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2002 J. Phys. A: Math. Gen. 35 8727

(http://iopscience.iop.org/0305-4470/35/41/307)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 8727–8742 PII: S0305-4470(02)38760-2

# Generalized comparison theorems in quantum mechanics

**Richard L Hall and Qutaibeh D Katatbeh**

Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8

E-mail: rhall@cicma.concordia.ca

Received 28 June 2002
Published 1 October 2002
Online at stacks.iop.org/JPhysA/35/8727

**Abstract**

This paper is concerned with the discrete spectra of Schrödinger operators $H = -\Delta + V$, where $V(r)$ is an attractive potential in $N$ spatial dimensions. Two principal results are reported for the bottom of the spectrum of $H$ in each angular-momentum subspace $\mathcal{H}_\ell$: (i) an optimized lower bound when the potential is a sum of terms $V(r) = V^{(1)}(r) + V^{(2)}(r)$, and the bottoms of the spectra of $-\Delta + V^{(1)}(r)$ and $-\Delta + V^{(2)}(r)$ in $\mathcal{H}_\ell$ are known, and (ii) a generalized comparison theorem which predicts spectral ordering when the graphs of the comparison potentials $V^{(1)}(r)$ and $V^{(2)}(r)$ intersect in a controlled way. Pure power-law potentials are studied and an application of the results to the Coulomb-plus-linear potential $V(r) = -a/r + br$ is presented in detail: for this problem an earlier formula for energy bounds is sharpened and generalized to $N$ dimensions.

PACS number: 03.65.Ge

## 1. Introduction

This paper has two principal aspects: the potential-sum approximation, and the generalization of the comparison theorem of quantum mechanics to cases where the comparison potentials intersect. We study spherically-symmetric problems in $N$ spatial dimensions. There is much interest in problems posed in arbitrary dimension $N$ [1–9], rather than specifically, say, for $N = 1$, or $N = 3$. References [1, 4] are useful for technical results such as the form of the Laplacian in $N$-dimensional spherical coordinates; the other papers are concerned with solving problems such as the hydrogen atom [3, 7] and the linear, harmonic-oscillator, hydrogen atom, and Morse potentials [8] in higher dimensions than $N = 3$. The geometrical methods we use in this paper are independent of dimension, which can usually be carried as a free parameter $N$. We consider examples with Hamiltonians of the form $H = -\Delta + v\,\mathrm{sgn}(q)r^q$ or with sums of such potential terms. We suppose that the Hamiltonian operators $H = -\Delta + V(r)$, $r = \|\boldsymbol{r}\|$,

0305-4470/02/418727+16$30.00  

have domains $\mathcal{D}(H) \subset L^2(R^N)$, they are bounded below, essentially self-adjoint, and have at least one discrete eigenvalue at the bottom of the spectrum. Because the potentials are spherically symmetric, the discrete eigenvalues $E_{n\ell}$ can be labelled by two quantum numbers, the total angular momentum $\ell = 0, 1, 2, \ldots$, and a 'radial' quantum number, $n = 1, 2, 3, \ldots$, which counts the eigenvalues in each angular-momentum subspace. Since the discrete spectrum may be characterized variationally [10, 12], the elementary *comparison theorem* $V^{(1)} < V^{(2)} \Rightarrow E^{(1)}_{n\ell} < E^{(2)}_{n\ell}$ immediately follows. The generalization we shall study (in section 3) involves comparison potentials whose graphs 'cross over' in such a way that spectral ordering is still guaranteed.

Before we study the generalized comparison theorem, we shall need some established results concerning 'kinetic potentials' [13] and 'envelope theory' [14, 15]. In order to fix ideas and simplify the presentation, let us suppose that $E$ is a discrete eigenvalue at the bottom of the spectrum of $H = -\Delta + V$ in $N$ dimensions. It follows that $E = \inf(\psi, H\psi)$ where $\psi \in \mathcal{D}(H)$ and $\|\psi\| = 1$. We perform the total minimization in two stages: first we constrain the process by fixing the mean kinetic energy $(\psi, -\Delta\psi) = s$, and then we minimize over $s > 0$. The mean potential-energy function under the constraint is called the 'kinetic potential' $\overline{V}(s)$ associated with the potential $V(r)$. Thus we define

$$\overline{V}(s) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} (\psi, V\psi) \quad \Rightarrow \quad E = \min_{s>0}\{s + \overline{V}(s)\}. \tag{1.1}$$

