Spinless Salpeter equation: Laguerre bounds on energy levels

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The spinless Salpeter equation may be considered either as a standard approximation to the Bethe-Salpeter formalism, designed for the description of bound states within a relativistic quantum field theory, or as the most simple, to a certain extent relativistic, generalization of the costumary nonrelativistic Schrödinger formalism. Because of the presence of the rather difficult-to-handle square-root operator of the relativistic kinetic energy in the corresponding Hamiltonian, very frequently the corresponding (discrete) spectrum of energy eigenvalues cannot be determined analytically. Therefore, we show how to calculate, by some clever choices of basis vectors in the Hilbert space of solutions, for the rather large class of power-law potentials, at least upper bounds on these energy eigenvalues. For the lowest-lying levels, this may be done even analytically. [S1050-2947(97)03107-7]

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I. INTRODUCTION: THE SPINLESS SALPETER EQUATION

One's attitude to the well-known ''spinless Salpeter equation'' may be reflected by either of the following two approaches (or points of view). On the one hand, this spinless Salpeter equation may be regarded as representing some standard approximation to the Bethe-Salpeter formalism for the description of bound states within a relativistic quantum field theory. It may be derived from the Bethe-Salpeter equation [1] by two steps: (i) Eliminate—in full accordance with the spirit of instantaneous interactions—any dependence on timelike variables to obtain in this way the so-called Salpeter equation [2]; (ii) Neglect any reference to all the spin degrees of freedom of the involved bound-state constituents and restrict your formalism exclusively to positive-energy solutions. On the other hand, this spinless Salpeter equation may be viewed as one of the most straightforward generalizations of the standard nonrelativistic quantum theory towards the reconciliation with all the requirements imposed by special relativity. To be precise, this generalization consists of incorporating the square-root operator of the relativistic expression for the kinetic energy of the involved particles. For the particular case of two particles of equal mass m and relative momentum $\mathbf{p}$, the kinetic-energy operator T is given by

$$T(\mathbf{p}) \equiv 2\sqrt{\mathbf{p}^2 + m^2}. \tag{1}$$

All the forces operating between the bound-state constituents are tacitly assumed to be described by an arbitrary static interaction potential V. For the special case of two particles, this interaction potential should depend only on the relative coordinate $\mathbf{x}$ of these particles, $V = V(\mathbf{x})$.

In any case, the self-adjoint Hamiltonian H governing the dynamics of any quantum system to be described by the spinless Salpeter equation will be of the form

$$H = T(\mathbf{p}) + V(\mathbf{x}). \tag{2}$$

The two-particle spinless Salpeter equation to be investigated here is then nothing else but the eigenvalue problem for this Hamiltonian H,

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

for Hilbert-space eigenvectors $|\chi_k\rangle$ corresponding to energy eigenvalues

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

For the sake of simplicity, we shall focus our attention to the physically most relevant case of central potentials, i.e., potentials which depend only on the modulus $|\mathbf{x}|$ of the configuration-space relative coordinate,

$$V = V(|\mathbf{x}|). \tag{3}$$

In the above form, the spinless Salpeter equation appears to be a very promising candidate for the (semi)relativistic description of hadrons as bound states of (constituent) quarks within the framework of potential models [3–5] or, at least, the first step in the correct direction [6,7].

However, the presence of the relativistic kinetic-energy operator (1) in Eq. (2) or, to do justice to the spinless Salpeter equation, the nonlocality of this operator H, that is, more precisely, of either the kinetic-energy operator T in configuration space or the interaction-potential operator V in momentum space, renders it difficult to arrive at rigorous analytical statements about the corresponding energy spectrum. In view of this, numerous attempts to circumvent these problems have been proposed. Some very brief accounts of the history of these attempts may be found, for instance, in Ref. [8]. These approaches include, among others, the development of elaborate numerical approximation methods [9–12] as well as the construction of effective Hamiltonians which, despite their apparently nonrelativistic form, incorporate relativistic effects by a sophisticated momentum dependence of the involved parameters [13]. A lot of information

on the solutions of the spinless Salpeter equation may even be gained by the application of a relativistic virial theorem [14], most easily derived from a rather general ''master virial theorem'' [15].

