Convexity and potential sums
for Salpeter-like Hamiltonians

Richard L. Hall 1, Wolfgang Lucha 2, and Franz F. Schöberl 3

1 Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8
2 Institut für Hochenergiephysik, Österreichische Akademie der Wissenschaften, Nikolsdorfgasse 18, A-1050 Wien, Austria
3 Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria

1 rhall@mathstat.concordia.ca, 2 wolfgang.lucha@oeaw.ac.at, 3 franz.schoeberl@univie.ac.at

Abstract

The semirelativistic Hamiltonian \( H = \beta \sqrt{m^2 + p^2} + V(r) \), where \( V(r) \) is a central potential in \( \mathbb{R}^3 \), is concave in \( p^2 \) and convex in \( p \equiv \sqrt{p^2} \). This fact enables us to obtain complementary energy bounds for the discrete spectrum of \( H \). By extending the notion of ‘kinetic potential’ we are able to find general energy bounds on the ground-state energy \( E \) corresponding to potentials with the form \( V = \sum_i a_i f^{(i)}(r) \). In the case of sums of powers and the log potential, where \( V(r) = \sum_{q \neq 0} a(q) \text{sgn}(q) r^q + a(0) \ln(r) \), the bounds can all be expressed in the semi-classical form

\[
E \approx \min_r \left\{ \beta \sqrt{m^2 + \frac{1}{r^2}} + \sum_{q \neq 0} a(q) \text{sgn}(q)(r P(q))^q + a(0) \ln(r P(0)) \right\}.
\]

‘Upper’ and ‘lower’ \( P \)-numbers are provided for \( q = -1, 1, 2 \), and for the log potential \( q = 0 \). Some specific examples are discussed, to show the quality of the bounds.

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1. Introduction

The Hamiltonian $H = K + V$ for the problems we study has the feature that either the kinetic energy $K$ or the potential energy $V$ is nonlocal. The most important example is the semirelativistic “spinless-Salpeter” Hamiltonian [1–4] given by

$$H = K(p) + V(r) = \sqrt{m^2 + p^2} + V(r), \quad (1.1)$$

where $r \equiv \|r\|$, $r \in \mathbb{R}^3$, and $p \equiv \|p\| = \sqrt{p^2}$. In this form at least $K(p)$ is nonlocal in configuration space and is defined as a multiplicative operator in momentum space. That is to say, $K\psi$ is defined to be what we get when $\psi$ is transformed to momentum space, the multiplicative operator $K$ is applied, and the result is transformed back to coordinate space. Nonlocality is the main source of difficulty for this class of problems. We study the discrete spectra of these Hamiltonians by the use of approaches that make use of convexity and of spectral information already obtained concerning related problems. In an earlier paper [4] we studied the relationship between $H_0 = K + h$ and $H = K + g \circ h$, where $g(h(r))$ is a smooth transformation of a ‘base’ potential $h(r)$. For cases in which $g$ had definite convexity, one could then employ the so-called ‘kinetic-potential’ [5] formalism and ‘envelope theory’ [6] to construct upper or lower bounds to the discrete eigenvalues of $H$ by using the known spectrum of $H_0$.

The present paper has two distinct aspects: we turn our attention firstly to the convexity of $K$, as a function of $p$ or $p^2$; and then we look at potentials that are a sum of terms $V = \sum_i V^{(i)}$. In Section 2 we extend the kinetic-potential formalism to include more general kinetic-energy operators than the Schrödinger form $K = p^2$ studied earlier [5]. We have already found [7] some implications of the fact that $K$ is concave in $p^2$. The spectral implications of the convexity of $K$ in $p$ demand a new analysis. By using Jensen’s inequality [8] we are able to construct a framework in Section 3 which accommodates both cases. Although it may not be immediately apparent, the treatment of potential sums also leads to an interesting convexity analysis of a completely different type [9, 10]. This in turn yields an optimized general lower bound for the bottom of the spectrum expressed in terms of the kinetic potentials generated by ‘component’ problems $K + V^{(i)}$. We discuss this in general terms in Section 4. In the special case in which the component
problems are pure-power potentials or the log potential, that is to say

\[ V(r) = \sum_{q \neq 0} a(q) \text{sgn}(q) r^q + a(0) \ln(r) , \]  

the lower bound (Section 5) and also upper bounds obtained by variational methods (Section 6) can all be expressed in terms of a semi-classical expression of the form

\[ E \approx \min_r \left\{ \sqrt{m^2 + \frac{1}{r^2}} + \sum_{q \neq 0} a(q) \text{sgn}(q) (r P(q))^q + a(0) \ln(r P(0)) \right\} . \]  

It is the goal of this paper to develop a general theory which leads to such a result and, in particular, to determine \( P \)-numbers which guarantee that the approximation (1.3) is an upper or lower bound. We shall find the appropriate upper and lower \( P(q) \) for the cases \( q = -1, 1, 2 \), and for the log potential \( q = 0 \). In Section 7 we apply our general results to some specific examples.

