

SPINLESS SALPETER EQUATION: ANALYTIC RESULTS

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Abstract

The spinless Salpeter equation is the combination of relativistic kinematics with some static interaction potential. The nonlocal nature of the Hamiltonian resulting from this approximation renders difficult to obtain rigorous analytic statements on resulting solutions. In view of this unsatisfactory state of affairs, we calculate analytic upper bounds on the involved energy levels, and, for the Coulomb potential, the ground-state energy at the critical coupling constant.

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1 Introduction: The Spinless Salpeter Equation

The most straightforward generalization of standard nonrelativistic quantum theory towards reconciliation with requirements imposed by special relativity is to describe a quantum system under consideration by the well-known *spinless Salpeter equation*. Consider a quantum system the dynamics of which is governed by a—by assumption self-adjoint—Hamiltonian H of the form

$$H = T + V , \quad (1)$$

where T denotes the square-root operator of the relativistic expression for the kinetic energy of some particle of mass m and momentum \mathbf{p} , that is, $T \equiv \sqrt{\mathbf{p}^2 + m^2}$, and $V = V(\mathbf{x})$ represents an arbitrary coordinate-dependent static interaction potential. The eigenvalue equation for this Hamiltonian H , $H|\chi_k\rangle = E_k|\chi_k\rangle$, $k = 0, 1, 2, \dots$, for Hilbert-space eigenvectors $|\chi_k\rangle$ corresponding to energy eigenvalues

$$E_k \equiv \frac{\langle \chi_k | H | \chi_k \rangle}{\langle \chi_k | \chi_k \rangle} ,$$

is the one-particle spinless Salpeter equation. However, because of the nonlocality of H , it is extremely hard to obtain analytic statements from this equation of motion.

Of particular importance in physics are “central” potentials, i.e., potentials which depend only on the radial coordinate $r \equiv |\mathbf{x}|$. Among these, the most prominent one is the Coulomb potential $V_C(r)$, which is parametrized by some coupling constant α :

$$V(\mathbf{x}) = V_C(r) = -\frac{\alpha}{r} , \quad \alpha > 0 . \quad (2)$$

The semirelativistic Hamiltonian (1) with the Coulomb interaction potential V in (2) defines the *spinless relativistic Coulomb problem*. In the past, the interest in this has undergone an eventful history. (For a rather comprehensive review, consult Ref. [1].)

By examining [2] the spectral properties of the Hamiltonian (1) with the potential (2) one infers the existence of a Friedrichs extension up to the critical value $\alpha_c = 2/\pi$ of α . As far as analytic statements about this spinless relativistic Coulomb problem, in particular, about the resulting energy levels, are concerned, up to now one has to be content with few series expansions of the energy eigenvalues in powers of α [3, 4], which then are, of course, only significant for some region of rather small values of α .

2 Variational Upper Bounds on Energy Levels

Variational upper bounds on the eigenvalues of the above Hamiltonian H are derived rather easily in the following way [5]. We introduce an arbitrary real parameter μ and make use of the positivity of the square of the (obviously self-adjoint) operator $T - \mu$,

$$0 \leq (T - \mu)^2 = T^2 + \mu^2 - 2\mu T = \mathbf{p}^2 + m^2 + \mu^2 - 2\mu T ,$$

in order to find, for the kinetic energy T , the operator inequality (see also Ref. [6])

$$T \leq \frac{\mathbf{p}^2 + m^2 + \mu^2}{2\mu} \quad \text{for all } \mu > 0 ,$$

and, therefore, for the semirelativistic Hamiltonian H in (1), the operator inequality

$$H \leq \widehat{H}_S(\mu) \quad \text{for all } \mu > 0 ,$$

with some Schrödinger-like Hamiltonian, denoted by $\widehat{H}_S(\mu)$ and given by the unusual form

$$\widehat{H}_S(\mu) = \frac{\mathbf{p}^2 + m^2 + \mu^2}{2\mu} + V .$$

Now, invoking the min–max principle, we infer that the set of energy eigenvalues E_k , $k = 0, 1, 2, \dots$, of the Hamiltonian H , if ordered according to $E_0 \leq E_1 \leq E_2 \leq \dots$, is bounded from above by the corresponding set of energy eigenvalues $\widehat{E}_{S,k}(\mu)$ of $\widehat{H}_S(\mu)$, if the latter are similarly ordered according to $\widehat{E}_{S,0}(\mu) \leq \widehat{E}_{S,1}(\mu) \leq \widehat{E}_{S,2}(\mu) \leq \dots$, i.e., $E_k \leq \widehat{E}_{S,k}(\mu)$ for all $\mu > 0$, and is, consequently, also bounded by the minimum of all these energy eigenvalues:

$$E_k \leq \min_{\mu > 0} \widehat{E}_{S,k}(\mu) .$$

For the Coulomb potential (2), these energy eigenvalues $\widehat{E}_{S,n}(\mu)$ are given by [5]

$$\widehat{E}_{S,n}(\mu) = \frac{1}{2\mu} \left[m^2 + \mu^2 \left(1 - \frac{\alpha^2}{n^2} \right) \right] ,$$

where the total quantum number n is defined according to $n = n_r + \ell + 1$. Minimizing the latter expression with respect to the parameter μ , we obtain as minimal bound [5]

$$\min_{\mu > 0} \widehat{E}_{S,n}(\mu) = m \sqrt{1 - \frac{\alpha^2}{n^2}} . \quad (3)$$