The (from the physical point of view perhaps most interesting) case of a Coulomb-type static interaction potential, the so-called relativistic Coulomb problem, has been investigated particularly carefully. For the corresponding lowest-lying energy eigenvalues, both lower [16,17] and upper [17–20] bounds have been derived and series expansions [21] in powers of the involved fine structure constant have been given. Specifically, Herbst [16] showed that the corresponding Hamiltonian is bounded from below up to some critical value of the Coulomb coupling constant and unbounded from below above this value.

Here, we intend to pave the way for the calculation of upper bounds on the energy eigenvalues of the spinless Salpeter equation with rather arbitrary interaction potentials. To this end, we apply the famous min-max principle—which controls any such attempt—in a particular basis of our trial space, characterized by generalized Laguerre polynomials.

II. MINIMUM-MAXIMUM PRINCIPLE AND RAYLEIGH-RITZ VARIATIONAL TECHNIQUE

The derivation of upper bounds on the eigenvalues of some operator H makes, of course, only sense for those operators H which are bounded from below. Accordingly, let us assume from now on that the arbitrary interaction potential (3) in our semirelativistic Hamiltonian (2) is such that this necessary prerequisite holds. For example, for the crucial case of a Coulomb-type static interaction potential, the so-called relativistic Coulomb problem, the demanded semiboundedness of the spectrum of the Hamiltonian H has been (rigorously) demonstrated by Herbst [16].

The theoretical basis as well as the primary tool for the derivation of rigorous upper bounds on the eigenvalues of some self-adjoint operator is, beyond doubt, the so-called min-max principle [22]. An immediate consequence of this min-max principle is the Rayleigh-Ritz technique: Let H be a semibounded self-adjoint operator. Let E_k, $k=0,1,2,\ldots$, denote the eigenvalues of H, ordered according to $E_0\leqslant E_1\leqslant E_2\leqslant\cdots$. Let D_d be some d-dimensional subspace of the domain of H and let $\hat{E}_k$, $k=0,1,\ldots,d-1$, denote all d eigenvalues of this operator H restricted to the space D_d, ordered according to $\hat{E}_0\leqslant\hat{E}_1\leqslant\cdots\leqslant\hat{E}_{d-1}$. Then the kth eigenvalue E_k (counting multiplicity[1]) of H satisfies the inequality

$$E_k\leqslant\hat{E}_k,\quad k=0,1,\ldots,d-1.$$

(For a discussion of the history of inequalities and variational methods for eigenvalue problems, see, e.g., Ref. [23]; for some applications, see, e.g., Ref. [24].)

[1]For instance, for a Hamiltonian H depending only on the moduli of momentum $\mathbf{p}$ and coordinate $\mathbf{x}$, respectively, states of given orbital angular momentum but different projections of the latter will be degenerate.

Now, let us assume that this d-dimensional subspace D_d is spanned by some set of d orthonormalized (and therefore beyond doubt linearly independent) basis vectors $|\psi_k\rangle$, $k=0,1,\ldots,d-1$:

$$\langle\psi_i|\psi_j\rangle=\delta_{ij},\quad i,j=0,1,\ldots,d-1.$$

Then the set of eigenvalues $\hat{E}$ may immediately be determined as the d roots of the characteristic equation

$$\det(\langle\psi_i|H|\psi_j\rangle-\hat{E}\,\delta_{ij})=0,\quad i,j=0,1,\ldots,d-1, \tag{4}$$

as becomes clear from an expansion of any eigenvector of the restricted operator H in terms of the set of basis vectors $|\psi_k\rangle$, $k=0,1,\ldots,d-1$, of the subspace D_d.