Although we obtain very concrete results in the end, our study begins with a somewhat abstract viewpoint. We now make a few general remarks that will help motivate these starting considerations. An idea that runs through the work is one well known to those who study non-linear problems: we try to use transformations to make the most of any soluble problem that is at hand, or, at least, one for which we have a good approximation. The setting for our ideas is geometrical. We suppose that we have an exact solution (or good bounds) for a ‘base’ problem with Hamiltonian \( \alpha p^2 + \beta h(r) \), and we are interested in a Hamiltonian of the form

\[ H = k(p^2) + g(h(r)) , \]

where \( k \) and \( g \) are monotone increasing smooth transformations. It follows that the ‘tangent spaces’ to \( H \) are Schrödinger operators with the general form

\[ H^{(t)} = a + b p^2 + c h(r) , \]

where the parameters \( \{a,b,c\} \) depend on the contact vector \( t \). What we look for is a theory that would allow us to deduce spectral information about \( H \) from the ‘known’ spectrum of its tangents \( H^{(t)} \). For example, if the transformation functions \( k \) and \( g \) are both concave, we would expect to obtain upper bounds via the spectral inequality

\[ H < H^{(t)} . \]

\textit{Mutatis mutandis}, a complimentary theory is possible with operator tangent spaces of the form \( H^{(t)} = a + b p + c h(r) \), where \( K(p) \) is convex in \( p \) and \( g(h) \) is convex in \( h \) : this leads to energy lower bounds. Since we have already explored [4] the potential transformation \( g \), the main thrust of the present paper concerns kinetic-energy transformations with ‘base problems’ respectively \( p^2 + h \) and \( p + h \) and to applications of the results when the potential in \( H \) is a sum of terms. The more
general case in which neither transformation $k(p)$ nor $g(h)$ is the identity follows immediately by combining the present and earlier results; hence we do not need to discuss this natural generalization in detail here. Coulomb ‘components’ present a special difficulty for a lower bound with kinetic energy $p$ because the operator $p - v/r$ has no discrete eigenvalues. However, for our main concern, the Salpeter Hamiltonian, we are able to make use of the very good Coulomb lower bound of Martin and Roy [11] and so incorporate the Coulomb contribution smoothly into our general formulation.

2. Variety of kinetic potentials

The discrete eigenvalues of the self-adjoint operators we study may be characterized variationally. Thus the bottom of the spectrum $E$ of $H = K + V$ is given by $E = \inf(\psi, H\psi)$, where the infimum is taken over all normalized functions in the domain $\mathcal{D}(H) \subset L^2(\mathbb{R}^3)$. The idea behind kinetic potentials is to perform the minimization in two stages: we first find the constrained minimum $\nabla(K; s)$ of $(\psi, V\psi)$, keeping the mean kinetic energy $(\psi, K\psi) = s$ constant; then, we recover $E$ by minimizing over the kinetic energy $s > 0$. Thus we have

$$\nabla(K; s) = \inf_{\psi \in \mathcal{D}(H)} (\psi, V\psi) \quad \Rightarrow \quad E = \min_{s > 0} \{s + \nabla(K; s)\}. \quad (2.1)$$

We call the function $\nabla(K; s)$ the kinetic potential of $V$ associated with the kinetic-energy operator $K$; we shall write simply $\nabla(s)$, if the kinetic-energy operator $K$ is fixed or is clear from the context. It follows immediately from the definition that the kinetic potentials absorb a positive coupling parameter in the sense that $c\nabla(s) = c\nabla(s)$. We note also that the elementary

Comparison Theorem

$$\nabla^{(1)}(s) < \nabla^{(2)}(s) \quad \Rightarrow \quad E^{(1)} < E^{(2)}$$

follows immediately from (2.1). The arguments we use are not restricted to dimension $N = 3$; this choice allows us to illustrate the general results with some explicit well-known examples, without the distraction of the operator dependencies on $N$.

The reason for using this description of the spectral problem is that it lends itself to some interesting approximations. Firstly, we have shown in the Schrödinger [5] and Salpeter [4] cases that, if $V(r) = g(h(r))$ and $g$ is monotone increasing and has
definite convexity, then the approximation $V(s) \approx g(h(s))$ leads to lower bounds if $g$ is convex and upper bounds if $g$ is concave. In Section 4 of the present paper we shall extend to general $K$ the result obtained earlier [10] for the Schrödinger case that kinetic potentials are subadditive, that is to say

$$ V(r) = h^{(1)}(r) + h^{(2)}(r) \Rightarrow V(s) \geq h^{(1)}(s) + h^{(2)}(s). $$

(2.2)

The lower energy bound then immediately follows from the above-mentioned comparison theorem for kinetic potentials. There is more to this result than meets the eye: it generates the optimum of a family of lower bounds; the details will be given in Section 4 below. Extensions to sums with more than two terms (or, further, to mixtures generated by an integral) are immediate. The principal limitation is that each potential term alone, when added to the kinetic energy, must, for large enough coupling, support a discrete eigenvalue. Thus $V(r) = -1/r + r$ is allowed but $V(r) = 1/r + r$ is not.

