Semirelativistic Potential Modelling of Bound States: Advocating Due Rigour

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Abstract. The Poincaré-covariant quantum-field-theoretic description of bound states by the homogeneous Bethe–Salpeter equation usually exhibits an intrinsic complexity that can be attenuated by allowing this formalism to undergo various simplifications. The resulting approximate outcome’s reliability can be assessed by applying several rigorous constraints on the nature of the bound-state spectra; most prominent here are existence, number and location of discrete eigenvalues.

1 Our Battlefield: Semirelativistic Bound States of Least Complexity

A popular (possibly even analytic) approach to semirelativistic bound states of scalar particles is known under the name spinless Salpeter equation, which is just the eigenvalue equation of a Hamiltonian $H$ encompassing both the relativistic kinetic term of the bound-state constituents and a static potential $V$ encoding all interactions. For the case of two bound-state constituents, of masses $m_1$ and $m_2$, and relative coordinates and momenta $x$ and $p$, this Hamiltonian $H$ reads

$$H = \sqrt{p^2 + m_1^2} + \sqrt{p^2 + m_2^2} + V(x),$$

which, for equal masses $m_1 = m_2 = m$ of its bound-state constituents, simplifies (a little bit) to

$$\tilde{H} = 2\sqrt{p^2 + m^2} + V(x).$$

The spinless Salpeter equation may be regarded as some approximation defined by a sequence of self-evident assumptions that serves to simplify the homogeneous Bethe–Salpeter equation [1], which constitutes within the framework of relativistic quantum field theories the adequate approach to bound states of the fundamental degrees of freedom of such quantum field theory:

1. The most decisive simplification is to disregard any reference to timelike coordinate and momentum variables, thereby defining an instantaneous Bethe–Salpeter formalism [2].
2. Enabling any bound-state constituent to propagate freely entails Salpeter’s equation [3].
3. Skipping impacts of negative-energy contributions gives the reduced Salpeter equation.
4. Ignoring the spins of all bound-state constituents leads to the spinless Salpeter equation.

2 General Insights: Elementary Constraints on Bound-State Spectra

Even if being not accessible analytically, the spectrum of the operator $\tilde{H}$ is tightly constrained.

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1. **Boundedness from below of Hamiltonian operators** is, as kinetic operators are positive, obvious if \( V(x) \) itself is bounded from below. If not, comparison with the relativistic Coulomb problem may prove advantageous. The Hamiltonian operator \( \hat{H} \) with the Coulomb interaction

\[
V(x) \equiv -\frac{\alpha}{|x|}, \quad \alpha > 0,
\]

will be bounded from below \([4,5]\) if and only if the coupling strength \( \alpha \) satisfies the constraint

\[
\alpha \leq \frac{4}{\pi} = 1.273239 \ldots.
\]

Within this interval, the spectrum, \( \sigma(\hat{H}) \), of this operator \( \hat{H} \) is subject to the lower bound \([4,5]\)

\[
\sigma(\hat{H}) \geq 2m \left( 1 - \frac{\pi \alpha^2}{4} \right). \quad (2)
\]

For Coulomb couplings \( \alpha \leq 1 \), the lower bound \((2)\) may, straightforwardly, be improved \([6]\) to

\[
\sigma(\hat{H}) \geq 2m \sqrt{1 + \sqrt{1 - \alpha^2}}.
\]

2. **Number of discrete eigenstates in the spectrum of \( \hat{H} \):** For all potentials \( V(x) \) that satisfy

\[
V(x) = V(r) \in L^{1/2}(|\mathbb{R}|) \cap L^3(|\mathbb{R}|), \quad V(x) \leq 0, \quad r \equiv |x|, \quad (3)
\]

the number of bound states of such operator \( \hat{H} \) may be shown to be bounded from above by \([7]\)

\[
N \leq \frac{C}{12 \pi} \int_0^\infty dr r^2 [\langle |V(x)| + 4m \rangle]^{3/2}.
\]

with the constant \( C \) given by \( C = 14.107590867 \) for \( m > 0 \) or \( C = 6.074898097 \) for \( m = 0 \) \([8]\).

3. **Upper bounds on the eigenvalues of \( \hat{H} \):** For all potentials \( V(x) \) that satisfy

\[
E_k \leq \tilde{E}_k \quad \forall \quad k = 0, 1, 2, \ldots, d - 1.
\]

Its eigenstates can be expanded in terms of some convenient basis \([10,11]\), e.g., in products of generalized-Laguerre polynomials, \( L_k^{(\gamma)} \), and spherical harmonics \( \gamma \) for angular momentum \( \ell \):

\[
\psi_k(x) \propto r^{\ell+\beta-1} \exp(-\mu r) L_k^{(2\ell+2\beta)}(2\mu r) \gamma, \quad k \in \mathbb{N}_0, \quad \ell \in \mathbb{N}_0, \quad (4)
\]

\[
L_k^{(\gamma)}(x) \equiv \sum_{t=0}^{k} \left( \begin{array}{c} k + \gamma \\gamma \end{array} \right) \left( \begin{array}{c} k - t \\mu \end{array} \right) \left( \begin{array}{c} -x \\beta \end{array} \right), \quad \mu > 0, \quad \beta > -\frac{1}{2}.
\]