III. GENERALIZED LAGUERRE BASIS

The crucial step in any investigation of the present type is the suitable choice of a basis in the subspace D_d. For the case of the semirelativistic Hamiltonian (2), we find it convenient to work in a basis which involves the so-called generalized Laguerre polynomials. The latter are specific orthogonal polynomials, defined by the power series [25]

$$L_k^{(\gamma)}(x)=\sum_{r=0}^{k}(-1)^r\binom{k+\gamma}{k-r}\frac{x^r}{r!}$$

and normalized according to [25]

$$\int_0^\infty dx\,x^\gamma\exp(-x)L_k^{(\gamma)}(x)L_{k'}^{(\gamma)}(x)=\frac{\Gamma(\gamma+k+1)}{k!}\,\delta_{kk'}.$$

Consequently, introducing two variational parameters, namely, one μ with the dimension of mass as well as a dimensionless one β, a generic trial vector $|\psi\rangle$ of the subspace D_d, with orbital angular momentum ℓ and its projection m, will be characterized by the following admittedly very suggestive ansatz for its coordinate-space representation $\psi_{k,\ell m}(\mathbf{x})$:

$$\psi_{k,\ell m}(\mathbf{x})=\mathcal{N}|\mathbf{x}|^{\ell+\beta-1}\exp(-\mu|\mathbf{x}|)L_k^{(\gamma)}(2\mu|\mathbf{x}|)\mathcal{Y}_{\ell m}(\Omega_{\mathbf{x}}), \tag{5}$$

where normalizability restricts the variational parameter μ to positive values,

$$\mu>0.$$

Here, $\mathcal{Y}_{\ell m}(\Omega)$ are the spherical harmonics for angular momentum ℓ and projection m depending on the solid angle Ω; they are orthonormalized according to

$$\int\mathrm{d}\Omega\,\mathcal{Y}_{\ell m}^*(\Omega)\mathcal{Y}_{\ell'm'}(\Omega)=\delta_{\ell\ell'}\delta_{mm'}. \tag{6}$$

The proper orthonormalization of the ansatz (5) fixes the parameter γ necessarily to the value $\gamma=2\ell+2\beta$ and determines the normalization constant $\mathcal{N}$:

$$\psi_{k,\ell m}(\mathbf{x}) = \sqrt{\frac{(2\mu)^{2\ell+2\beta+1}k!}{\Gamma(2\ell+2\beta+k+1)}}|\mathbf{x}|^{\ell+\beta-1} \times \exp(-\mu|\mathbf{x}|)L_k^{(2\ell+2\beta)}(2\mu|\mathbf{x}|)\mathcal{Y}_{\ell m}(\Omega_{\mathbf{x}})$$

satisfies the normalization condition

$$\int \mathrm{d}^3x\, \psi^*_{k,\ell m}(\mathbf{x})\psi_{k',\ell' m'}(\mathbf{x}) = \delta_{kk'}\delta_{\ell\ell'}\delta_{mm'}.$$

Rather obviously, normalizability constrains the variational parameter β too, namely, to a range characterized by $2\beta > -1$, i.e., to the range

$$\beta > -\frac{1}{2}.$$

Clearly, any particular choice for the value of the variational parameter β will yield (nonoptimized) upper bounds on the energy eigenvalues. Below, we shall find that—for the case of radial excitations, at least—we may evaluate these upper bounds analytically for 2β integer, i.e., for $2\beta = 0,1,2,\ldots$. A numerical analysis for $\beta = \frac{1}{2},1,2$ indicates that $\beta = 1$ is a reasonable choice, which we shall use occasionally in order to illustrate our general findings. For this choice of β, our Laguerre basis functions reduce to the well-known nonrelativistic Coulomb functions. The Fourier transform $\tilde{\psi}_{k,\ell m}(\mathbf{p})$ of the above trial function involves the hypergeometric series F, defined with the help of the gamma function Γ by [25]

$$F(u,v;w;z) = \frac{\Gamma(w)}{\Gamma(u)\Gamma(v)}\sum_{n=0}^{\infty}\frac{\Gamma(u+n)\Gamma(v+n)}{\Gamma(w+n)}\frac{z^n}{n!};$$

it reads

$$\tilde{\psi}_{k,\ell m}(\mathbf{p}) = \sqrt{\frac{(2\mu)^{2\ell+2\beta+1}k!}{\Gamma(2\ell+2\beta+k+1)}}\frac{(-i)^\ell|\mathbf{p}|^\ell}{2^{\ell+1/2}\Gamma(\ell+3/2)}\sum_{r=0}^{k}\frac{(-1)^r}{r!}\binom{k+2\ell+2\beta}{k-r}\frac{\Gamma(2\ell+\beta+r+2)(2\mu)^r}{(\mathbf{p}^2+\mu^2)^{(2\ell+\beta+r+2)/2}} \times F\left(\frac{2\ell+\beta+r+2}{2},-\frac{\beta+r}{2};\ell+\frac{3}{2};\frac{\mathbf{p}^2}{\mathbf{p}^2+\mu^2}\right)\mathcal{Y}_{\ell m}(\Omega_{\mathbf{p}})$$