The ‘component’ kinetic potential $\overline{h}(s) = \overline{h}(K; s)$ can be constructed by use of a Legendre transformation from the eigenvalue function $E = F(v)$, in which $F(v)$ is the bottom of the spectrum of $H = K + vh(r)$, as a function of the coupling $v$. In the Schrödinger case $H = p^2 + vh(r)$ we have shown that $F(v)$ is concave [5] and moreover the kinetic potential for $K = p^2$ is given in terms of $F(v)$ by the transformation

$$ s = F(v) - vF'(v), \quad \overline{h}(K; s) = F'(v). $$

(2.3)

The concavity of the eigenvalue function $F(v)$ has been proved for the Schrödinger case [5] and the Salpeter case [4] by the application of a simple variational argument. By exactly similar reasoning we can show that the eigenvalue function for the operator $p + vh(r)$ is also concave in $v$. Moreover, the Legendre transformation (2.3) is generic: it is valid for all kinetic-energy operators $K$. This is an immediate consequence of the concavity of $F(v)$, as the following equations clearly demonstrate:

$$ F(v) = \min_{u>0}\{F(u) - uF'(u) + vF'(u)\} = \min_{s>0}\{s + v\overline{h}(K; s)\}. $$

Our principal assumption concerning $K$ is that it is at once a convex function of $p$ and a concave function of $p^2$. This convexity is clearly true for our most important example, the relativistic kinetic energy $K = \sqrt{m^2 + p^2}$; however, we shall use this specific form only when we need to.
We now turn from the general to some very specific results. We shall need to have at our disposal some ‘component’ kinetic potentials for the operators $K + v \text{ sgn}(q)r^q$, where $K = p$, or the Schrödinger case $K = p^2$. By elementary scaling arguments we can show that the dependence of the energy functions on the coupling $v$ are given by

\[ p + v \text{ sgn}(q)r^q \Rightarrow E = F^{(1)}(q; v) = F^{(1)}(q; 1)v^{\frac{1}{1+q}} \]  

(2.4a)

and

\[ p^2 + v \text{ sgn}(q)r^q \Rightarrow E = F^{(2)}(q; v) = F^{(2)}(q; 1)v^{\frac{2}{1+q}} \]  

(2.4b)

The Legendre transformation $F \leftrightarrow \overline{h}$ given above in (2.3) now allows us to deduce the precise forms of the corresponding kinetic potentials. For convenience we choose to write the kinetic potentials so obtained in a special way. We change variables for the mean kinetic energy $s$ in the two cases respectively to $s = 1/r$ and $s = 1/r^2$. It then follows from (2.3) by straightforward algebraic computations that the kinetic potentials for $h(r) = \text{ sgn}(q)r^q$ have similar convenient forms, namely

\[ \overline{h}(p; 1/r) = \text{ sgn}(q)(P^{(1)}(q)r)^q \]  

(2.5a)

and

\[ \overline{h}(p^2; 1/r^2) = \text{ sgn}(q)(P^{(2)}(q)r)^q, \]  

(2.5b)

where the $P$-numbers are defined in terms of the $v = 1$ eigenvalues $E^{(i)}(q) = F^{(i)}(q; 1), \ i = 1, 2$, respectively by the explicit formulas

\[ K = p \Rightarrow P^{(1)}(q) := \left| \frac{E^{(1)}(q)}{1+q} \right|^{1+\frac{1}{q}} |q|, \ q > -1, q \neq 0 \]  

(2.6a)

and

\[ K = p^2 \Rightarrow P^{(2)}(q) := \left| \frac{E^{(2)}(q)}{1+q/2} \right|^{\frac{1}{2}+\frac{1}{q}} \left| \frac{q}{2} \right|^{\frac{1}{2}}, \ q > -2, q \neq 0. \]  

(2.6b)

The energies are related to the kinetic potentials by specific realizations of the general formula (2.1): for example, we have in this spectral representation

\[ p + v \text{ sgn}(q)r^q \Rightarrow E = \min_{r > 0} \left\{ \frac{1}{r} + v \text{ sgn}(q) \left( P^{(1)}(q)r \right)^q \right\}, \ q > -1, q \neq 0. \]  

(2.7)
One of our side goals is purely esthetic, namely we wish to end up with ‘attractive formulas’: after the changes of variable from \( s \) to \( r \), the kinetic potentials look like the original power potentials themselves, but with the \( P \)-factors inserted. We turn now to the base potential \( h(r) = \ln(r) \) and find by scaling arguments that

\[
p + v \ln(r) \quad \Rightarrow \quad F^{(1)}(v) = vF^{(1)}(1) - v \ln(v) \quad (2.8a)
\]

and

\[
p^2 + v \ln(r) \quad \Rightarrow \quad F^{(2)}(v) = vF^{(2)}(1) - \frac{1}{2}v \ln(v). \quad (2.8b)
\]