The variational definition of the kinetic potentials implies that (i) $\overline{cV}(s) = c\overline{V}(s)$ and (ii) $\overline{V}^{(1)}(s) \leqslant \overline{V}^{(2)}(s) \Rightarrow E^{(1)} \leqslant E^{(2)}$. Kinetic potentials can be defined [13] for higher eigenvalues and they can then be reconstructed from 'energy trajectories', the functions which describe how the eigenvalues vary with the coupling parameter $v > 0$. We have, in general, for coupling

$$H = -\Delta + vf(r) \quad \rightarrow \quad E_{n\ell} = F_{n\ell}(v) \tag{1.2a}$$

and

$$s = F_{n\ell}(v) - vF'_{n\ell}(v) \qquad \overline{f}_{n\ell}(s) = F'_{n\ell}(v) \tag{1.2b}$$

where $E_{n\ell}$ is the $n$th eigenvalue in the angular-momentum space labelled by $\ell$ and $F_{n\ell}(v)$ describes how this eigenvalue depends on the coupling $v > 0$; the corresponding kinetic potentials may then be defined by (1.2*b*). The relationship $F(v) \leftrightarrow \overline{f}(s)$ is essentially a Legendre transformation [16]: for the ground state (or the bottom $E_{1\ell}$ of each angular-momentum subspace) $F(v)$ is concave [11–13] and consequently $\bar{f}(s)$ is convex; it follows [17] immediately from (1.2*b*) that $F''(v)\bar{f}''(s) = -v^{-3} < 0$ whenever $F''(v) \neq 0$; thus in general $F(v)$ and $\bar{f}(s)$ have opposite convexities almost everywhere. For the important class of examples $H = -\Delta + v\,\mathrm{sgn}(q)r^q$, corresponding to pure powers $q > -2$, we know that $F(v)$ is *concave* for every (discrete) eigenvalue since, by scaling arguments, we have $F_{n\ell}(v) = F_{n\ell}(1)v^{\frac{2}{2+q}}$, and $\mathrm{sgn}(F_{n\ell}(1)) = \mathrm{sgn}(q)$.

The main purpose for this two-step reformulation of 'min-max' is that certain spectral approximations are very effectively developed in terms of kinetic potentials. We shall consider first the 'envelope approximation', which in its most succinct form can be summarized as follows:

$$f(r) = g(h(r)) \quad \Rightarrow \quad \overline{f_{n\ell}}(s) \approx g(\overline{h_{n\ell}}(s)). \tag{1.3}$$

Here $f(r)$ is a smooth transformation of a 'base' potential $h(r)$. We suppose that the transformation $g$ is monotone increasing and, if it also has definite convexity, the following important conclusions may be drawn: if $g$ is concave, we get an upper bound $\approx = \leqslant$; and,

**Table 1.** The 'input' $P$-values $P^N_{n0}(1)$ used in the general formula (1.4), for $N = 2, 3, \ldots, 12$. The same data apply to $\ell > 0$ since by theorem 2 we have $P^N_{n\ell} = P^{N+2\ell}_{n0}$.

| $N$ | $n=1$ | $n=2$ | $n=3$ | $n=4$ |
|---|---|---|---|---|
| 2 | 0.9348 | 2.8063 | 4.6249 | 6.4416 |
| 3 | 1.3761 | 3.1813 | 4.9926 | 6.8051 |
| 4 | 1.8735 | 3.6657 | 5.4700 | 7.2783 |
| 5 | 2.3719 | 4.1550 | 5.9530 | 7.7570 |
| 6 | 2.8709 | 4.6472 | 6.4398 | 8.2396 |
| 7 | 3.3702 | 5.1413 | 6.9291 | 8.7251 |
| 8 | 3.8696 | 5.6367 | 7.4204 | 9.2129 |
| 9 | 4.3692 | 6.1330 | 7.9130 | 9.7024 |
| 10 | 4.8689 | 6.6299 | 8.4068 | 10.1932 |
| 11 | 5.3686 | 7.1274 | 8.9053 | 10.7453 |
| 12 | 5.8684 | 7.6253 | 9.4045 | 11.2744 |

if $g$ is convex, we obtain a lower bound $\approx = \geqslant$. These results may also be derived by the use of families of upper and lower 'tangential' potentials [18]. In section 2, we shall apply this result to study the Coulomb-plus-linear potential $V(r) = -1/r + \lambda r$ which is clearly at once a convex transformation of the hydrogenic potential $h(r) = -1/r$ and a concave transformation of the linear potential $h(r) = r$. We shall show that we are also able to express both the upper and lower bounds for the entire discrete spectrum in the form of explicit rational functions $\lambda = \lambda(E_{n\ell})$.

The base potentials used for the Coulomb-plus-linear potential are both pure powers. Thus we shall need to use the corresponding base kinetic potentials. In fact, we have shown in general [14] that

$$-\Delta + \mathrm{sgn}(q)r^q \quad \Rightarrow \quad E^N_{n\ell} = \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(q)}{r}\right)^2 + \mathrm{sgn}(q)r^q\right\} \tag{1.4}$$

where, for example, $P^N_{n\ell}(-1) = (n + \ell + N/2 - 3/2)$ and $P^N_{n\ell}(2) = (2n + \ell + N/2 - 2)$. These $P$-numbers and the underlying eigenvalues $E^N_{n\ell}$ satisfy the relation $E^N_{n\ell} = E^{N+2\ell}_{n0}$: this is generally true for central potentials and is the content of theorem 2, which we prove in section 4. Numerical values for $P^N_{n0}(1)$ are given in table 1 for $N = 2, \ldots, 12$. It is interesting that the case $q = 0$ corresponds *exactly* to the $\ln(r)$ potential [15]. The expression in (1.4) is derived by a change of variable $s \to (P^N/r)^2$ in the kinetic-potential formalism. The application to the Coulomb-plus-linear potential is not our only interest in these $P^N$-numbers. They provide through (1.4) a nice representation for the pure-power eigenvalues since the $P^N$-numbers vary smoothly with $q$ through $q = 0$ whereas the eigenvalues themselves do not [14]. We have proved [14] that $P^N_{n\ell}(q)$ are monotone increasing in $q$. This result was obtained by using envelope theory: we considered one power $q$ as a smooth transformation of another $p$ and then took the limit $p \to q$.