and satisfies the normalization condition

$$\int \mathrm{d}^3p\, \tilde{\psi}^*_{k,\ell m}(\mathbf{p})\tilde{\psi}_{k',\ell' m'}(\mathbf{p}) = \delta_{kk'}\delta_{\ell\ell'}\delta_{mm'}.$$

In principle, it is straightforward to calculate the expectation values

$$H_{ij} \equiv \langle\psi_i|H|\psi_j\rangle$$

of the Hamiltonian (2), necessary for applying the min-max principle. Due to the orthonormalization (6) of the spherical harmonics $\mathcal{Y}_{\ell m}(\Omega)$, however, only matrix elements taken between states of identical orbital angular momentum ℓ and its projection m will be nonvanishing.

IV. POWER-LAW POTENTIALS

When speculating about the possible shape of a physically meaningful (or phenomenologically acceptable) interaction potential, the very first idea which unavoidably comes to one's mind as a reasonable candidate is an interaction potential of the power-law form, the power being only constrained by requiring that the Hamiltonian is bounded from below,

$$V(|\mathbf{x}|) = \sum_n a_n|\mathbf{x}|^{b_n}, \tag{7}$$

with sets of arbitrary real constants a_n and b_n, the latter only subject to the constraint

$$b_n \geqslant -1 \quad \text{if } a_n < 0.$$

For the Coulomb problem, defined by $b_n \equiv b_C = -1$ and $a_n \equiv -\kappa < 0$, according to the above-mentioned analysis of Herbst [16], the coupling parameter κ has to be bounded by

$$|a_n| \equiv \kappa < \frac{4}{\pi}.$$

This bound, as arising from the requirement of operator boundedness, applies to the whole spectrum of the Hamiltonian under consideration. In general, the bounds on the coupling constant will differ for different levels of excitation: the one for the ground state is the most stringent one; the bounds for arbitrary values of the orbital angular momentum ℓ have been derived both in Ref. [26] and, more rigorously, in Ref. [9]. By close inspection of our ansatz (5) it should become clear that we are able to handle even potentials of the type ''power-times-exponential,'' that is, potentials of the form

$$V(|\mathbf{x}|) = \sum_n a_n|\mathbf{x}|^{b_n}\exp(c_n|\mathbf{x}|), \quad b_n \geqslant -1 \quad \text{if } a_n < 0.$$

It is a rather simple task to write down the matrix elements for the power-law potential (7):

TABLE I. Energy eigenvalues of the spinless Salpeter equation with harmonic-oscillator potential $V(|\mathbf{x}|)=\omega|\mathbf{x}|^2$, for the parameter values $\mu=m=1$ GeV, $\omega=0.5$ GeV^3, $\beta=1$, and a size $d\times d$ of the energy matrix (H_{ij}). Numbers in italics (for small matrix sizes) indicate analytically obtained results. All eigenvalues are given in units of GeV.

State	1×1	2×2	25×25	Schrödinger
1S	*4.2162*	*3.9276*	3.8249	3.8249
2S		*8.1085*	5.7911	5.7911
3S			7.4829	7.4823
4S			9.0215	9.0075

$$V_{ij}\equiv\langle\psi_i|V(|\mathbf{x}|)|\psi_j\rangle=\sum_n a_n\int \mathrm{d}^3x\,\psi^*_{i,\ell m}(\mathbf{x})|\mathbf{x}|^{b_n}\psi_{j,\ell m}(\mathbf{x})$$
$$=\sqrt{\frac{i!\,j!}{\Gamma(2\ell+2\beta+i+1)\Gamma(2\ell+2\beta+j+1)}}$$
$$\times\sum_n\frac{a_n}{(2\mu)^{b_n}}\sum_{r=0}^{i}\sum_{s=0}^{j}\frac{(-1)^{r+s}}{r!\,s!}\binom{i+2\ell+2\beta}{i-r}$$
$$\times\binom{j+2\ell+2\beta}{j-s}\Gamma(2\ell+2\beta+b_n+r+s+1).$$