Consequently we obtain from the transformation (2.3)

\[
\bar{h}(p; 1/r) = \ln(P^{(1)}(0)r), \quad \bar{h}(p^2; 1/r^2) = \ln(P^{(2)}(0)r), \quad (2.9)
\]

where

\[
P^{(1)}(0) = \exp(E^{(1)}(0) - 1), \quad P^{(2)}(0) = \frac{1}{\sqrt{2}} \exp \left( E^{(2)}(0) - \frac{1}{2} \right). \quad (2.10)
\]

For the discussion of examples we shall need to have some specific \( P \) values. For the cases \( q = -1, 0, 1, 2 \) we supply some of these numerical values in Table 1. This table has an eigenvalue symmetry because of the operator equivalence \( p + r^2 \sim p^2 + r \); it also has two omissions corresponding to \( q = -1 \), because \( p - 1/r \) has no discrete eigenvalues. We offer now a solution to this Coulomb difficulty. As we shall make clear in Section 4, viable Coulomb \( P \)-numbers are needed for lower bounds. For our most important application \( K = \sqrt{p^2 + m^2} \), a lower bound to the bottom of the spectrum of \( H = K - v/r \) is provided by the Martin–Roy bound [11]

\[
E \geq e_L(v) = m \left( \frac{1 + \sqrt{1 - 4v^2}}{2} \right)^{1/2}, \quad v < \frac{1}{2}. \quad (2.11)
\]

The condition \( v < \frac{1}{2} \) is a little more restrictive than the fundamental operator restriction \( v < 2/\pi \); it was proved by Herbst [12] that a Friedrichs extension exists for \( H \) only if the Coulomb coupling is sufficiently small. The Coulomb lower bound has the same scaling law with respect to \( m \) as does the exact energy: although \( m \) originates in the Hamiltonian inside the square root of the kinetic-energy term, it appears in the eigenvalue and in its lower approximation simply as an overall
factor [4]. Now we construct a $v$-dependent $P$-representation for this lower bound. We write (as a definition of $P_L(v)$)

$$e_L(v) = \min_r \left\{ \sqrt{m^2 + \frac{1}{r^2}} - \frac{v}{P_L(v)r} \right\}.$$  \hfill (2.12)

An elementary calculation then shows that (2.11) and (2.12) imply $P_L(v) = e_L(v)/m$. This serendipitous discovery fills the gaps in Table 1, and will allow us to include the Coulomb component in our lower-bound energy formula for sums of potential terms: we must make the substitution

$$-\frac{v}{P^{(1)}(-1)r} = -\frac{v}{P_L(v)r} = -\frac{mv}{e_L(v)r}, \quad v < \frac{1}{2}.$$  \hfill (2.13)

3. Complementary convexity: $p + V$ and $p^2 + V$

The principal result of this section is best expressed in terms of kinetic potentials by the following

**Theorem 1.** If $E$ is the bottom of the spectrum of the Hamiltonian $H = K + V$, and the kinetic-energy operator $K$ is at once convex in $p$ and concave in $p^2$, then it follows that

$$\min_{s > 0} \{ K(s) + \overline{V}(p; s) \} \leq E \leq \min_{s > 0} \{ K(s) + \overline{V}(p^2; s^2) \}. \hfill (3.1)$$

It makes sense here to speak of $K(p)$ as though $p$ were a real variable since, by definition, the action of the operator $K$ is effected via the Fourier transform. We shall now prove this result by an application of Jensen’s inequality [8] and kinetic potentials defined in (2.1). We consider first the left-hand inequality of the theorem. If $\psi$ is a normalized function in the domain $\mathcal{D}(H)$ of $H = K + V$, then, since $K = K(p)$ is convex in $p$, by Jensen’s inequality, we have

$$E = \inf_{\psi \in \mathcal{D}(H)} \{(\psi, K(p)\psi) + (\psi, V\psi)\} \geq \inf_{\psi \in \mathcal{D}(H)} \{K((\psi, p\psi)) + (\psi, V\psi)\}.$$  \hfill \smallskip

That is to say,

$$E \geq \min_{s > 0} \inf_{\psi \in \mathcal{D}(H)} \{K((\psi, p\psi)) + (\psi, V\psi)\} = \min_{s > 0} \{K(s) + \overline{V}(p; s)\}.$$
The proof of the upper-bound inequality is very similar: we write $K(p) = k(p^2)$, where $k$ is concave; then, setting $t = s^2$, we arrive at the inequality

$$E \leq \min_{t > 0} \{ k(t) + \overline{V}(p^2; t) \} = \min_{s > 0} \{ K(s) + \overline{V}(p^2; s^2) \},$$

which establishes the theorem.