In section 3 we prove theorem 1 which provides a lower bound for the bottom of the spectrum in each angular-momentum subspace using the sum approximation. In section 4 we prove theorem 2, which establishes the invariance of the eigenvalues with respect to changes in $\ell$ and $N$ that leave the sum $N + 2\ell$ invariant. This allows us to restrict our considerations to the ground state in sufficiently high dimension $N$. We reformulate the *refined comparison theorem* (theorem 3 of [19]) which becomes theorem 3 here. We first prove the monotonicity of the ground-state wavefunction in $N$ dimensions; then we prove theorem 4, which extends theorem 3 to $N \geqslant 2$ dimensions. Finally, we prove theorems 5–7 which provide simple

explicit sufficient conditions for the application of theorem 4 under a variety of crossing schemes. In section 4, we apply theorem 5 to sharpen the envelope bounds already found in section 2 for the bottom of the spectrum $E$ of $H$ when $V$ is the Coulomb-plus-linear potential $V(r) = -a/r + br$.

## 2. Coulomb-plus-linear potential: an eigenvalue formula

The Coulomb-plus-linear potential $V(r) = -a/r + br$ is of interest in physics because it serves as a nonrelativistic model for the principal part of the quark–quark interaction. First, we will use the envelope method to derive a simple formula for upper and lower bounds for all the eigenvalues $E_{n\ell}$, $n = 1, 2, 3, \ldots$, $\ell = 0, 1, 2, \ldots$. Because the linear potential, rather than the harmonic oscillator, is used as a basis for the upper bound, the new bounds are sharper than those of the earlier paper [20].

If we denote the eigenvalues of $H = -\omega\Delta - \alpha/r + \beta r$ by $E(\omega, \alpha, \beta)$ and consider a scale of change of the form $r' = r/\sigma$, and if we further choose $\sigma = \alpha/\omega$, then it is easy to show that

$$E(\omega, \alpha, \beta) = \alpha^2\omega^{-1}E(1, 1, \lambda) \qquad \lambda = \frac{\beta\omega^2}{\alpha^3}. \tag{2.1}$$

Thus it is sufficient to study the special case $H = -\Delta - 1/r + \lambda r$.

We need a solvable model which we can use as an envelope basis. The natural bases to use in the present context are the hydrogenic and linear potentials

$$h(r) = \mathrm{sgn}(q)r^q \qquad \text{where} \quad q = -1, 1. \tag{2.2}$$

The spectrum generated by the potential $h(r)$ is represented precisely by means of the semi-classical expression (1.1) as follows:

$$\mathcal{E}_{n\ell}(v) = \min_{s>0}\{s + v\bar{h}_{n\ell}(s)\} \tag{2.3}$$

where the 'kinetic potentials' $\bar{h}_{n\ell}(s)$ associated with the power-law potentials (1.1) are given [15] by

$$\bar{h}_{n\ell}(s) = \frac{2}{q}\left|\frac{q\mathcal{E}^{(q)}_{n\ell}}{2+q}\right|^{\frac{q+2}{2}} s^{-q/2} \tag{2.4}$$

and $\mathcal{E}^{(q)}_{n\ell}$ is the eigenvalue of $-\Delta + \mathrm{sgn}(q)r^q$ in $N$ dimensions, that is to say, corresponding to the pure-power potential with coupling 1. If we use the potential $h(r) = -\frac{1}{r}$ as an envelope basis, then $V(r) = -\frac{1}{r} + \lambda r = g\left(-\frac{1}{r}\right)$ implies $g$ is convex. And if we use the linear potential $h(r) = r$ as an envelope basis, then $g$ is concave. A weaker upper bound is provided by the harmonic oscillator $h(r) = r^2$, for which again $g(h)$ is convex.

For the power-law potentials $h(r) = \mathrm{sgn}(q)r^q$ we can simplify (2.3) by changing the minimization variable $s$ to $r$ defined in each case by the equation $\bar{h}_{n\ell}(s) = h(r)$ so that $g(h(r)) = f(r) = -\frac{1}{r} + \lambda r$. The minimization on the other hand, which yields eigenvalue approximations for the Hamiltonian $H = -\omega\Delta + f(r)$ ($\omega > 0$), can be expressed in the form

$$E^N_{n\ell} \approx \min_{r>0}\left\{\omega\left(\frac{P^N_{n\ell}(q)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \tag{2.5}$$

where

$$P^N_{n\ell}(q) = \left|E^{(q)}_{n\ell}\right|^{\frac{2+q}{2q}}\left[\frac{2}{2+q}\right]^{\frac{1}{q}}\left|\frac{q}{2+q}\right|^{\frac{1}{2}} \qquad q \neq 0. \tag{2.6}$$