For instance, considering merely radial excitations by letting $\ell=0$ and choosing, just for the sake of definiteness, for the variational parameter β the value $\beta=1$, the explicit form of the potential matrix $V\equiv(V_{ij})$ is

$$V=\frac{1}{6}\sum_n\frac{a_n}{(2\mu)^{b_n}}\Gamma(3+b_n)\begin{pmatrix}3 & -\sqrt{3}b_n & \cdots\\ -\sqrt{3}b_n & 3+b_n+b_n^2 & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}.$$

V. ANALYTICALLY EVALUATABLE SPECIAL CASES

It should really be no great surprise that the evaluation of the matrix elements of the kinetic-energy operator T,

$$T_{ij}\equiv\langle\psi_i|T(\mathbf{p})|\psi_j\rangle=\int \mathrm{d}^3p\,\tilde\psi^*_{i,\ell m}(\mathbf{p})T(\mathbf{p})\tilde\psi_{j,\ell m}(\mathbf{p}),$$

is somewhat more delicate than the previous calculation of the matrix elements of the power-law potentials V. Consequently, let us focus our attention to those situations which allow for a fully analytic evaluation of the above kinetic-energy matrix elements.

TABLE II. Energy eigenvalues of the spinless Salpeter equation with Coulomb potential $V(|\mathbf{x}|)=-\kappa/|\mathbf{x}|$, for the parameter values [7] $\mu=m=1$ GeV, $\beta=1$, $\kappa=0.456$, and the size $d\times d$ of the energy matrix (H_{ij}). Numbers in italics (for small matrix sizes) indicate analytically obtained results. All eigenvalues are given in units of GeV.

State	1×1	2×2	25×25
1S	*2.2602*	*2.0539*	1.9450
2S		*3.0702*	1.9868
3S			2.0015
4S			2.0238

TABLE III. Energy eigenvalues of the spinless Salpeter equation with linear potential $V(|\mathbf{x}|)=a|\mathbf{x}|$, for the parameter values [7] $\mu=m=1$ GeV, $\beta=1$, $a=0.211$ GeV^2, and the size $d\times d$ of the energy matrix (H_{ij}). Numbers in italics (for small matrix sizes) indicate analytically obtained results. All eigenvalues are given in units of GeV.

State	1×1	2×2	20×20
1S	*3.0327*	*2.8034*	2.7992
2S		*4.0767*	3.3629
3S			3.8079
4S			4.1905

A. Orbital excitations

On the one hand, we may restrict our formalism to the case $i=j=0$, but allow, nevertheless, for still arbitrary values of the orbital angular momentum ℓ (which means considering arbitrary orbital excitations), and set $\beta=1$. Then the matrix elements V_{ij} of the power-law potential (7) reduce to

$$V_{00}=\frac{1}{\Gamma(2\ell+3)}\sum_n\frac{a_n}{(2\mu)^{b_n}}\Gamma(2\ell+b_n+3),$$

whereas for the matrix elements T_{ij} of the kinetic energy (1) we obtain

$$T_{00}=\frac{4^{\ell+2}[\Gamma(\ell+2)]^2}{\sqrt{\pi}\Gamma(2\ell+7/2)}\mu F\left(-\frac{1}{2},\ell+2;2\ell+\frac{7}{2};1-\frac{m^2}{\mu^2}\right).\tag{8}$$

At this point, our primary aim must be to get rid of the hypergeometric series F in the above intermediate result.

In the ultrarelativistic limit, realized in the case of vanishing mass m of the involved particles, that is, for $m=0$, the hypergeometric series F in Eq. (8) may be simplified with the help of the relation [25]

$$F(u,v;w;1)=\frac{\Gamma(w)\Gamma(w-u-v)}{\Gamma(w-u)\Gamma(w-v)}$$

for

TABLE IV. Energy eigenvalues of the spinless Salpeter equation with funnel potential $V(|\mathbf{x}|)=-\kappa/|\mathbf{x}|+a|\mathbf{x}|$, for the parameter values [7] $\mu=m=1$ GeV, $\beta=1$, $\kappa=0.456$, $a=0.211$ GeV^2, and the size $d\times d$ of the energy matrix (H_{ij}). Numbers in italics (for small matrix sizes) indicate analytically obtained results. All eigenvalues are given in units of GeV.