This result is an essential ingredient in the proof of the sum approximation in the next section. We now look at an example, namely the Salpeter problem with a linear potential. We have

$$H = \sqrt{m^2 + p^2} + V(r), \quad V(r) = vh(r) = vr,$$

(3.2)

where $v$ is a positive coupling parameter. In terms of the convenient variable $r > 0$ the two kinetic potentials from (2.5) are

$$\overline{h}(p; 1/r) = P^{(1)}(1)r, \quad \overline{h}(p^2; 1/r^2) = P^{(2)}(1)r,$$

(3.3)

where the $P$-numbers are provided in Table 1. Theorem 1 then immediately yields the bounds

$$\min_{r > 0} \left\{ \sqrt{m^2 + r^2} + vP^{(1)}(1)r \right\} \leq E \leq \min_{r > 0} \left\{ \sqrt{m^2 + r^2} + vP^{(2)}(1)r \right\}. \quad (3.4)$$

In Figure 1 we plot these bounds as a function of $m$ for the case $v = 1$. If we combine Theorem 1 here with Theorem 2 of Ref. [4] (to the effect that $g \circ h > g \circ h$ when $g$ is convex) we obtain the following class of examples. We suppose that $V(r)$ is monotone increasing and convex in $h(r) = r$ then the two theorems together yield the lower bound

$$E \geq \min_{r > 0} \left\{ \sqrt{m^2 + \frac{1}{r^2}} + vV(P^{(1)}(1)r) \right\}. \quad (3.5)$$

Of course, if $V(r)$ is concave, then we get an upper bound by the same expression provided we use $P^{(2)}(1)$. It is perhaps important to note that with $P = P^{(2)}(r)$ an upper bound would be obtained for every choice of $r$ in the expression on the right-hand side; the expression in (3.5) is however only a lower bound a priori at the minimum point.

4. The sum approximation: lower bounds

Since further generalization easily follows, we first look at the problem of the sum of two potential terms. We assume that each potential $vh^{(i)}(r)$ alone, when
added to the kinetic-energy operator $K$, has a discrete eigenvalue at the bottom of the spectrum for sufficiently large ‘coupling’ $v$. We express our result in terms of kinetic potentials and prove the following

**Theorem 2** If $E$ is the bottom of the spectrum of the Hamiltonian $H = K + V$, and the potential $V$ is the sum $V(r) = h^{(1)}(r) + h^{(2)}(r)$, then it follows that the sum of the component kinetic potentials yields a lower bound to $V$, that is to say

$$
\nabla(K; s) \geq h^{(1)}(K; s) + h^{(2)}(K; s).
$$

We shall now prove this theorem, which is in effect an optimized Weyl lower bound [13–15]; this remark will be clarified below, after the proof of the theorem. From the definition (2.1) of kinetic potentials we have

$$
\nabla(K; s) = \inf_{\psi \in \mathcal{D}(H)} \left( \psi, V\psi \right) = \inf_{\psi \in \mathcal{D}(H)} \left( \psi, \left( h^{(1)} + h^{(2)} \right) \psi \right).
$$

But the latter minimum mean-value is clearly bounded below by the sum of the separate minima. Thus we have

$$
\nabla(K; s) \geq \inf_{\psi \in \mathcal{D}(H)} \left( \psi, h^{(1)} \psi \right) + \inf_{\psi \in \mathcal{D}(H)} \left( \psi, h^{(2)} \psi \right) = h^{(1)}(K; s) + h^{(2)}(K; s),
$$

which inequality establishes the theorem. 

Another approach, which would eventually yield an alternative proof of the theorem, exhibits the relationship between Theorem 2 and the classical Weyl lower bound [13–15] for the eigenvalues of the sum of two operators. Let us suppose that $\Psi$ is the exact normalized lowest eigenfunction of $H = K + V$, so that $H\Psi = E\Psi$. If the positive real parameter $w$ is bounded by 1, $0 < w < 1$, then $E = (\Psi, (K + V)\Psi)$ may be written as follows:

$$
E = w \left( \Psi, \left( K + \frac{1}{w} h^{(1)}(r) \right) \Psi \right) + (1 - w) \left( \Psi, \left( K + \frac{1}{1 - w} h^{(2)}(r) \right) \Psi \right)
$$

$$
\geq w \inf_{\psi \in \mathcal{D}(H)} \left( \psi, \left( K + \frac{1}{w} h^{(1)}(r) \right) \psi \right)
$$

$$
+ (1 - w) \inf_{\psi \in \mathcal{D}(H)} \left( \psi, \left( K + \frac{1}{1 - w} h^{(2)}(r) \right) \psi \right).
$$
That is to say, in terms of component kinetic potentials, we arrive at Weyl’s inequality for the lowest eigenvalue of the sum $H = wK + h^{(1)} + (1 - w)K + h^{(2)}$:

$$E \geq w \min_{s > 0} \left\{ s + \frac{1}{w} h^{(1)}(K; s) \right\} + (1 - w) \min_{s > 0} \left\{ s + \frac{1}{1 - w} h^{(2)}(K; s) \right\}.$$ 

