ISSN 1330–0016
CODEN FIZBE7

BOUND STATES BY THE SPINLESS SALPETER EQUATION[1]

WOLFGANG LUCHA[a] and FRANZ F. SCHÖBERL[b]

[a] *Institut für Hochenergiephysik, Österreichische Akademie der Wissenschaften, Nikolsdorfergasse 18, A-1050 Wien, Austria, E-mail: v2032dac@vm.univie.ac.at, wolfgang.lucha@oeaw.ac.at*

[b] *Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria, E-mail: franz.schoeberl@univie.ac.at*

Received 8 January 1999; Accepted 7 June 1999

In quantum theory, bound states are described by eigenvalue equations which usually cannot be solved exactly. However, some simple general theorems allow to derive rigorous statements about the corresponding solutions, that is, energy levels and wave functions. These theorems are applied to the prototype of all relativistic wave equations, the spinless Salpeter equation.

PACS numbers: 11.10.St, 03.65.Pm, 03.65.Ge, 12.39.Ki UDC 530.145
Keywords: spinless Salpeter equation, bound states, energy levels and wave functions

1. Introduction

In quantum theory, exact statements on solutions of eigenvalue equations, which describe bound states, may be obtained by some rather simple and elementary methods. Here, these methods are reviewed and illustrated with the simplest nontrivial (semi-)relativistic wave equation, the spinless Salpeter equation, which represents a well-defined standard approximation to the famous Bethe–Salpeter formalism. For more details, see Ref. 1.

1.1. Relativistic wave equation: spinless Salpeter equation

1.1.1. Bound states in quantum field theory: Bethe–Salpeter (BS) formalism

The appropriate framework for the description of bound states within relativistic quantum field theory is the Bethe–Salpeter formalism. There, a bound state $|\mathrm{M}\rangle$ (with momentum K and energy E) of, say, fermion and antifermion (with masses

[1] Invited plenary talk by W. Lucha at the International Conference "Nuclear & Particle Physics with CEBAF at Jefferson Lab," November 3 – 10, 1998, Dubrovnik, Croatia

M_1, M_2 and momenta P_1, P_2, respectively) is represented by its *Bethe–Salpeter amplitude* Ψ, defined, in momentum space, in terms of the time-ordered product of the field operators of the two bound-state constituents between vacuum and bound state by

$$\Psi(P) = \exp(\mathrm{i}\,K\,X_{\mathrm{CM}}) \int \mathrm{d}^4X\, \exp(\mathrm{i}\,P\,X)\, \langle 0|\mathrm{T}(\psi_1(X_1)\,\bar{\psi}_2(X_2))|\mathrm{M}(K)\rangle \ ,$$

with the total momentum $K = P_1 + P_2$, relative momentum P, center-of-momentum coordinate X_{CM}, and relative coordinate $X \equiv X_1 - X_2$ of the bound-state constituents. The Bethe–Salpeter amplitude Ψ satisfies the *Bethe–Salpeter equation*

$$S_1^{-1}(P_1)\,\Psi(P)\,S_2^{-1}(-P_2) = \frac{\mathrm{i}}{(2\pi)^4} \int \mathrm{d}^4Q\,\mathcal{K}(P,Q)\,\Psi(Q) \ ,$$

which involves two dynamical ingredients:

- The full fermion propagator $S_i(P)$ of some particle i $(i = 1, 2)$ of momentum P and mass M_i is usually approximated by its free form, $S_{i,0}^{-1}(P) = (-\mathrm{i}\gamma_\mu\,P^\mu - M_i)$, with M_i interpreted as some effective ("constituent") mass and the propagator understood as an effective one.
- The *BS kernel* $\mathcal{K}(P,Q)$ is defined perturbatively as the sum of all two-particle (BS-) irreducible Feynman diagrams for two-particle into two-particle scattering (and thus gauge-dependent!); it is given, e.g., in the lowest order QED from one-photon exchange (in Feynman gauge) by

$$\mathcal{K}(P,Q) = \frac{e^2}{(P-Q)^2}\,\gamma^\mu \otimes \gamma_\mu \ .$$

The BS equation is formally exact. Nevertheless, it faces some well-known **problems**:

- There are no means to compute the BS kernel beyond perturbation theory.
- In general, it is not possible to find the exact solutions of the BS equation (except for very few special cases, like the famous Wick–Cutkosky model for two scalar particles interacting by exchange of some massless scalar particle).
- In non-Abelian gauge theories like QCD, free propagators are incompatible with a confining BS kernel because Dyson–Schwinger equations connect the propagators and the kernel.