We obtain a lower bound with $P^N_{n\ell}(-1) = (n + \ell + N/2 - 3/2)$ and the harmonic-oscillator upper bound (of [20]) with $P^N_{n\ell}(2) = 2n+\ell+N/2-2$, and a sharper upper bound with $P^N_{n\ell}(1)$; the $P^N_{n0}(1)$-numbers are provided in table 1 for $N = 2, \ldots, 12$. This table allows $\ell > 0$ since $P^N_{n\ell} = P^{N+2\ell}_{n0}$: it is clear that $E^N_{n\ell}(-1)$ and $E^N_{n\ell}(2)$, and the corresponding $P$-numbers, are invariant with respect to changes in $\ell$ and $N$ which preserve the sum $2\ell + N$; this symmetry is also true for $E^N_{n\ell}(1)$, indeed for *all* eigenvalues generated by a central potential. This property is the content of theorem 2, which we state and prove in section 4. We thus obtain the following energy bounds:

$$\min_{r>0}\left\{\left(\frac{P^N_{n\ell}(-1)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \leqslant E_{n\ell} \leqslant \min_{r>0}\left\{\left(\frac{P^N_{n\ell}(1)}{r}\right)^2 - \frac{1}{r} + \lambda r\right\} \tag{2.7}$$

for $n = 1, 2, 3, \ldots, \ell = 0, 1, 2, \ldots$. Consequently, the energy bounds are given by the parametric equations

$$E_{n\ell} = -\frac{1}{2\nu t} + \frac{3\lambda\mu t}{2} \tag{2.8a}$$

$$1 = \frac{t}{2\nu} + \frac{\lambda\mu t^3}{2} \qquad t = r P^N_{n\ell}(q) \qquad q = -1, 1 \tag{2.8b}$$

wherein the lower and upper bounds take the values $\nu = \mu = P^N_{n\ell}(-1)$ and $\nu = \mu = P^N_{n\ell}(1)$, respectively. It is interesting that we can actually solve equations (2.8*a*) and (2.8*b*) to obtain $\lambda$ as an explicit function of $E = E^N_{n\ell}$; the result namely is

$$\lambda = \frac{\left\{2(\nu E)^3 - \nu E^2\left[(1+3\nu^2 E)^{\frac{1}{2}} - 1\right]\right\}}{\mu\left[(1+3\nu^2 E)^{\frac{1}{2}} - 1\right]^3} \tag{2.9}$$

with $E \geqslant -\frac{1}{4\nu^2}$ (corresponding to $\lambda = 0$ for the pure hydrogenic spectrum). We emphasis that these bounds are valid for all the discrete eigenvalues in arbitrary dimension $N \geqslant 2$. The bounds are weak for $n > 1$, but at the bottom of each angular-momentum subspace $n = 1$ they are sharp and improve with increasing $\ell$, $N$ and $\lambda$. The lower bound for the bottom of each angular-momentum subspace ($n = 1$) can be improved by the use of the 'sum approximation' ([21] and section 3 below) in which $\nu = P^N_{n\ell}(1)$ (table 1) and $\mu = P^N_{n\ell}(-1) = (n + \ell + N/2 - 3/2)$. In figure 1 we exhibit these bounds for $n = 1$, $N = 3$ and $\ell = 0, 1, 2, 3$.

## 3. The sum approximation: lower bounds

We now consider potentials which are sums of terms. Since further generalizations easily follow, we first look at the problem of the sum of only two potential terms. We assume that each potential $vh^{(i)}(r)$ alone, when added to the kinetic-energy operator $-\Delta$, has a discrete eigenvalue $E$ at the bottom of the spectrum for sufficiently large coupling $v$. We note that the proof is unchanged if we restrict the problem to a given angular-momentum subspace labelled by $\ell$; our claim then concerns the bottom of the spectrum of $H$ in such a subspace; in the more general case, all the kinetic potentials would be labelled by $\ell$. We express our result in terms of kinetic potentials and prove (for the case $\ell = 0$) the following:

**Theorem 1.** *If $E$ is the bottom of the spectrum of the Hamiltonian $H = -\Delta + V$, 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 $\overline{V}$, that is to say*

$$\overline{V}(s) \geqslant \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s). \tag{3.1}$$

We shall now prove this theorem, which is in effect an optimized Weyl lower bound [22–24].