Since $w$ is an essentially free parameter in the last expression, we may optimize the Weyl lower bound with respect to the choice of $w$ and this forces the individual values of $s$ at the minima, $\{s_1(w), s_2(w)\}$, to be related. More specifically we find from the individual minimizations over $s$,

$$E \geq \mathcal{E}(w) = w s_1(w) + (1 - w) s_2(w) + \bar{h}^{(1)}(K; s_1(w)) + \bar{h}^{(2)}(K; s_2(w)),$$

where

$$w = -\frac{\partial \bar{h}^{(1)}}{\partial s}(K; s_1(w)), \quad \text{and} \quad 1 - w = -\frac{\partial \bar{h}^{(2)}}{\partial s}(K; s_2(w)).$$

The critical condition $\mathcal{E}'(w) = 0$ for the subsequent maximization of the lower bound over $w$ then yields $s_1(w) = s_2(w)$. Thus the best lower energy bound is given by

$$E \geq \min_{s > 0} \left\{ s + \bar{h}^{(1)}(K; s) + \bar{h}^{(2)}(K; s) \right\}.$$

The kinetic-potential inequality of Theorem 2 leads, of course, to the same energy lower bound: the optimization just performed above is therefore seen to be automatically ‘built in’ by the formalism.

It follows immediately from the above kinetic-potential comparison theorem and coupling-parameter absorption that a lower bound to the lowest energy $E$ of the Hamiltonian $H = K + \sum_i c_i h^{(i)}(r)$, $\{c_i > 0\}$, is provided by the formula

$$E \geq \min_{s > 0} \left\{ s + \sum_i c_i \bar{h}^{(i)}(K; s) \right\}.$$  \hspace{1cm} (4.2)$$

Similarly we can extend this result to ‘continuous sums’ such as $V(r) = \int_{t_1}^{t_2} c(t) h^{(t)}(r) dt$.

This general theory becomes practically useful when we have good information concerning the components. More particularly, we must have some exact component kinetic potentials, or lower bounds to them. Outside the well-explored Schrödinger case $K = p^2$, such analytical results are rather sparse. We look at the interesting class of power-law potentials in the next section.
5. Sums of powers and the log potential

For power-law potentials and the relativistic kinetic energy \( K = \sqrt{m^2 + p^2} \) we have discussed some lower bounds in Section 3 and we shall now turn these to our advantage. The link between Theorem 1 and Theorem 2 derives from the observation that the equation \( K(s) = \sqrt{m^2 + s^2} \) allows us to change the minimization variable \( s \rightarrow r = 1/s \). In the first stage of minimization, we have used Jensen’s inequality for the lower bound (see proof of Theorem 1); this allows us to keep \((\psi, p\psi) = s = 1/r\) constant at first, and then later minimize over \( s \), or, equivalently, over \( r \). We can also easily accommodate a further positive kinetic-energy parameter \( \beta \). Thus we immediately arrive at

**Theorem 3** \( A \) lower bound to the lowest eigenvalue of the semirelativistic spinless-Salpeter operator

\[
H = \beta \sqrt{m^2 + p^2} + \sum_{q \neq 0} a(q) \text{sgn}(q) r^q + a(0) \ln(r),
\]

where \( \beta > 0 \) and the potential coefficients \( a(q) \geq 0 \) are not all zero, is given by

\[
E \geq \min_{r > 0} \left\{ \beta \sqrt{m^2 + \frac{1}{r^2}} + \sum_{q \neq 0} a(q) \text{sgn}(q) (P^{(1)}(q) r)^q + a(0) \ln(P^{(1)}(0) r) \right\}, \quad (5.1)
\]

where, for the Coulomb component \( q = -1 \), we make the substitution

\[
- \frac{a(-1)}{P^{(1)}(-1) r} = - \frac{\beta^2 m v}{e_L(v) r} = - \frac{\beta v}{r \left( 1 + \sqrt{1 - 4v^2} \right)^{1/2}}, \quad v = \frac{a(-1)}{\beta} < \frac{1}{2} \quad (5.2)
\]

The problem presented for the lower bound by the fact that \( p = \sqrt{v^2} \) has no discrete spectrum was discussed in Section 2. We have no simple \( P \)-number \( P(-1) \) but we could derive a ‘running’ \( P \) \((2.13)\) from the Martin–Roy energy bound \((2.11)\); the positive factor \( \beta \) has been inserted in \((5.2)\) by elementary scaling. We shall look at applications of Theorem 3 in Section 7 when we also have at our disposal the upper-bound \( P \)-numbers derived in Section 6.