The usual way out is the **reduction** of the BS equation by a series of approximations:

1) Eliminate any dependence on timelike variables:

- Adhere to the *static approximation* to the BS kernel, i.e., assume that the kernel depends only on the relative *three*-momenta of initial and final state: $\mathcal{K}(P,Q) = \mathcal{K}(\mathbf{P},\mathbf{Q})$. (This is tantamount to ignoring all retardation effects by assuming instantaneous interactions.)
- Define the *equal-time wave function* $\Phi(\mathbf{P}) \equiv \int \mathrm{d}P_0\, \Psi(\mathbf{P},P_0)$.

This leads to the *Salpeter equation*

$$\Phi(\mathbf{P}) = \int \frac{\mathrm{d}^3Q}{(2\pi)^3} \left[\frac{\Lambda_1^+\,\gamma_0\,\mathcal{K}(\mathbf{P},\mathbf{Q})\,\Phi(\mathbf{Q})\,\gamma_0\,\Lambda_2^-}{E-\sqrt{\mathbf{P}_1^2+M_1^2}-\sqrt{\mathbf{P}_2^2+M_2^2}} - \frac{\Lambda_1^-\,\gamma_0\,\mathcal{K}(\mathbf{P},\mathbf{Q})\,\Phi(\mathbf{Q})\,\gamma_0\,\Lambda_2^+}{E+\sqrt{\mathbf{P}_1^2+M_1^2}+\sqrt{\mathbf{P}_2^2+M_2^2}} \right],$$

with the positive/negative-energy projection operators for particle i ($i=1,2$)

$$\Lambda_i^\pm \equiv \frac{\sqrt{\mathbf{P}_i^2+M_i^2} \pm \gamma_0\,(\boldsymbol{\gamma}\cdot\mathbf{P}_i+M_i)}{2\sqrt{\mathbf{P}_i^2+M_i^2}}\ .$$

The Salpeter equation is the equation of motion for the equal-time wave function Φ with full relativistic kinematics but in static approximation for the kernel $\mathcal{K}$.

2) Neglect the second term on the r.h.s. of the Salpeter equation by assuming

$$E-\sqrt{\mathbf{P}_1^2+M_1^2}-\sqrt{\mathbf{P}_2^2+M_2^2} \ll E+\sqrt{\mathbf{P}_1^2+M_1^2}+\sqrt{\mathbf{P}_2^2+M_2^2}\ .$$

This leads to the *reduced Salpeter equation*

$$\left(E-\sqrt{\mathbf{P}_1^2+M_1^2}-\sqrt{\mathbf{P}_2^2+M_2^2}\right)\Phi(\mathbf{P}) = \int \frac{\mathrm{d}^3Q}{(2\pi)^3}\,\Lambda_1^+\,\gamma_0\,\mathcal{K}(\mathbf{P},\mathbf{Q})\,\Phi(\mathbf{Q})\,\gamma_0\,\Lambda_2^-\ .$$

3) Neglect all spin degrees of freedom of the involved bound-state constituents.

4) Assume that the BS kernel $\mathcal{K}(\mathbf{P},\mathbf{Q})$ depends only on the difference of the relative momenta, which means that it is of convolution type: $\mathcal{K}(\mathbf{P},\mathbf{Q}) = \mathcal{K}(\mathbf{P}-\mathbf{Q})$.

5) Restrict the whole formalism exclusively to positive-energy solutions ψ.

Under these simplifying assumptions and approximations, the BS equation reduces to the *spinless Salpeter equation*

$$\left[\sqrt{\mathbf{P}_1^2+M_1^2}+\sqrt{\mathbf{P}_2^2+M_2^2}+V(\mathbf{X})\right]\psi=E\,\psi\ ,$$

involving an interaction potential, $V(\mathbf{X})$, which arises as the Fourier transform of $\mathcal{K}(\mathbf{P}-\mathbf{Q})$. In the center-of-momentum frame of the two bound-state constituents, i.e., for $\mathbf{K}=\mathbf{0}$, this equation reads $H|\psi\rangle=E|\psi\rangle$, with the Hamiltonian

$$H=\sqrt{\mathbf{P}^2+M_1^2}+\sqrt{\mathbf{P}^2+M_2^2}+V(\mathbf{X})\ .$$

1.1.2. Equal-mass case

For equal masses of the two bound-state constituents (i.e., assuming $M_1=M_2=M$), the two-particle spinless Salpeter equation is equivalent to its one-particle form. To see this, consider the two-particle Hamiltonian H with an interaction represented, e.g., by a central potential of the power-law form:

$$H=2\,\sqrt{\mathbf{P}^2+M^2}+\sum_{n\in Z}k_n\,R^n\ ,\quad R\equiv|\mathbf{X}|\ .$$