State	1×1	2×2	20×20
1S	*2.5767*	*2.5182*	2.5162
2S		*3.4499*	3.1570
3S			3.6337
4S			4.0348

TABLE V. Energy eigenvalues for the 1P states of the spinless Salpeter equation with harmonic-oscillator potential $V(|\mathbf{x}|)=\omega|\mathbf{x}|^2$, Coulomb potential $V(|\mathbf{x}|)=-\kappa/|\mathbf{x}|$, linear potential $V(|\mathbf{x}|)=a|\mathbf{x}|$, and funnel potential $V(|\mathbf{x}|)=-\kappa/|\mathbf{x}|+a|\mathbf{x}|$, respectively, for the parameter values [7] $\mu=m=1$ GeV, $\beta=1$, $\omega=0.5$ GeV^3, $\kappa=0.456$, $a=0.211$ GeV^2, and the size $d\times d$ of the energy matrix (H_{ij}). Numbers in italics (for small matrix sizes) indicate analytically obtained results. All eigenvalues are given in units of GeV.

Potential	1×1	20×20	Schrödinger
Harmonic oscillator	*6.5094*	4.9015	4.9015
Coulomb	*2.5314*	1.9875	
Linear	*3.2869*	3.1414	
Funnel	*3.0589*	2.9816	

$$w\neq0,-1,-2,\ldots,\quad \Re(w-u-v)>0,$$

in order to yield for the kinetic-energy matrix element T_{00}, Eq. (8), the much more innocent expression

$$T_{00}=\frac{2[\Gamma(\ell+2)]^2}{\Gamma(\ell+3/2)\Gamma(\ell+5/2)}\mu.$$

The resulting upper bounds H_{00} can be optimized by minimizing H_{00} with respect to the variational parameter μ. For instance, for a linear potential $V(|\mathbf{x}|)=a|\mathbf{x}|$, this minimization procedure thus yields

$$\min_{\mu>0}H_{00}=2\Gamma(\ell+2)\sqrt{\frac{(2\ell+3)a}{\Gamma(\ell+3/2)\Gamma(\ell+5/2)}}.$$

In the limit of large orbital angular momenta ℓ, that is, for $\ell\to\infty$, this minimal upper bound turns out not to be in conflict with the experimentally well-established linearity of ''Regge trajectories,''

$$\lim_{\ell\to\infty}\ \min_{\mu>0}(H_{00})^2=8a\ell,$$

which is in striking accordance with all previous findings [27,28].

Fixing the variational parameter μ to the particular value $\mu=m$ allows us to take advantage of the fact that

$$F(u,v;w;0)=1,$$

whence the kinetic-energy matrix element T_{00}, Eq. (8), reduces to

$$T_{00}=\frac{4^{\ell+2}[\Gamma(\ell+2)]^2}{\sqrt{\pi}\Gamma(2\ell+7/2)}m.$$

B. Radial excitations

On the other hand, considering only states of vanishing orbital angular momentum ℓ, i.e., only states with $\ell=0$, confines our investigation to the analysis of radial excitations. In this case, we may use the relation [25]

$$F\left(u,1-u;\frac{3}{2};\sin^2z\right)=\frac{\sin[(2u-1)z]}{(2u-1)\sin z}$$

in order to recast the hypergeometric series F in the momentum-space representation $\tilde{\psi}_{k,00}(|\mathbf{p}|)$ of our trial states into the form

$$F\left(\frac{\beta+r+2}{2},-\frac{\beta+r}{2};\frac{3}{2};\frac{\mathbf{p}^2}{\mathbf{p}^2+\mu^2}\right)=\frac{\sqrt{\mathbf{p}^2+\mu^2}}{(\beta+r+1)|\mathbf{p}|}\sin\left[(\beta+r+1)\arctan\frac{|\mathbf{p}|}{\mu}\right].$$