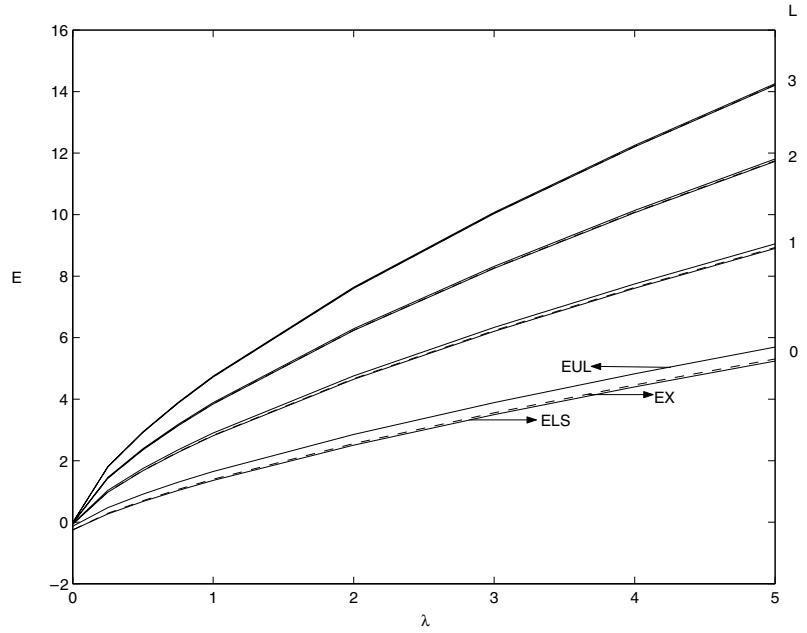


**Figure 1.** The eigenvalues $E(\lambda)$ of the Hamiltonian $H = -\Delta - 1/r + \lambda r$ for $N = 3$, $n = 1$ and $\ell = L = 0, 1, 2, 3$. The continuous curves show the upper bound EUL given by the envelope formula (2.9) with $\nu = \mu = P^3_{1\ell}(1)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P^3_{1\ell}(1)$ and $\mu = P^3_{1\ell}(-1)$. The dashed curve EX represents accurate numerical data.

**Proof.** From the definition (1.1) of kinetic potentials we have

$$\overline{V}(s) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi, V\psi) = \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,K\psi)=s}} (\psi, (h^{(1)} + h^{(2)})\psi).$$

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

$$\overline{V}(s) \geqslant \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} (\psi, h^{(1)}\psi) + \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1\\(\psi,-\Delta\psi)=s}} (\psi, h^{(2)}\psi) = \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s)$$

which inequality establishes the theorem. □

Another approach, which would eventually yield an alternative proof of the theorem, exhibits the relationship between theorem 1 and the classical Weyl lower bound [24–26] for the eigenvalues of the sum of two operators. Let us suppose that $\Psi$ is the exact normalized lowest eigenfunction of $H = -\Delta + V$, so that $H\Psi = E\Psi$. If the positive real parameter $w$ satisfies $0 < w < 1$, then $E = (\Psi, (-\Delta + V)\Psi)$ may be written as follows:

$$\begin{aligned} E &= w\left(\Psi, \left(-\Delta + \frac{1}{w}h^{(1)}(r)\right)\Psi\right) + (1-w)\left(\Psi, \left(-\Delta + \frac{1}{1-w}h^{(2)}(r)\right)\Psi\right) \\ &\geqslant w \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}} \left(\psi, \left(-\Delta + \frac{1}{w}h^{(1)}(r)\right)\psi\right) \\ &\quad + (1-w) \inf_{\substack{\psi\in\mathcal{D}(H)\\(\psi,\psi)=1}} \left(\psi, \left(-\Delta + \frac{1}{1-w}h^{(2)}(r)\right)\psi\right). \end{aligned}$$

That is to say, in terms of component kinetic potentials, we arrive at Weyl's inequality for the lowest eigenvalue $E$ of the operator sum $H$, where

$$H = -w\Delta + h^{(1)} + (-(1-w)\Delta + h^{(2)})$$

and we conclude

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

Since $w$ is an essentially free parameter in the last expression, we may optimize the Weyl lower bound with respect to the choice of $w$: 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 $s$,

$$E \geqslant \mathcal{E}(w) = ws_1(w) + (1-w)s_2(w) + \overline{h}^{(1)}(s_1(w)) + \overline{h}^{(2)}(s_2(w))$$

where

$$w = -\frac{\partial\overline{h}^{(1)}}{\partial s}(s_1(w)) \qquad \text{and} \qquad 1-w = -\frac{\partial\overline{h}^{(2)}}{\partial s}(s_2(w)).$$

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

$$E \geqslant \min_{s>0}\{s + \overline{h}^{(1)}(s) + \overline{h}^{(2)}(s)\}.$$

The kinetic-potential inequality of theorem 1 leads, of course, to the same energy lower bound: the optimization just performed above is therefore seen to be automatically 'built in' by the kinetic-potential 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 $H = -\Delta + \sum_i c_i h^{(i)}(r)$, $\{c_i > 0\}$ is provided by the formula

$$E \geqslant \min_{s>0}\left\{s + \sum_i c_i\overline{h}^{(i)}(s)\right\}. \tag{3.2}$$

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

Meanwhile, since the proof is identical, the bound is valid for the bottom of each angular-momentum subspace. Thus, more generally, the fundamental inequality becomes

$$\overline{V}_{1\ell}(s) \geqslant \overline{h}^{(1)}_{1\ell}(s) + \overline{h}^{(2)}_{1\ell}(s) \qquad \ell = 0, 1, 2, \ldots. \tag{3.3}$$

## 4. Generalized comparison theorems

The proof of our generalized comparison theorem (theorem 4) depends on monotone behaviour of the wavefunction induced by the assumed monotonicity of the potential. We are able to establish this monotonicity for the lowest eigenfunction in arbitrary many spatial dimensions $N \geqslant 1$. We shall then be able to apply our eigenvalue results to the case $\ell > 0$ and $n = 1$ because of theorem 2 which claims that $E^N_{n\ell} = E^{N+2\ell}_{n0}$; this general result is then employed in the special case $n = 1$.

