Variational approach to the spinless relativistic Coulomb problem

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By application of a straightforward variational procedure, we derive a simple, analytic upper bound on the ground-state energy eigenvalue of a semirelativistic Hamiltonian for (one or two) spinless particles which experience some Coulomb-type interaction.

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I. INTRODUCTION

A standard (semi) relativistic description of bound states built up by particles of spin zero is provided by a Hamiltonian H which incorporates relativistic kinematics by involving the "square-root" operator of the relativistic kinetic energy, $\sqrt{\mathbf{p}^2+m^2}$ for a particle of mass m and momentum $\mathbf{p}$, but describes the forces acting between the bound-state constituents by some coordinate-dependent static interaction potential $V(\mathbf{x})$.

For the case of bound states consisting of two particles of equal mass m, the generic Hamiltonian in the center-of-momentum frame of these constituents, expressed in terms of relative momentum $\mathbf{p}$ and relative coordinate $\mathbf{x}$, reads

$$H = 2\sqrt{\mathbf{p}^2+m^2} + V(\mathbf{x}). \tag{1}$$

The equation of motion resulting from this type of Hamiltonian is the well-known "spinless Salpeter equation." It may be obtained from the so-called Salpeter equation [1] by ignoring all spin degrees of freedom and considering positive-energy solutions only. The Salpeter equation, in turn, approximates the Bethe–Salpeter equation [2] for bound states within a relativistic quantum field theory by eliminating, according to the spirit of an instantaneous interaction, any dependence on timelike variables. A central role in physics is played by the Coulomb potential, a spherically symmetric potential, i.e., one which depends only on the radial coordinate $r \equiv |\mathbf{x}|$, parametrized by some coupling strength κ:

$$V(\mathbf{x}) = V_C(r) = -\frac{\kappa}{r}, \qquad \kappa > 0. \tag{2}$$

The bound-state problem defined by the semirelativistic Hamiltonian (1) with the Coulomb potential (2) is what we call the "spinless relativistic Coulomb problem."

Over the past years, this spinless relativistic Coulomb problem, in both the one- and two-particle formulations, has been the subject of intense study.[1] First of all, Herbst [3], in a rigorous mathematical discussion, developed the complete spectral theory of the one-particle counterpart of the operator (1), (2), from which one may directly deduce for the two-particle relativistic "Coulombic" Hamiltonian under consideration its essential self-adjointness for $\kappa \leq 1$ and the existence of its Friedrichs extension up to the critical value $\kappa_{\rm cr} = 4/\pi$ of the coupling constant, and derived a strict lower bound on the energy E_0 of the ground state which translates in the two-particle case to

$$E_0 \geq 2m\sqrt{1-\left(\frac{\pi\kappa}{4}\right)^2} \qquad \text{for} \quad \kappa < \frac{4}{\pi}. \tag{3}$$

Durand and Durand [4] obtained, in a certainly rather involved analysis of the spinless relativistic Coulomb problem for the particular case of vanishing relative orbital angular momentum of the bound-state constituents, as a by-product of the explicit construction of the corresponding wave function, a closed analytic expression for the exact energy eigenvalues. Castorina and co-workers [5] generalized, for small relative distances of the bound-state constituents, this wave function to arbitrary values of the orbital angular momentum. Hardekopf and Sucher [6] performed a comprehensive numerical analysis of one- and two-particle relativistic wave equations for both spin-0 as well as spin-$\frac{1}{2}$ particles, in the course of which they were able to show that the result reported in Ref. [4] for the energy eigenvalues must necessarily be wrong. Mar-

[1]The semirelativistic Coulombic Hamiltonians for one- and two-particle problems, $H^{(1)} = \sqrt{\mathbf{P}^2+M^2} - \alpha/R$ and $H^{(2)} = 2\sqrt{\mathbf{p}^2+m^2} - \kappa/r$, respectively, may be easily equated. Relate their respective phase-space variables $(\mathbf{X},\mathbf{P})$ and $(\mathbf{x},\mathbf{p})$ by rescaling them by some scale factor λ according to $\mathbf{P} = \lambda\,\mathbf{p}$ and $\mathbf{X} = \mathbf{x}/\lambda$, which preserves their fundamental commutation relations: $[\mathbf{X},\mathbf{P}] = [\mathbf{x},\mathbf{p}]$. Let $\lambda = 2$ and identify both mass and Coulomb coupling strength parameters according to $M = 2\,m$ and $\alpha = \kappa/2$.

tin and Roy [7] improved the lower bound (3) somewhat to

$$E_0 \geq 2m\sqrt{\frac{1+\sqrt{1-\kappa^2}}{2}} \quad \text{for} \quad \kappa < 1. \tag{4}$$

Finally, Raynal and co-workers [8] succeeded in restricting numerically the ground-state energy eigenvalue of the semirelativistic Hamiltonian (1), (2), considered as a function of the coupling strength κ, to some remarkably narrow band.

The aim of the present paper is to find some simple and, in any case, analytically given upper bound on the ground-state energy level of the above semirelativistic "Coulombic" Hamiltonian.