One may always perform a scale transformation of the phase-space variables $\mathbf{X}$, $\mathbf{P}$ by some arbitrary scale factor λ,

$$\mathbf{p}=\lambda\,\mathbf{P}\ ,\quad \mathbf{x}=\frac{\mathbf{X}}{\lambda}\ ,$$

since this rescaling certainly preserves the fundamental commutation relations: $[\mathbf{x},\mathbf{p}]=[\mathbf{X},\mathbf{P}]$. Fix λ to $\lambda=2$, which implies

$$H=\sqrt{4\,\mathbf{P}^2+4\,M^2}+\sum_{n\in Z}k_n\,R^n=\sqrt{\mathbf{p}^2+4\,M^2}+\sum_{n\in Z}k_n\,2^n\,r^n\ ,$$

identify the one- and two-particle mass and coupling-strength parameters according to $m=2\,M$ and $a_n=2^n\,k_n$, $n\in Z$, and arrive at the equivalent one-particle Hamiltonian

$$H=\sqrt{\mathbf{p}^2+m^2}+\sum_{n\in Z}a_n\,r^n\ ,\quad r\equiv|\mathbf{x}|\ .$$

1.1.3. Prototype: (one-particle) spinless Salpeter equation

In view of the above, it is sufficient to consider the self-adjoint Hamiltonian $H=T+V$, with the "square-root" operator of the relativistic kinetic energy of a particle of mass m and momentum $\mathbf{p}$,

$$T=T(\mathbf{p})\equiv\sqrt{\mathbf{p}^2+m^2}\ ,$$

and arbitrary coordinate-dependent, static interaction-potential operators $V = V(\mathbf{x})$. The **spinless Salpeter equation** is then nothing else but the eigenvalue equation for H, i.e., $H|\chi_k\rangle = E_k|\chi_k\rangle$, $k = 0, 1, 2, \ldots$, for Hilbert-space eigenvectors $|\chi_k\rangle$ and energy eigenvalues

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

It represents the simplest relativistic generalization of the Schrödinger equation of standard nonrelativistic quantum theory. **N.B.** The semirelativistic Hamiltonian H is a *nonlocal* operator, i.e.,

- either T *in configuration space*
- or, in general, V *in momentum space*

is nonlocal. Therefore, it is rather difficult to obtain rigorous *analytic* statements on the solutions of this equation of motion.

1.2. Example: the (spinless) relativistic Coulomb problem

For illustrative purposes, let us consider the (spherically symmetric) Coulomb potential, with interaction strength parametrized by some (dimensionless) coupling constant α:

$$V(\mathbf{x}) = V_{\rm C}(r) = -\frac{\alpha}{r} \ , \quad r \equiv |\mathbf{x}| \ , \quad \alpha > 0 \ .$$

For this case, some important pieces of knowledge have been accumulated until now:

- An examination of the spectral properties of H with a Coulomb potential reveals [2]
  - the *essential self-adjointness* of H (i.e., its closure is self-adjoint) for $\alpha \leq \frac{1}{2}$;
  - the existence of the *Friedrichs extension* of H up to the critical value $\alpha_{\rm c} = \frac{2}{\pi}$;
  - a strict *lower bound* on the ground-state energy E_0 (that is, on H), given by
$$E_0 \geq m\sqrt{1 - \left(\frac{\pi\,\alpha}{2}\right)^2} \quad \text{for } \alpha < \frac{2}{\pi} \ .$$

In this sense, the Coulombic Hamiltonian H is a reasonable operator up to $\alpha_{\rm c}$.