**Theorem 2.** *Suppose that $H = -\Delta + V(r)$, where $V(r)$ is a central potential in $N \geqslant 2$ dimensions, has a discrete eigenvalue $E^N_{n\ell}$ with $n-1$ radial nodes in the angular-momentum subspace labelled by $\ell$, then $E^N_{n\ell} = E^{N+2\ell}_{n0}$.*

**Proof.** We suppose that $\psi$ is the eigenfunction corresponding to $E^N_{n\ell}$. We express $-\Delta$ in spherical coordinates [1–9] and write the radial eigenequation explicitly as

$$-\psi''(r) - \frac{(N-1)}{r}\psi'(r) + \frac{\ell(\ell+N-2)}{r^2}\psi(r) + V(r)\psi(r) = E^N_{n\ell}\psi(r).$$

If we now define the reduced radial function $u(r) \in L^2(R^+)$ by $\psi(r) = u(r)r^{-(N-1)/2}$, $r > 0$, and $u(0) = 0$, we obtain

$$-u''(r) + \left[\frac{\frac{(N-1)}{2}\frac{(N-3)}{2} + \ell(\ell+N-2)}{r^2} + V(r)\right]u(r) = E^N_{n\ell}u(r). \tag{4.1}$$

If we consider the spherically-symmetric potential $V(r)$ in $M$ dimensions such that $(M-1)(M-3)/4 = \ell(\ell+N-2) + (N-1)(N-3)/4$, we find that $M = 2\ell + N$. The eigenequation (4.1) then may be written equivalently as

$$-u''(r) + \left[\frac{\frac{(M-1)}{2}\frac{(M-3)}{2}}{r^2} + V(r)\right]u(r) = E^N_{n\ell}u(r). \tag{4.2}$$

It therefore follows immediately that $E^N_{n\ell} = E^M_{n0} = E^{2\ell+N}_{n0}$. □

For the purpose of our comparison theory we may now consider the special case $n = 1, \ell = 0$ in arbitrary $N \geqslant 1$ spatial dimensions: the energy results which we derive will then be applicable to the family of equivalent problems in $N'$ spatial dimensions with $n = 1$, $\ell > 0$ and $N = N' + 2\ell$. In order to prove an appropriate extension of the comparison theorem in $N$ dimensions, we shall first need to establish an elementary monotonicity property for the ground state $\psi$. We prove the following:

**Lemma.** *Suppose $\psi = \psi(r)$, $r = \|\boldsymbol{r}\|$, $\boldsymbol{r} \in R^N$, satisfies Schrödinger's equation*

$$H\psi(r) = (-\Delta + V(r))\psi(r) = E\psi(r) \tag{4.3}$$

*where $V(r)$ is a central potential which is monotone increasing for $r > 0$. Suppose that $E$ is a discrete eigenvalue at the bottom of the spectrum of the operator $H = -\Delta + V$, defined on some suitable domain $\mathcal{D}(H)$ in $L^2(R^N)$. Suppose that $\psi(r)$ has no nodes, so that, without loss of generality, we can assume $\psi(r) > 0, r > 0$. Then $\psi'(r) \leqslant 0, r > 0$.*

**Proof.** The proof for the case $N = 1$ is given in [19], equation (2.2). Henceforth, we shall now assume $N \geqslant 2$. If we express $-\Delta$ in spherical coordinates in $N$ spatial dimensions, then we have

$$-\Delta\psi + V\psi = E\psi \qquad -\frac{1}{t^{N-1}}\frac{\partial}{\partial t}\left(t^{N-1}\frac{\partial}{\partial t}\right)\psi(t) + V(t)\psi(t) = E\psi(t).$$

We now multiply both sides by $t^{N-1}$ and integrate with respect to $t$ to obtain

$$\psi'(r) = (1/r^{N-1})\int_0^r [V(t) - E]\psi(t)t^{N-1}\,\mathrm{d}t.$$

Since $V$ is monotone increasing, it follows that there is one point $\hat{r} > 0$ satisfying $V(\hat{r}) = E$. First, we prove that $s(r) = \int_{\hat{r}}^r [V(t) - E]\psi(t)t^{N-1}\,\mathrm{d}t$ is monotone increasing and bounded. For $t > \hat{r}$, $[V(t) - E]\psi(t)t^{N-1} > 0$, because $V(t) > E$ and hence $s(r)$ is increasing as $r \to \infty$. If there exists $r_1 < \infty$ such that $s(r_1) = -\int_0^{\hat{r}} [V(t) - E]\psi(t)t^{N-1}\,\mathrm{d}t$, then $\int_0^r [V(t) - E]\psi(t)t^{N-1}\,\mathrm{d}t > 0, r > r_1$ and $\psi'(r) > 0, r > r_1$; this contradicts the fact that the wavefunction $\psi(r)$ is positive and belongs to $L^2(R^N)$. This means that $\int_0^r [V(t) - E]\psi(t)t^{n-1}\,\mathrm{d}t \leqslant 0, \forall r > 0$. Consequently $\psi'(r) \leqslant 0, \forall r > 0$. □