II. A VARIATIONAL UPPER BOUND

In order to derive an analytic upper bound on the energy eigenvalue of the ground state of the spinless relativistic Coulomb problem, we make use of a rather standard variational technique. The basic idea of this variational technique is (i) to calculate the expectation values of the Hamiltonian H under consideration with respect to a suitably chosen set of trial states $|\lambda\rangle$ distinguished from each other by some variational parameter λ, which yields the λ-dependent expression $E(\lambda) \equiv \langle\lambda|H|\lambda\rangle$, and (ii) to minimize $E(\lambda)$ with respect to λ in order to obtain the upper bound to the proper energy eigenvalue E of the Hamiltonian H in the Hilbert-space subsector of the employed trial states $|\lambda\rangle$ as the above λ-dependent expression $E(\lambda)$ evaluated at the point of the minimizing value $\lambda_{\min}$ of the variational parameter: $E \leq E(\lambda_{\min})$.

For the Coulomb potential, the most reasonable choice of trial states is obviously the one for which the coordinate-space representation $\psi(\mathbf{x})$ of the states $|\lambda\rangle$ for vanishing radial and orbital angular momentum quantum numbers is given by the hydrogenlike trial functions ($\lambda > 0$)

$$\psi(\mathbf{x}) = \sqrt{\frac{\lambda^3}{\pi}}\,\exp(-\lambda r).$$

For this particular set of trial functions we obtain for the expectation values we shall be interested in, namely, the ones of the square of the momentum $\mathbf{p}$ and of the inverse of the radial coordinate r, respectively, with respect to the trial states $|\lambda\rangle$,

$$\langle\lambda\,|\mathbf{p}^2|\,\lambda\rangle = \lambda^2$$

and

$$\left\langle\lambda\left|\frac{1}{r}\right|\lambda\right\rangle = \lambda.$$

Let us follow this line of argument in some detail. As an immediate consequence of the fundamental postulates of any quantum theory, the expectation value of a given Hamiltonian H taken with respect to any normalized Hilbert-space state and, therefore, in particular, taken with respect to any of the above trial states, must necessarily be larger than or equal to that eigenvalue E_0 of the Hamiltonian H which corresponds to its ground state:

$$E_0 \leq E(\lambda) \equiv \langle\lambda|H|\lambda\rangle.$$

The application to the semirelativistic Hamiltonian of Eq. (1) yields, for the right-hand side of this inequality,

$$E(\lambda) = 2\left\langle\lambda\left|\sqrt{\mathbf{p}^2+m^2}\right|\lambda\right\rangle + \langle\lambda|V(\mathbf{x})|\lambda\rangle.$$

Here, the rather cumbersome although (for convenient trial states) not impossible evaluation of the expectation value of the square-root operator may be circumvented very easily by taking advantage of a trivial but nevertheless fundamental inequality. This inequality relates the expectation values, taken with respect to arbitrary Hilbert-space vectors $|\rangle$ normalized to unity, of both the first and second powers of a self-adjoint but otherwise arbitrary operator $\mathcal{O} = \mathcal{O}^\dagger$; it reads

$$|\langle\mathcal{O}\rangle| \leq \sqrt{\langle\mathcal{O}^2\rangle}.$$

For the purposes of the present discussion it is sufficient to replace, in turn, $E(\lambda)$ by its upper bound obtained by applying this inequality:

$$E(\lambda) \leq 2\sqrt{\langle\lambda\,|\mathbf{p}^2|\,\lambda\rangle + m^2} + \langle\lambda|V(\mathbf{x})|\lambda\rangle.$$

Identifying in this, as far as its evaluation is concerned, simplified, upper bound the until-now general potential $V(\mathbf{x})$ with the Coulomb potential (2) and inserting both of the λ-dependent expectation values given above implies

$$E(\lambda) \leq 2\sqrt{\lambda^2+m^2} - \kappa\,\lambda. \tag{5}$$

From this intermediate result, by inspection of the limit $\lambda \to \infty$, we may state already at this very early stage that, for the semirelativistic Hamiltonian (1), (2) to be bounded from below at all, the Coulombic coupling strength κ has to stay below a certain critical value: $\kappa \leq 2$.

The value of the variational parameter λ which minimizes the upper bound on the right-hand side of Eq. (5) may be determined from the derivative of this expression with respect to λ:

$$\lambda_{\min} = \frac{m\,\kappa}{2\sqrt{1-\frac{\kappa^2}{4}}}.$$

For this value of λ, by shuffling together all our previous inequalities, we find that the energy eigenvalue corresponding to the ground state of the semirelativistic Hamiltonian (1) with the Coulomb potential (2), E_0, is bounded from above by

$$E_0 \leq 2m\sqrt{1-\frac{\kappa^2}{4}}. \tag{6}$$

The reality of this upper bound requires again $\kappa \leq 2$.

III. SUMMARY

Within the framework of a simple variational technique we derived an analytic upper bound, Eq. (6), to the ground-state energy level of the spinless relativistic Coulomb problem. However, for any nonvanishing value of the Coulombic coupling strength κ, this upper bound (6) turns out, in fact, to be violated by the lowest energy eigenvalue obtainable from the analytic expression given in Ref. [4]. This provides, of course, further confirmation of the corresponding findings of Ref. [6]; a similar observation has been made in Ref. [9].

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