- For part of the allowed range of α, an improved lower bound may be derived [3]:

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

- Lower bounds on the spectrum of H may be found numerically with the help of the **generalized "local-energy" theorem** [4]: Assume that

  1) the Fourier transform $\widetilde{V}(\mathbf{p})$ of $V(\mathbf{x})$ is strictly negative, except at infinity, as is the case for an attractive Coulomb potential,
  2) the spectrum of H is discrete, and
  3) the ground state of H exists.

  Define the "local energy"

$$\mathcal{E}(\mathbf{p}) \equiv T(\mathbf{p}) + \frac{\displaystyle\int \mathrm{d}^3q\, \widetilde{V}(\mathbf{p}-\mathbf{q})\, \phi(\mathbf{q})}{\phi(\mathbf{p})} \ ,$$

  with some suitably chosen, positive trial function $\phi(\mathbf{p}) > 0$. Then[2]

$$\inf_{\mathbf{p}} \mathcal{E}(\mathbf{p}) \leq E_0 < \sup_{\mathbf{p}} \mathcal{E}(\mathbf{p}) \ .$$

  This theorem restricts the ground-state energy $E_0(\alpha)$ as a function of α to some remarkably narrow band. In particular, at α_c, one finds

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

  Consequently, $E_0(\alpha = \alpha_\mathrm{c})$ is definitely nonvanishing.

However, even for the Coulomb potential, the eigenvalues of H are not known exactly!

2. Analytic upper bounds on energy levels [5]

We are interested in exact analytic expressions for upper bounds on the eigenvalues of H. This only makes sense if the operator under consideration is bounded from below. Consequently, assume that the potential V is such that H is bounded from below. For the **Coulomb potential**, this has been rigorously proven [2].

[2] The lower bound even holds if the spectrum is not purely discrete.

2.1. Bounds on eigenvalues: minimum–maximum principle

The primary tool for the derivation of rigorous upper bounds on the eigenvalues of a self-adjoint operator is the well-known *minimum–maximum principle*. Among several equivalent formulations, the most convenient one for practical purposes is the following: Let H be a self-adjoint operator bounded from below, with eigenvalues E_k, $k = 0, 1, \ldots$, ordered according to $E_0 \leq E_1 \leq E_2 \leq \ldots$, and let D_d be some d-dimensional subspace of the domain of H. Then the kth eigenvalue E_k (when counting multiplicity) satisfies

$$E_k \leq \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \quad \text{for } k = 0, 1, 2, \ldots \ .$$

2.2. Operator inequalities

We would like to replace the problematic kinetic-energy square-root operator in H by some more tractable operator. One way to achieve this is to use the min–max principle in order to compare eigenvalues of operators:

- Assume the validity of a (generic) operator inequality of the form $H \leq \mathcal{O}$. Then,
$$E_k \leq \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \leq \sup_{|\psi\rangle \in D_{k+1}} \frac{\langle\psi|\mathcal{O}|\psi\rangle}{\langle\psi|\psi\rangle} \ .$$

- Assume that D_{k+1} is spanned by the first $k+1$ eigenvectors of $\mathcal{O}$ (corresponding to the first $k+1$ eigenvalues $\widehat{E}_0, \widehat{E}_1, \ldots, \widehat{E}_k$ of $\mathcal{O}$ if the latter are ordered according to $\widehat{E}_0 \leq \widehat{E}_1 \leq \widehat{E}_2 \leq \ldots$). Then
$$\sup_{|\psi\rangle \in D_{k+1}} \frac{\langle\psi|\mathcal{O}|\psi\rangle}{\langle\psi|\psi\rangle} = \widehat{E}_k \ .$$

Every eigenvalue of H is bounded from above by the related eigenvalue of $\mathcal{O}$: $E_k \leq \widehat{E}_k$.

2.3. The "Schrödinger" bound

The simplest upper bound on the eigenvalues of H may be easily found by exploiting the positivity of the square of the (self-adjoint, since T is self-adjoint) operator $T - m$:

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

Assuming m to be positive, this may be converted into an operator inequality for T, $T \leq m + \mathbf{p}^2/(2\,m)$, which entails an operator inequality for H:

$$H \leq m + \mathbf{p}^2/(2\,m) + V \ .$$

For the **Coulomb potential**, the required Schrödinger energy eigenvalues are given by

$$E_{\mathrm{S},n} = m\left(1 - \frac{\alpha^2}{2\,n^2}\right),$$

with the total quantum number n, expressed in terms of the radial quantum number n_{r} ($n_{\mathrm{r}} = 0, 1, 2, \ldots$) and the orbital angular momentum ℓ ($\ell = 0, 1, 2, \ldots$) by $n = n_{\mathrm{r}} + \ell + 1$.