Comparing with the results obtained in the framework of perturbation theory [4], which read, for instance, for the level $n = 2$, $\ell = 1$,

$$\frac{E}{m} = 1 - \frac{\alpha^2}{8} - \frac{7\alpha^4}{384} + \frac{727\alpha^6}{82944} + \dots ,$$

we observe that our upper bound (3) not only possesses the elegance of a particularly simple form but is also valid for all $\alpha \leq \alpha_c$ and arbitrary levels of excitation. A quick glance at Table 1 shows that the relative error of our bound is always less than 0.1 %.

Table 1: Comparison of the perturbatively computed [4] energy eigenvalues for, e.g., the level $n = 2$ and $\ell = 1$ with our variational upper bounds, extracted from Eq. (3)

α	E/m	
	Perturbation Theory [4]	Variational Procedure, Eq. (3)
0.0155522	0.999969765	0.999969766
0.1425460	0.997452	0.997457
0.2599358	0.99147	0.99152
0.3566678	0.9838	0.9840
0.4359255	0.975	0.976
0.5	0.967	0.9682

3 The Energy at the Critical Coupling Constant

Let us apply again the min–max principle. Our particular (somewhat sophisticated) choice for the basis vectors $|\psi_k\rangle$ to be adopted here is defined by trial functions $\psi_k(r)$ given in configuration-space representation (with the radial coordinate $r \equiv |\mathbf{x}|$) by [7]

$$\psi_k(r) = \sqrt{\frac{(2m)^{2k+2\beta+1}}{4\pi\Gamma(2k+2\beta+1)}} r^{k+\beta-1} \exp(-mr), \quad \beta \geq 0, \quad m > 0.$$

Whereas k indicates a positive integer, $k = 0, 1, 2, \dots$, the parameter β is introduced to allow, for some given value of the coupling constant α , of a total cancellation of the divergent contributions to the expectation values of kinetic energy T and interaction potential $V_C(r)$: $\beta = \beta(\alpha)$. More precisely: in order to provide for that cancellation, the parameter β has to be adjusted for the ground state according to the relation [8]

$$\alpha = \beta \cot\left(\frac{\pi}{2}\beta\right),$$

which implicitly determines β as a function of the coupling constant α . In particular, this relation tells us that the critical coupling constant, α_c , is approached for $\beta \rightarrow 0$. From the behaviour of the matrix elements $\langle\psi_i|T|\psi_j\rangle$ of the kinetic energy T for large momenta p and of the matrix elements $\langle\psi_i|V_C(r)|\psi_j\rangle$ of the Coulomb potential $V_C(r)$ at small distances r , respectively, it should become evident that, for our particular choice of basis states $|\psi_k\rangle$, these singularities can arise only in matrix elements taken with respect to the ground state $|\psi_0\rangle$, that is, merely in $\langle\psi_0|T|\psi_0\rangle$ and $\langle\psi_0|V_C(r)|\psi_0\rangle$.

The remainder of our way is straightforward. With the above basis functions, we obtain, by calculating the 2×2 energy matrix (and performing very carefully the limit $\beta \rightarrow 0$), for the roots of the corresponding characteristic equation the expression [9]

$$\frac{\hat{E}}{m} = \frac{2}{15\pi} \left(60 \ln 2 - 23 \pm \sqrt{(60 \ln 2)^2 - 4800 \ln 2 + 1649} \right),$$

which yields the upper bound $\hat{E}_0/m = 0.484288\dots$ for the ground-state eigenvalue of the Coulombic Hamiltonian. In principle, the d roots of the characteristic equation may be determined algebraically up to and including the case $d = 4$. For $d = 4$, our method constrains the lowest-lying energy level by the bound $\hat{E}_0/m = 0.4842564\dots$. On the other hand, at the critical coupling constant α_c the best numerically obtained bounds are given by [8]

$$0.4825 \leq \frac{E_0}{m} \leq 0.4842910 \quad \text{for } \alpha = \alpha_c.$$

Comparing these only numerically determined bounds on the ground-state energy E_0 with the above upper bound, we realize that even our 2×2 analytical bound lies well within the numerically obtained range. Consequently, we obtain a clear improvement of the best upper bound available up to now for the ground-state energy level of the spinless relativistic Coulomb problem at the critical value of the coupling constant.

References

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