We now consider two potentials $V_1(r)$ and $V_2(r)$, both of the type described above. We have two Schödinger equations for the respective ground states $\psi_1$ and $\psi_2$ and the corresponding discrete eigenvalues $E_1$ and $E_2$ at the bottoms of the spectra. Thus we have the following pair of eigenequations:

$$(-\Delta + V_1(r))\psi_1(r) = E_1\psi_1(r) \tag{4.4}$$

$$(-\Delta + V_2(r))\psi_2(r) = E_1\psi_2(r). \tag{4.5}$$

The radial wavefunctions in the present paper satisfy the normalization condition $\int_0^\infty \psi_i^2(r)r^{N-1}\,\mathrm{d}r < \infty$, $i = 1, 2$. With this notation and $N = 3$, theorem 3 of [19] becomes

**Theorem 3.**

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^2\,\mathrm{d}t \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \quad \Rightarrow \quad E_1 \leqslant E_2. \tag{4.6}$$

We shall now generalize this theorem to general dimension $N \geqslant 1$. We first establish a fundamental comparison formula (equation (4.7)) below.

By multiplying (4.4) by $\psi_2$ and (4.5) by $\psi_1$, and subtracting, we find

$$\psi_1\Delta\psi_2 - \psi_2\Delta\psi_1 + [V_1 - V_2]\psi_1\psi_2 = [E_1 - E_2]\psi_1\psi_2.$$

Integrating over $R^N$ and using the following identity:

$$\nabla \cdot (\psi_1\nabla\psi_2) = \nabla\psi_1 \cdot \nabla\psi_2 + \psi_1\nabla^2\psi_2$$

we find that

$$\int_{R^N} \nabla \cdot [\psi_1\nabla\psi_2 - \psi_2\nabla\psi_1]\,\mathrm{d}^N r + \int_{R^N} [V_1 - V_2]\psi_1\psi_2\,\mathrm{d}^N r = [E_1 - E_2]\int_{R^N} \psi_1\psi_2\,\mathrm{d}^N r.$$

Now by Gauss's theorem [27] we find that the first term becomes a surface integral which vanishes because $\psi_i \in L^2(R^N)$. In the remaining integrals the angular factors yield $2\pi^{N/2}/\Gamma(N/2)$. Hence we find

$$\frac{2\sqrt{\pi^N}}{\Gamma(N/2)}\int_0^\infty [V_1(r) - V_2(r)]\psi_1(r)\psi_2(r)r^{N-1}\,\mathrm{d}r$$

$$= \frac{2\sqrt{\pi^N}}{\Gamma(N/2)}[E_1 - E_2]\int_0^\infty \psi_1(r)\psi_2(r)r^{N-1}\,\mathrm{d}r$$

which implies

$$s = \int_0^\infty [V_1 - V_2]\psi_1\psi_2 r^{N-1}\,\mathrm{d}r = [E_1 - E_2]\int_0^\infty \psi_1\psi_2 r^{N-1}\,\mathrm{d}r. \tag{4.7}$$

Now we may state our generalization of theorem 3 to $N$ dimensions:

**Theorem 4.**

$$k(r) = \int_0^r (V_1(t) - V_2(t))\psi_i(t)t^{N-1}\,\mathrm{d}t \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \quad \Rightarrow \quad E_1 \leqslant E_2. \tag{4.8}$$

**Proof.** For definiteness we assume that $i = 1$; the proof is just the same with the other choice. We study the integral $s$ on the left side of (4.7). Integrating by parts we find that

$$s = [k(r)\psi_2(r)]_0^\infty - \int_0^\infty k(r)\psi_2'(r)r^{N-1}\,\mathrm{d}r. \tag{4.9}$$

Since $k(0) = \psi_2(\infty) = 0$, the first term vanishes, and $s$ is therefore equal to the negative of the integral of the right side of (4.9). But the integrand of this integral is positive because $k(r) \leqslant 0$, by hypothesis, and we know that $\psi_2'(r) \leqslant 0$ by the above lemma. This proves that $s \leqslant 0$. Consequently, by (4.7), we obtain $E_1 \leqslant E_2$. □

It may be difficult to apply theorem 4 in practice. Thus it would be helpful to establish some simpler sufficient conditions, depending on the number and nature of the crossings of the two comparison potentials. We treat three useful cases: theorem 5, one potential crossing, with the use of the wavefunction; theorem 6, two crossings and the use of the wavefunction; theorem 7, two crossings and no wavefunction used. In these theorems we shall assume that the integrals $\int_0^\infty (V_1(r) - V_2(r))\psi_i(r) r^{N-1}\,\mathrm{d}r$, $i = 1, 2$, exist for the given problem, even though we use at most one wavefunction factor.