2.4. A straightforward generalization

A real improvement is made by considering the positivity of the square of the (obviously self-adjoint) operator $T-\mu$, where μ is an arbitrary real parameter (with the dimension of mass):

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

implies a set of operator inequalities for T (see also Ref. 3), $T \leq (\mathbf{p}^2+m^2+\mu^2)/(2\,\mu)$ $\forall\ \mu > 0$. This translates into an operator inequality for H: $H \leq (\mathbf{p}^2 + m^2 + \mu^2)/(2\,\mu) + V\ \forall\ \mu > 0$. Hence, according to the min–max principle, E_k is bounded from above by the eigenvalue $\widehat{E}_{\mathrm{S},k}(\mu)$ of the Schrödinger-like Hamiltonian on the r.h.s. of this inequality, $E_k \leq \widehat{E}_{\mathrm{S},k}(\mu)\ \forall\ \mu > 0$, and thus also by the minimum of these Schrödinger-like bounds:

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

For the **Coulomb potential**, the corresponding "Schrödinger" energy eigenvalues are

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

with the total quantum number $n = n_{\mathrm{r}} + \ell + 1$. Minimizing $\widehat{E}_{\mathrm{S},n}(\mu)$ w.r.t. μ then yields

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

These bounds hold for all $\alpha \leq \alpha_{\mathrm{c}}$ and arbitrary levels of excitation, and they improve definitely the Schrödinger bounds, for any n:

$$\min_{\mu>0} \widehat{E}_{\mathrm{S},n}(\mu) < E_{\mathrm{S},n} \quad \text{for } \alpha \neq 0\ .$$

(For $\mu = m$, one necessarily recovers the Schrödinger case.) The **comparison** of these analytic (!) upper bounds with their numerically obtained counterparts shows that the relative error of these analytic bounds (for $\alpha \leq 0.5$) is for the ground state ($n_{\mathrm{r}} = \ell = 0$) less than 4.5 % and for the level $n_{\mathrm{r}} = 0$, $\ell = 1$ less than 0.1 %.

2.5. Rayleigh–Ritz variational technique

An **immediate consequence of the min–max principle** is the famous Rayleigh–Ritz technique: Restrict the operator H to the subspace D_d by orthogonal projection P onto D_d: $\widehat{H} := P\,H\,P$. Let $\widehat{E}_k$, $k = 0, 1, \ldots, d-1$, denote all d eigenvalues of $\widehat{H}$, ordered according to $\widehat{E}_0 \leq \widehat{E}_1 \leq \ldots \leq \widehat{E}_{d-1}$. The kth eigenvalue (counting multiplicity) of H, E_k, then satisfies $E_k \leq \widehat{E}_k$, $k = 0, 1, \ldots, d-1$.

Now, if D_d is spanned by linearly a set of independent basis vectors $|\psi_k\rangle$, $k = 0, 1, \ldots, d-1$, the eigenvalues $\widehat{E}$ are simply determined by diagonalizing the $d \times d$ matrix $(\langle\psi_i|\widehat{H}|\psi_j\rangle)$, $i, j = 0, 1, \ldots, d-1$, i.e., as the d roots of the characteristic equation

$$\det\left(\langle\psi_i|\widehat{H}|\psi_j\rangle - \widehat{E}\,\langle\psi_i|\psi_j\rangle\right) = 0\ , \quad i, j = 0, 1, \ldots, d-1\ .$$

2.6. Variational bound for the ground state

As a first test, let us apply the Rayleigh–Ritz variational technique to the ground state, by considering the case $k = 0$ (i.e., an only one-dimensional subspace). In this case, the min–max principle reduces to

$$E_0 \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$

(i.e., the ground-state energy E_0 is less than or equal to any expectation value of H). However, one may consider simultaneously more than one one-dimensional trial spaces in order to obtain an optimized upper bound according to the following **prescription**:

1) Choose some suitable set of trial states $\{|\psi_\lambda\rangle\}$ (with elements distinguished from each other by some variational parameter λ).

2) Calculate all the expectation values $E(\lambda) \equiv \langle\psi_\lambda|H|\psi_\lambda\rangle/\langle\psi_\lambda|\psi_\lambda\rangle$ of H w.r.t. $|\psi_\lambda\rangle$.