6. Variational upper bounds

The lower bound for sums discussed in the previous two sections has the attractive feature that if the component kinetic potentials are exact and only one term is present, then the result is exact. We are unable to construct a general upper bound
with this feature. Instead we use a trial wave function \( \phi = c \exp(-\frac{1}{2} \alpha r^\nu) \) with a scale parameter \( \alpha > 0 \) and two other parameters \( \{c, \nu\} \), and we apply this wave function to the entire problem. One degree of freedom \( c \) is used to guarantee normalization, and the scale parameter \( \alpha > 0 \) is expressed in terms of a new variable \( t > 0 \) chosen in such a way that the scale minimization is of an expression with the same form as the lower bound. Initially we use here \( t \) rather than \( r \) since, during the discussion, we shall need to refer to the potential function \( V(r) \). The choice of the remaining parameter \( \nu > 0 \) is left for later optimization.

If we suppose that \( c \) has already been chosen so that \( \|\phi\| = 1 \), and, for computational convenience, we use Jensen’s inequality, we then obtain the following upper energy bound:

\[
E < \mathcal{E} = \beta \sqrt{m^2 + (\phi, p^2 \phi)} + \left( \phi, \left\{ \sum_{q \neq 0} a(q) \text{sgn}(q) r^q + a(0) \ln(r) \right\} \phi \right) .
\] (6.1)

Now, for each fixed \( \nu > 0 \), we define a new scale variable \( t > 0 \) by the following:

\[
(\phi, p^2 \phi) = (\phi, -\Delta \phi) = \alpha^{2/\nu} \left( \frac{\nu}{2} \right)^2 \frac{\Gamma(2 + \frac{1}{\nu})}{\Gamma(\frac{4}{\nu})} \equiv \frac{1}{t^2}.
\] (6.2)

Using this definition of \( t \), we can go on to define the ‘upper’ \( P \)-numbers \( P(\nu, q) \) by the relations

\[
(\phi, r^q \phi) = \frac{1}{\alpha^{\nu/\nu}} \frac{\Gamma(\frac{q+3}{\nu})}{\Gamma(\frac{4}{\nu})} \equiv (P(\nu, q)t)^q , \quad q \neq 0,
\] (6.3a)

and

\[
(\phi, \ln(r) \phi) = \ln \left( P(\nu, 0)t \right) .
\] (6.3b)

If we now rename the scale variable \( t = r \), and minimize the upper bound \( \mathcal{E} \) with respect to scale, we arrive at

**Theorem 4**  For each \( \nu > 0 \), an upper bound to the lowest eigenvalue \( E \) of the Salpeter operator

\[
H = \beta \sqrt{m^2 + p^2} + \sum_{q \neq 0} a(q) \text{sgn}(q) r^q + a(0) \ln(r),
\]

where \( \beta > 0 \) and the potential coefficients \( a(q) \geq 0 \) are not all zero, is given by

\[
E \leq \min_{r > 0} \left\{ \beta \sqrt{m^2 + \frac{1}{r^2}} + \sum_{q \neq 0} a(q) \text{sgn}(q) (P(\nu, q)r)^q + a(0) \ln(P(\nu, 0)r) \right\} ,
\] (6.4)
where the upper $P$-numbers are provided by the formulas

$$P(\nu, q) = \frac{\nu}{2} \left( \frac{\Gamma(2 + \frac{1}{\nu})}{\Gamma(\frac{3}{\nu})} \right)^{\frac{1}{2}} \left( \frac{\Gamma(\frac{q+3}{\nu})}{\Gamma(\frac{q}{\nu})} \right)^{\frac{1}{q}}, \quad q \neq 0, \quad (6.5a)$$

$$P(\nu, 0) = \frac{\nu}{2} \left( \frac{\Gamma(2 + \frac{1}{\nu})}{\Gamma(\frac{3}{\nu})} \right)^{\frac{1}{2}} \exp \left( \frac{1}{\nu} \psi \left( \frac{3}{\nu} \right) \right), \quad (6.5b)$$

and $\psi$ is the digamma function $\psi(t) = \frac{\Gamma'(t)}{\Gamma(t)}$.

Apart from the special Coulomb considerations pertaining to the lower bound (5.1), that formula is essentially identical to the upper bound (6.4): we simply have to use the correct $P$-numbers in each case.

7. Examples

We have now assembled the $P$-numbers for our energy-bound formulas (5.1) and (6.4). We shall use the lower $P$-numbers in Table 1, lower ‘running’ $P$-formula for the Coulomb component (2.13), and the formulas (6.5) for the $P(\nu, q)$ corresponding to the variational upper bound (6.4). The class of problems we are thus immediately able to consider have the following explicit Hamiltonian form:

$$H = \beta \sqrt{m^2 + p^2} - a/r + b \ln(r) + cr + dr^2 , \quad a, b, c, d \geq 0, \quad (7.1)$$

where $\beta > 0$, and the potential parameters $\{a, b, c, d\}$ are not all zero. We look at two examples. In the first, illustrated in Figure 2, we look at the linear-plus-Coulomb potential $V(r) = -0.1/r + 0.25r$ and compare the energy bounds $\{L, U\}$ we find, as functions of the mass $m$, with some very accurate numerical values (center curve) obtained by minimizing the expectation value of the Hamiltonian in a 25-dimensional trial space. In the next graph, Figure 3, we plot the energy bounds alone, for the same potential and a wider range of values of the mass $m$. As a second example we consider the broad linear combination $V(r) = -0.1/r + 0.25 \ln(r) + 0.25r + 0.25r^2$ and plot in Figure 4 the energy bounds as functions of the mass. These illustrations give a clear indication of the quality of the bounds that the theory yields.