Simplifying the momentum-space trial function $\tilde{\psi}_{k,00}(|\mathbf{p}|)$ in this way,

$$\tilde{\psi}_{k,00}(|\mathbf{p}|)=\sqrt{\frac{k!}{\mu\Gamma(2\beta+k+1)}}\frac{2^\beta}{\pi|\mathbf{p}|}\sum_{r=0}^{k}\frac{(-2)^r}{r!}\binom{k+2\beta}{k-r}\Gamma(\beta+r+1)\left(1+\frac{\mathbf{p}^2}{\mu^2}\right)^{-(\beta+r+1)/2}\sin\left[(\beta+r+1)\arctan\frac{|\mathbf{p}|}{\mu}\right],$$

the matrix elements T_{ij} of the kinetic energy (1) immediately become

$$T_{ij}=\sqrt{\frac{i!j!}{\Gamma(2\beta+i+1)\Gamma(2\beta+j+1)}}\frac{4^{\beta+1}}{\pi}\mu\sum_{r=0}^{i}\sum_{s=0}^{j}\frac{(-2)^{r+s}}{r!s!}\binom{i+2\beta}{i-r}\binom{j+2\beta}{j-s}\Gamma(\beta+r+1)\Gamma(\beta+s+1)I_{rs},$$

where I_{rs} denotes the only remaining integration,

$$I_{rs}\equiv\int_0^\infty dy\,\sqrt{y^2+\frac{m^2}{\mu^2}}\frac{\cos[(r-s)\arctan y]-\cos[(2\beta+r+s+2)\arctan y]}{(1+y^2)^{(2\beta+r+s+2)/2}}.$$

This integration may, of course, always be performed by some standard numerical integration procedure. However, for $\mu=m$, the integral I_{rs} simplifies to

$$I_{rs}=\int_0^\infty dy\frac{\cos[(r-s)\arctan y]-\cos[(2\beta+r+s+2)\arctan y]}{(1+y^2)^{(2\beta+r+s+1)/2}},$$

which, for 2β integer and, because of the previous normalizability constraint $2\beta>-1$, non-negative, i.e., for the values $2\beta=0,1,2,\ldots$, may be evaluated with the help of the expansion

$$\cos(N\arctan y)=\frac{1}{(1+y^2)^{N/2}}\sum_{n=0}^{N}\binom{N}{n}\cos\left(\frac{n\pi}{2}\right)y^n \quad \text{for } N=0,1,2,\ldots,$$

with the result

$$\begin{aligned}I_{rs}=&\frac{1}{2}\left[\Gamma\left(\frac{2\beta+r+s+|r-s|+1}{2}\right)\right]^{-1}\sum_{n=0}^{|r-s|}\binom{|r-s|}{n}\\&\times\Gamma\left(\frac{n+1}{2}\right)\Gamma\left(\frac{2\beta+r+s+|r-s|-n}{2}\right)\cos\left(\frac{n\pi}{2}\right)\\&-\frac{1}{2}\left[\Gamma\left(2\beta+r+s+\frac{3}{2}\right)\right]^{-1}\sum_{n=0}^{2\beta+r+s+2}\binom{2\beta+r+s+2}{n}\\&\times\Gamma\left(\frac{n+1}{2}\right)\Gamma\left(2\beta+r+s+1-\frac{n}{2}\right)\cos\left(\frac{n\pi}{2}\right).\end{aligned}$$

The case $\beta=0$, however, requires special care for the following reason. For $\beta=0$, the integral I_{00} and therefore also the kinetic-energy matrix element T_{00} become singular, as may be read off from the explicit expression for the integral I_{rs} above. This singularity may be cancelled by the contribution of a Coulomb-type term $\kappa|\mathbf{x}|^{-1}$ in the power-law potential (7) if the involved coupling constant κ takes some particular, ''critical'' value. This cancellation can then be made manifest by observing that [20]

$$\begin{aligned}\lim_{\beta\to 0}\int_0^\infty dy\frac{1-\cos[(2+2\beta)\arctan y]}{(1+y^2)^{1/2+\beta}}&\\=2\lim_{\beta\to 0}\int_0^\infty dy\frac{y^2}{(1+y^2)^{3/2+\beta}}&.\end{aligned}$$