3) Determine (from the first derivative of $E(\lambda)$ w.r.t. λ) that value $\lambda_{\min}$ of λ which minimizes $E(\lambda)$.

4) Compute $E(\lambda_{\min})$ (i.e., the minimal expectation value of H in the Hilbert-space subsector of the chosen trial states).

The outcome of this procedure will be an optimized upper bound on E_0, viz., $E_0 \leq E(\lambda_{\min})$.

In order to get rid of the troublesome square-root operator in H, we adopt a trivial but fundamental inequality for the expectation values of some self-adjoint

operator $\mathcal{O}$ and its square w.r.t. any state $|\psi\rangle$ in the domain of $\mathcal{O}$:

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

We consider this inequality, of course, for T, and apply the resulting inequality to H:

$$E_0 \leq \frac{\langle\psi|T+V|\psi\rangle}{\langle\psi|\psi\rangle} \leq \sqrt{\frac{\langle\psi|T^2|\psi\rangle}{\langle\psi|\psi\rangle}} + \frac{\langle\psi|V|\psi\rangle}{\langle\psi|\psi\rangle} \equiv \sqrt{\frac{\langle\psi|\mathbf{p}^2|\psi\rangle}{\langle\psi|\psi\rangle} + m^2} + \frac{\langle\psi|V|\psi\rangle}{\langle\psi|\psi\rangle} \; .$$

For the **Coulomb potential**, a special choice for the coordinate-space representation of trial vectors is suggestive: the well-known (normalized) hydrogen-like trial functions

$$\psi_\lambda(\mathbf{x}) = \sqrt{\frac{\lambda^3}{\pi}} \, \exp(-\lambda\, r) \; , \quad \lambda > 0 \; .$$

This leads to a one-parameter set of upper bounds, $E_0 \leq \sqrt{\lambda^2 + m^2} - \alpha\,\lambda$ for all $\lambda > 0$, with the absolute minimum $E_0 \leq m\sqrt{1-\alpha^2}$, which is identical to the previous generalized (operator) bound for $n = 1$ and, for $\alpha \neq 0$, lower and thus better than the Schrödinger bound

$$E_{\mathrm{S},0} = m\left(1 - \frac{\alpha^2}{2}\right) .$$

Thus, the variational technique yields indeed improved upper bounds on the energy levels.

2.7. Energy levels at the critical coupling constant of the relativistic Coulomb problem

In order to find, for the **Coulomb potential**, upper bounds on the energy levels at α_{c}, we employ basis vectors $|\psi_k\rangle$ (labelled by a positive integer $k = 0, 1, 2, \ldots$) of D_d, given in configuration-space representation by

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

For a given α, the parameter β allows the complete cancellation of the divergent contributions to the expectation values of the kinetic energy T for large momenta p and the Coulomb potential $V_{\mathrm{C}}(r)$ at small distances r: $\beta = \beta(\alpha)$. β is implicitly determined as a function of α, e.g., for the ground state by [6] $\alpha = \beta\cot(\beta\,\pi/2)$. Consequently, α_{c} is approached for $\beta \to 0$. For our $|\psi_k\rangle$, singularities arise only

in the ground-state matrix elements, i.e., in $\langle\psi_0|T|\psi_0\rangle$ and $\langle\psi_0|V_{\rm C}(r)|\psi_0\rangle$. It is a simple task to evaluate all relevant matrix elements for arbitrary β.

For simplicity, introduce a dimensionless energy eigenvalue ε by $\widehat{E} =: (2/\pi)\, m\, \varepsilon$. The resulting characteristic equation for $\beta = 0$ is typically of the form

$$\det \begin{pmatrix} 4\ln 2 - 2 - \varepsilon & \dfrac{\sqrt{2}}{3} - \dfrac{\varepsilon}{\sqrt{2}} & \cdots \\ \dfrac{\sqrt{2}}{3} - \dfrac{\varepsilon}{\sqrt{2}} & \dfrac{17}{15} - \varepsilon & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} = 0 \ .$$

The roots of this equation (which may be calculated algebraically up to $d = 4$) read, for $d = 1$, $\varepsilon = 2\,(2\ln 2 - 1)$, entailing the ground-state upper bound $\widehat{E}_0/m = 0.4918\ldots$, for $d = 2$,

$$\varepsilon = \frac{1}{15}\left(60\ln 2 - 23 \pm \sqrt{(60\ln 2)^2 - 4800\ln 2 + 1649}\right) ,$$

entailing the ground-state upper bound $\widehat{E}_0/m = 0.484288\ldots$, while, for $d = 4$, some lengthy expression implies the ground-state upper bound $\widehat{E}_0/m = 0.4842564\ldots$. From $d = 2$ on, all these analytic bounds lie well within the numerical "local-energy range."