8. Conclusion

The principal theoretical results of this paper are the complementary bounds of Theorem 1, and the sum-approximation lower bound, Theorem 2. In order to arrive
at these results we needed first to extend the notion of ‘kinetic potential’ to allow for more general kinetic-energy operators than the Schrödinger form $K = p^2$. The complementary bounds are based on the assumption that $K$ is a convex function of $p$ and also a concave function of $p^2$, assumptions clearly satisfied by our prime example and principal motivation, the relativistic kinetic energy $K = \beta \sqrt{m^2 + p^2}$. The inequality of Jensen then allows us to learn approximately how special mean values of the problem, the eigenvalues of $H$, depend on the operator parameters.

By combining Theorem 1 of this paper with Theorem 2 of our earlier paper [4] we obtain a general theory applicable to ‘operator manifolds’ of the form $H = K(p) + g(h)$ with, on the one hand, tangent spaces spanned by the Schrödinger operators $ap^2 + bh(r) + c$, and, on the other, by complementary operators of the form $ap + bh(r) + c$. Given the correct convexities of $K$ and $g$, energy bounds immediately follow. We looked at one example of this type of problem near the end of Section 3; and the results were exhibited in Figure 1.

A completely different lower bound is provided by Theorem 2, which may be thought of as a spectral expression of the sum structure of the potential, namely the subadditivity of the corresponding kinetic potential, as a sum of components.

In order to make practical use of these theoretical results we need some definite spectral information about component problems. This is provided by the family of pure-power potentials $V(r) = \text{sgn}(q)r^q$. For this family we are able to take advantage of known eigenvalues, or bounds to them, and of simple upper bounds obtained with the aid of Jensen’s inequality and a two-parameter family of trial functions. All our component results can then be expressed in terms of certain $P$-numbers (or, for the lower Coulomb case, $q = -1$, by a $P$-function), which are required by the general lower- and upper-bound formulas of Theorems 3 and 4. These formulas illustrate the effectiveness of the theoretical results and provide recipes for approximate solutions to an interesting class of semirelativistic spectral problems.

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Table 1. Eigenvalues for $v = 1$ and corresponding $P$-numbers [given by (2.6) and (2.10)] for the Coulomb, log, linear and harmonic-oscillator potentials. The eigenvalues have been computed numerically and are rounded so that the $E^{(1)}(q)$ are lower bounds and the $E^{(2)}(q)$ are upper bounds (and similarly for the derived $P$-numbers). The Coulomb lower bound is treated differently because $H = p - 1/r$ has no discrete spectrum.

| $q$ | $E^{(1)}(q)$ | $P^{(1)}(q)$ | $E^{(2)}(q)$ | $P^{(2)}(q)$ |
|-----|---------------|---------------|---------------|---------------|
| $-1$ | $-$           | $-$           | $-\frac{1}{4}$ | $1$          |
| $0$  | $1.06365$     | $1.0657$      | $1.0443325$   | $1.218669$   |
| $1$  | $2.23225$     | $1.2457$      | $2.3381075$   | $1.376084$   |
| $2$  | $2.338107$    | $1.366687$    | $3$           | $\frac{3}{2}$ |
Figure 1.

Complementary upper (U) and lower (L) bounds (3.4) on the lowest eigenvalue $E(m)$ of $H = \sqrt{m^2 + p^2} + r$ plotted against $m$. 
Figure 2.

Lower bounds (L) by (5.1) and upper bounds (U) by (6.4) for the lowest eigenvalue $E(m)$ of $H = \sqrt{m^2 + p^2} - 0.1/r + 0.25r$ plotted against $m$. The upper bound (U) used the wave-function parameter $\nu = 1.6$. The central curve is a very accurate upper bound found by a variational exploration in a 25-dimensional trial space.
Figure 3.

Lower bounds (L) by (5.1) and upper bounds (U) by (6.4) for the lowest eigenvalue $E(m)$ of $H = \sqrt{m^2 + p^2} - 0.1/r + 0.25r$ plotted against $m$: this is a continuation of the graph in Figure 2 to larger $m$. 
Figure 4.

Lower bounds (L) by (5.1) and upper bounds (U) by (6.4) for the lowest eigenvalue $E(m)$ of $H = \sqrt{m^2 + p^2} - 0.1/r + 0.25 \ln(r) + 0.25r + 0.25r^2$ plotted against $m$. The upper bound (U) used the wave-function parameter $\nu = 1.4$. 

Convexity and potential sums for Salpeter-like Hamiltonians