Only for a harmonic-oscillator potential the momentum-space representation of the semirelativistic Hamiltonian $H$ is therefore of the form of a nonrelativistic Hamiltonian with a square-root interaction potential:

$$H = -a \Delta p + 2 \sqrt{p^2 + m^2}.$$  

The resulting (nonrelativistic) Schrödinger equation is then solved with a standard numerical procedure designed exactly for this purpose. (For details, in particular, for exact analytical upper and lower bounds on the energy levels, see, for instance, Refs. [10].)

Table 1: Eigenvalues (in units of GeV) of the semirelativistic Hamiltonian $H = 2 \sqrt{p^2 + m^2} + V(r)$ with a harmonic-oscillator potential $V(r) = a r^2$, for states of principal quantum number $n = 1, 2, 3, 4$ and orbital angular momentum $\ell = 0$ or $\ell = 1$ (called $nS$ or $nP$ in the usual spectroscopic notation) obtained by the “semianalytical matrix method” for increasing matrix sizes $d = 1, 3, 10, 25$, compared with the corresponding “exact” eigenvalues obtained from the momentum-space representation of the spinless Salpeter equation, which, for the special case of a harmonic-oscillator potential, resembles a nonrelativistic Schrödinger equation (as discussed in the text). The chosen physical parameter values are $m = 1$ GeV for the particle mass and $a = 0.5$ GeV$^3$ for the harmonic-oscillator coupling strength.

$$
\begin{array}{cccccccc}
\text{d} = N + 1 & \text{ell} = 0 & & & & \text{ell} = 1 & & \\
 & 1S & 2S & 3S & 4S & 1P & 2P & 3P & 4P \\
1 & 4.14531 & — & — & — & 5.12166 & — & — & — \\
3 & 3.91571 & 7.08622 & 11.94458 & — & 5.03946 & 7.68220 & 14.80138 & — \\
10 & 3.82522 & 5.80930 & 7.76609 & 9.90246 & 4.89944 & 6.72710 & 8.54739 & 11.20168 \\
25 & 3.82494 & 5.79112 & 7.48323 & 9.01617 & 4.90149 & 6.69298 & 8.28585 & 9.74304 \\
\text{exact} & 3.82493 & 5.79102 & 7.48208 & 9.00749 & 4.90145 & 6.69305 & 8.28464 & 9.74276 \\
\end{array}
$$

Table 1 demonstrates the rapid convergence for increasing matrix size of the lowest-lying energy eigenvalues of the spinless Salpeter equation with a harmonic-oscillator potential.
References

[1] E. E. Salpeter and H. A. Bethe, Phys. Rev. 84 (1951) 1232.

[2] W. Lucha and F. F. Schöberl, Int. J. Mod. Phys. A 7 (1992) 6431.

[3] W. Lucha and F. F. Schöberl, Int. J. Mod. Phys. A 14 (1999) 2309, \texttt{hep-ph/9812368};
W. Lucha and F. F. Schöberl, Fizika B 8 (1999) 193, \texttt{hep-ph/9812526}.

[4] W. Lucha, F. F. Schöberl, and D. Gromes, Phys. Rep. 200 (1991) 127.

[5] W. Lucha, H. Rupprecht, and F. F. Schöberl, Phys. Rev. D 45 (1992) 1233.

[6] L. J. Nickisch, L. Durand, and B. Durand, Phys. Rev. D 30 (1984) 660; 30 (1984) 1995 (E).

[7] Handbook of Mathematical Functions, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1964).

[8] H. Rupprecht, Semirelativistische Behandlung von Potentialmodellen, Ph. D. thesis, University of Vienna (1991).

[9] W. Lucha and F. F. Schöberl, Int. J. Mod. Phys. C 10 (1999) 607, \texttt{hep-ph/9811453}.

[10] W. Lucha and F. F. Schöberl, Phys. Rev. A 60 (1999) 5091, \texttt{hep-ph/9904391};
W. Lucha and F. F. Schöberl, Int. J. Mod. Phys. A (in print), \texttt{hep-ph/9909451}.