2.8. Generalized Laguerre basis

Upper bounds on eigenvalues may be improved by enlarging D_d to higher dimensions d or by spanning it by a more sophisticated set of basis states. A rather popular choice of trial functions involves the generalized Laguerre polynomials $L_k^{(\gamma)}(x)$ for the parameter γ: these are orthogonal polynomials defined by the power series

$$L_k^{(\gamma)}(x) = \sum_{t=0}^{k} (-1)^t \begin{pmatrix} k+\gamma \\ k-t \end{pmatrix} \frac{x^t}{t!}$$

and normalized, with the weight function $x^\gamma \exp(-x)$, according to

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

To construct a trial vector corresponding to a state with orbital angular momentum ℓ and its projection m, introduce two variational parameters: μ (with dimension of mass) and β (dimensionless). This state is defined by the configuration-space

representation

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

with the orthonormalized spherical harmonics $\mathcal{Y}_{\ell m}(\Omega)$, depending on the solid angle Ω. Normalizability of the trial states requires $\mu > 0$ and $\beta > -1/2$; $\psi_{k,\ell m}(\mathbf{x})$ then satisfies the (standard) orthonormalization condition $\int \mathrm{d}^3x\,\psi^*_{k,\ell m}(\mathbf{x})\,\psi_{k',\ell' m'}(\mathbf{x}) = \delta_{kk'}\,\delta_{\ell\ell'}\,\delta_{mm'}$.

2.8.1. Power-law potentials

Let us investigate interaction potentials of power-law form: $V(r) = \sum_n a_n\,r^{b_n}$, $r \equiv |\mathbf{x}|$, where the real constants a_n and b_n are only constrained by the semiboundedness of H: $b_n \geq -1$ if $a_n < 0$. The matrix elements of V are easily worked out:

$$\begin{aligned}\langle\psi_i|V|\psi_j\rangle &= \sqrt{\frac{i!\,j!}{\Gamma(2\,\ell+2\,\beta+i+1)\,\Gamma(2\,\ell+2\,\beta+j+1)}}\\ &\times \sum_n \frac{a_n}{(2\,\mu)^{b_n}}\sum_{t=0}^{i}\sum_{s=0}^{j}\frac{(-1)^{t+s}}{t!\,s!}\\ &\times \begin{pmatrix} i+2\,\ell+2\,\beta \\ i-t \end{pmatrix}\begin{pmatrix} j+2\,\ell+2\,\beta \\ j-s \end{pmatrix}\Gamma(2\,\ell+2\,\beta+b_n+t+s+1)\,.\end{aligned}$$

2.8.2. Analytically evaluable special cases

Orbital excitations

Consider just orbital excitations by restricting to $i = j = 0$, but allowing for arbitrary ℓ. Only for definiteness, fix β to $\beta = 1$. In this case, the matrix elements of T are given by

$$\langle\psi_0|T|\psi_0\rangle = \frac{4^{\ell+2}\,[\Gamma(\ell+2)]^2}{2\sqrt{\pi}\,\Gamma\left(2\,\ell+\frac{7}{2}\right)}\,\mu\,F\left(-\frac{1}{2},\ell+2;2\,\ell+\frac{7}{2};1-\frac{m^2}{\mu^2}\right),$$

with the hypergeometric series

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

There are several possibilities to get rid of F. For example, in the ultrarelativistic limit ($m = 0$), the kinetic-energy matrix element becomes

$$\langle\psi_0|T|\psi_0\rangle = \frac{[\Gamma(\ell+2)]^2}{\Gamma\left(\ell+\frac{3}{2}\right)\Gamma\left(\ell+\frac{5}{2}\right)}\,\mu\ .$$