Explicitly, for $\beta=1$, the kinetic-energy matrix $T\equiv(T_{ij})$ is given by

$$T=\frac{128}{15\pi}m\begin{pmatrix}1 & \frac{\sqrt{3}}{7} & \cdots\\ \frac{\sqrt{3}}{7} & \frac{11}{9} & \cdots\\ \vdots & \vdots & \ddots\end{pmatrix}.$$

In any case, our approach yields analytic expressions for the matrix elements H_{ij} of our semirelativistic Hamiltonian H with an interaction potential out of the rather large class given by the power-law form (7). In principle, the d (real) roots of the characteristic equation (4) may be determined algebraically up to and including the case $d=4$, entailing, of course, analytic expressions of rather rapidly increasing complexity. For larger values of the dimension d of our trial space D_d, the resulting energy matrix (H_{ij}) may be easily diagonalized numerically without the necessity of applying time-consuming integration procedures.

In order to be able to estimate and appreciate the quality of all the upper bounds obtained in this way, we apply the above results to four prototype potentials, namely, to the harmonic-oscillator potential

$$V(|\mathbf{x}|)=\omega|\mathbf{x}|^2,\quad \omega>0,$$

the Coulomb potential

$$V(|\mathbf{x}|)=-\frac{\kappa}{|\mathbf{x}|},\quad 0<\kappa<\frac{4}{\pi},$$

the linear potential

$$V(|\mathbf{x}|)=a|\mathbf{x}|,\quad a>0,$$

and the funnel potential

$$V(|\mathbf{x}|)=-\frac{\kappa}{|\mathbf{x}|}+a|\mathbf{x}|,\quad 0<\kappa<\frac{4}{\pi},\quad a>0,$$

for typical values [7] of the involved coupling parameters ω, κ, and a. The upper bounds on the energy eigenvalues of the lowest-lying radial excitations (1S, 2S, 3S, and 4S in usual spectroscopic notation) for the harmonic-oscillator, Coulomb, linear, and funnel potentials are shown in Tables I through IV, respectively; the upper bounds on the respective energy eigenvalues of just the first orbital excitation (1P again in usual spectroscopic notation) for the above potentials are listed in Table V.

For the case of the harmonic-oscillator potential, the corresponding Hamiltonian H in its momentum-space representation is equivalent to a nonrelativistic Hamiltonian with some effective interaction potential, which clearly is reminiscent of that troublesome square-root operator.[2] In this form, it is then rather easily accessible to numerical procedures for solving a nonrelativistic Schrödinger equation [30]. For comparison we quote in Tables I and V the eigenvalues obtained along these lines. We find a very encouraging rapid convergence of the upper bounds.[3]

VI. SUMMARY

By the application of the well-known min-max principle, which represents the theoretical foundation of any computation of upper bounds on the eigenvalues of self-adjoint operators, to trial spaces spanned by sets of basis states which enable us to handle the square-root operator of the relativistic kinetic energy T in a satisfactory manner, we demonstrated how to derive (even analytically for lowest-lying states) up-

[2]For a brief account of these relationships, see, e.g., Ref. [9]. For a numerical study of the relativistic harmonic-oscillator problem in momentum space, see, e.g., Ref. [29].

[3]Needless to say, in the case of the Coulomb potential, the deviation of our upper bounds, computed for some given matrix size $d\times d$, from the exact energy eigenvalues will increase as the coupling constant κ approaches its critical value. Comparing our approach with the best set of corresponding upper bounds known so far [31], we find that, for instance, up to $\kappa\simeq 1.1$ this deviation is less than 0.8% for a 25×25 matrix.

per bounds on the energy levels of the spinless Salpeter equation with some (linear combination of) power-law potentials. Interestingly, in the case of the funnel potential, which is the prototype of almost all of the ''realistic,'' that is, phenomenologically acceptable, interquark potentials used for the description of hadrons as bound states of (constituent) quarks, the obtained lowest-order approximation to the upper bound on, e.g., the ground-state energy is merely some 2% above the corresponding value. Of course, all the bounds derived here may be improved numerically by a minimization with respect to the variational parameters introduced.

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