4. **Quality of eigenstates** \([12,13]\) tentatively localized by whatever technique forms a crucial aspect that may be quantified by the relativistic generalization \([14,15]\) of the virial theorem of nonrelativistic quantum theory, which relates, for any of the eigenstates \( |\psi \rangle \) of the operator \((1)\), the expectation values of the radial derivatives of both the kinetic terms and the potential \( V(x) \):

\[
\left\langle x \left| \frac{p^2}{\sqrt{p^2 + m_1^2}} + \frac{p^2}{\sqrt{p^2 + m_2^2}} \right| x \right\rangle = \left\langle x \right| x \cdot \frac{\partial V}{\partial x}(x) \left| x \right\rangle.
\]
All of this proved useful in locating the discrete spectra of problems defined by spherically symmetric (central) potentials \( V(x) = V(r) \) (where \( r \equiv |x| \)) of Woods–Saxon \([14,17]\), Hulthéen \([17,18]\), Yukawa \([19]\), kink-like \([8]\) or generalized-Hellmann \([20,21]\) type. As an illustration, an application of all these tools is sketched for the totality of generalized-Hellmann potentials.

### 3 Application: Class of Potentials Generalizing Hellmann’s Proposal

Let us take the liberty to generalize the form proposed by Hellmann \([22,23]\) to a superposition

\[
V_H(r) \equiv V_C(r) + V_Y(r) = -\frac{\kappa}{r} - \nu \frac{\exp(-b r)}{r}
\]

of a definitely attractive Coulomb potential \( V_C(r) \) and a Yukawa-inspired potential \( V_Y(r) \), with Coulomb coupling \( \kappa \) and Yukawa coupling \( \nu \) and slope parameter \( b \), subject to the constraints

\[
\kappa \geq 0, \quad \nu \gtrless 0, \quad b > 0.
\]

Within the obtained class of generalized Hellmann potentials \( V_H(r) \), the qualitative behaviour of any of its members depends on the relative sign and size of the two coupling strengths \( \kappa \) and \( \nu \) that govern the Coulomb and Yukawa contributions to such generalized Hellmann potential. These potentials show a significant diversity: they may be unbounded \([\text{Fig.1(a,b)}]\) or bounded \([\text{Fig.1(c,d)}]\) from below, and be singular \([\text{Fig.1(a,b,d)}]\) or finite \([\text{Fig.1(c)}]\) at the origin, \( r = 0 \).

Needless to stress, using the tools sketched in Sect.2 it is a breeze to rough out the spectra of the entirety of relativistic Hellmann problems (for some relevant details, consult Ref. \([20]\)).

- Evidently, boundedness from below is the question to be answered first and foremost: Since any of our generalized Hellmann potentials is trivially bounded from below by conveniently selected Coulomb potentials, suboptimal bounds on the spectrum \( \sigma(\tilde{H}) \) necessarily exist for

\[
\kappa + \nu \leq \frac{4}{\pi}.
\]

For the sum of couplings non-positive, i.e., \( \kappa + \nu \leq 0 \), this lower bound of Coulomb origin is easily improvable: \( V_H(r) \) is bounded from below and hence \( \sigma(\tilde{H}) \) by the minimum of \( V_H(r) \).

### Table 1

| Bound state | Upper bounds |
|-------------|--------------|
| \( n_r \) | \( \ell \) | \( \kappa = \nu = \frac{1}{2} \) | \( \kappa = 1, \nu = -1 \) | \( \kappa = 1, \nu = -2 \) |
|-------------|--------------|
| 0 | 0 | -0.11673 | -0.17951 | -0.14410 |
| 0 | 1 | -0.01579 | -0.06294 | -0.06157 |
| 0 | 2 | -0.00616 | -0.02813 | -0.02812 |
| 1 | 0 | -0.02107 | -0.05464 | -0.04786 |
| 1 | 1 | -0.00509 | -0.02810 | -0.02762 |
| 2 | 0 | -0.00688 | -0.02566 | -0.02338 |
| Lower bound | -0.58578... | -1 | -0.37336... |
Figure 1. Representatives of four (out of the in total seven) different categories of generalized Hellmann potentials $V_H(r)$, specified by the (in)equalities of their couplings (a) $\nu > \kappa$, (b) $\nu = \kappa$, (c) $\nu = -\kappa$, and (d) $\nu < -\kappa$, obtained as sums (solid black) of Coulombic (dashed magenta) and Yukawa (dotted blue) terms. The systematic classification of all generalized Hellmann potentials can be found in Table 1 of Ref. [21].
The number of discrete eigenstates of any generalized-Hellmann Hamiltonian may never be bounded from above because any generalized Hellmann potential becomes Coulomb-like at large distances, in the limit \( r \to \infty \). More technically, any generalized relativistic Hellmann problem fails \([20]\) to satisfy the prerequisite \([3]\) that guarantees finiteness \([7]\) of the number.

Upper bounds on the eigenvalues corresponding to lowest-lying discrete eigenstates may be conveniently calculated numerically upon spanning that \( d \)-dimensional subspace referred to by the minimum–maximum theorem by a Laguerre basis \([4]\), as exemplified in Table \([1]\), they can be optimized by increasing the dimension \( d \) and adapting the two parameters \( \mu \) and/or \( \beta \).

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