For instance, for the **linear potential** $V(r) = a\,r$, $a > 0$, minimizing $\langle\psi_0|H|\psi_0\rangle$ w.r.t. μ leads to the minimal upper bound

$$\min_{\mu>0}\langle\psi_0|H|\psi_0\rangle = 2\sqrt{a}\,\frac{\Gamma(\ell+2)}{\Gamma\left(\ell+\frac{3}{2}\right)}\ .$$

In the limit $\ell \to \infty$, this reduces to

$$\lim_{\ell\to\infty}\left(\min_{\mu>0}\langle\psi_0|H|\psi_0\rangle\right)^2 = 4\,a\left(\ell+\frac{5}{4}\right),$$

describing linear Regge trajectories, i.e., $[E(\ell)]^2 \sim \ell$, in striking accordance with other findings based on different considerations [7,8].

Radial excitations

Consider pure radial excitations by focusing to states with $\ell = 0$. The matrix elements of T then typically take the form

$$\begin{aligned}\langle\psi_i|T|\psi_j\rangle &= \sqrt{\frac{i!\,j!}{\Gamma(2\,\beta+i+1)\,\Gamma(2\,\beta+j+1)}}\,\frac{4^{\beta+1}}{2\pi}\,\mu\sum_{t=0}^{i}\sum_{s=0}^{j}\frac{(-2)^{t+s}}{t!\,s!}\\ &\times \left(\begin{array}{c} i+2\,\beta \\ i-t \end{array}\right)\left(\begin{array}{c} j+2\,\beta \\ j-s \end{array}\right)\Gamma(\beta+t+1)\,\Gamma(\beta+s+1)\,I_{ts}\ ,\end{aligned}$$

with I_{ts}, for $\mu = m$, and for $2\,\beta$ integer (and therefore non-negative), i.e., $2\,\beta = 0, 1, 2, \ldots$, given by

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

By this, analytic expressions for the matrix elements $\langle\psi_i|H|\psi_j\rangle$ of H with a power-law potential may be found. Up to $d = 4$, these matrix elements are, at least in principle, algebraically accessible. For $d > 4$, the energy matrix $(\langle\psi_i|H|\psi_j\rangle)$ must be diagonalized numerically, however, without the need of (time-consuming!) integration procedures.

References

1) W. Lucha and F. F. Schöberl, HEPHY-PUB 701/98 (1998), hep-ph/9812368; Int. J. Mod. Phys. A (in print);

2) I. W. Herbst, Commun. Math. Phys. **53** (1977) 285; **55** (1977) 316 (addendum);

3) A. Martin and S. M. Roy, Phys. Lett. B **233** (1989) 407;

4) J. C. Raynal, S. M. Roy, V. Singh, A. Martin and J. Stubbe, Phys. Lett. B **320** (1994) 105;

5) W. Lucha and F. F. Schöberl, Phys. Rev. D **50** (1994) 5443; Phys. Rev. A **54** (1996) 3790; Phys. Lett. B **387** (1996) 573; Phys. Rev. A **56** (1997) 139;

6) B. Durand and L. Durand, Phys. Rev. D **28** (1983) 396; **50** (1994) 6662 (E); P. Castorina, P. Cea, G. Nardulli and G. Paiano, Phys. Rev. D **29** (1984) 2660; L. J. Nickisch, L. Durand and B. Durand, Phys. Rev. D **30** (1984) 660, 1995 (E); G. Hardekopf and J. Sucher, Phys. Rev. A **31** (1985) 2020;

7) J. S. Kang and H. J. Schnitzer, Phys. Rev. D **12** (1975) 841; A. Martin, Z. Phys. C **32** (1986) 359; Yu. A. Simonov, Phys. Lett. B **226** (1989) 151;

8) W. Lucha, H. Rupprecht and F. F. Schöberl, Phys. Lett. B **261** (1991) 504; W. Lucha and F. F. Schöberl, Z. Phys. C **53** (1992) 83.

VEZANA STANJA PREMA SALPETEROVOJ JEDNADŽBI BEZ SPINA

U kvantnoj se teoriji vezana stanja opisuju svojstvenim jednadžbama koje se obično ne mogu egzaktno riješiti. Međutim, izvjesni jednostavni i opći teoremi dozvoljavaju izvođenje strogih tvrdnji o odgovarajućim rješenjima, tj. o energijskim stanjima i valnim funkcijama. Ti se teoremi primjenjuju na prototip svih relativističkih valnih jednadžbi, Salpeterovu jednadžbu bez spina.