**Theorem 5.** *If the potentials $V_1(r)$ and $V_2(r)$ cross exactly once for $r > 0$ at $r = r_1$, with,*

*(i)* $V_1(r) < V_2(r)$ $(0 < r < r_1)$ *and*
*(ii)* $\int_0^\infty [V_1(t) - V_2(t)]\psi_i(t) t^{N-1}\,\mathrm{d}t \leqslant 0$, $i = 1$ or 2,

*then*

$$k(r) = \int_0^r [V_1(t) - V_2(t)] t^{N-1} \psi_i(r)\,\mathrm{d}t \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \tag{4.10}$$

*from which $E_1 \leqslant E_2$ follows, by theorem 4.*

**Remark.** The best bound is obtained with the equality in hypothesis (ii).

**Proof of theorem 5.** We choose $i = 1$: the proof is identical for $i = 1$ or 2. First, we show that $s(r) = \int_{r_1}^r [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t$ is monotone increasing. For $t > r_1$, $s'(r) = [V_1(r) - V_2(r)]\psi_1(r) r^{N-1} > 0$, because $V_1(r) > V_2(r)$; hence $s(r)$ is increasing on $(r_1, \infty)$. Moreover, (ii) implies that the maximum value of $s(r)$ is reached at $r = \infty$, i.e. $s(r) \leqslant s(\infty)$; we have therefore

$$\int_0^\infty [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t$$
$$= \int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t + \int_{r_1}^\infty [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t \leqslant 0$$

and therefore

$$\lim_{r\to\infty} s(r) \leqslant -\int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t.$$

Now, we have the following two cases to consider:

*Case* 1. For $r < r_1$, $k(r) = \int_0^r [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t \leqslant 0$, since $V_1(t) < V_2(t)$ for $0 < t < r$.

*Case* 2. If $r > r_1$, then

$$k(r) = \int_0^{r_1} [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t + \int_{r_1}^r [V_1(t) - V_2(t)]\psi_1(t) t^{N-1}\,\mathrm{d}t$$
$$= s(r) - s(\infty) < 0.$$

Therefore, $k(r) \leqslant 0$, $\forall r > 0$. □

**Theorem 6.** *If the potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1, r = r_2$ $(r_1 < r_2)$ with*

*(i)* $V_1(r) < V_2(r)$ *for* $0 < r < r_1$ *and*

*(ii)* $\int_0^{r_2}(V_1(t)-V_2(t))\psi_i(t)t^{N-1}\,\mathrm{d}t \leqslant 0$, $i = 1$ or 2,

*then*

$$k(r) = \int_0^r (V_1(t)-V_2(t))\psi_i(t)t^{N-1}\,\mathrm{d}t \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \tag{4.11}$$

*from which* $E_1 \leqslant E_2$ *follows, by theorem 4.*

**Remark.** The best bound is obtained with the equality in hypothesis (ii).

**Proof of theorem 6.** We choose $i = 1$; the proof is the same if $i = 2$. $k'(r) = (V_1(r)-V_2(r))r^{N-1}\psi_1(r)$, now $k(0) = 0$, $k'(r) < 0, 0 < r < r_1$ implies $k(r) < 0$, $0 < r < r_1$. Next, $k(r_2) = 0$, $k'(r) > 0, r_1 < r < r_2$ implies $k(r) < 0, r_1 < r < r_2$. Lastly, $k(r_2) = 0, k'(r) < 0, r > r_2$ implies $k(r) \leqslant 0, r > r_2$. □

**Theorem 7.** *If the potentials* $V_1(r)$ *and* $V_2(r)$ *cross twice for* $r > 0$ *at* $r = r_1, r_2$ $(r_1 < r_2)$ *with*

*(i)* $V_1(r) < V_2(r)$ *for* $0 < r < r_1$ *and*
*(ii)* $\int_0^{r_2}(V_1(t)-V_2(t))t^{N-1}\,\mathrm{d}t \leqslant 0$

*then*

$$k(r) = \int_0^r [V_1(t)-V_2(t)]\psi_i(t)t^{N-1}\,\mathrm{d}t \leqslant 0 \qquad \forall r > 0 \quad i = 1 \text{ or } 2 \tag{4.12}$$

*from which* $E_1 < E_2$ *follows, by theorem 4.*

**Remark.** The best bound is obtained with the equality in hypothesis (ii).

**Proof of theorem 7.** We choose $i = 1$: the proof is identical if $i = 2$. Define $h(r) = \int_0^r (V_1(t)-V_2(t))t^{N-1}\,\mathrm{d}t$, the proof of theorem 3 shows that $h(r) \leqslant 0, 0 \leqslant r \leqslant r_2$. But

$$\begin{aligned} k(r) &= \int_0^r (V_1(t)-V_2(t))\psi_1(t)t^{N-1}\,\mathrm{d}t \\ &= [h(t)\psi_1(t)]_0^r - \int_0^r h(t)\psi_1'(t)\,\mathrm{d}t \\ &= h(r)\psi_1(r) - \int_0^r h(t)\psi_1'(t)\,\mathrm{d}t < 0 \end{aligned}$$

meanwhile, $k'(r) < 0, r > r_2$. Therefore, $k(r) \leqslant 0, \forall r > 0$. □

## 5. Application to the Coulomb-plus-linear potential

As an example, we employ the comparison theorems to improve the bounds obtained in section 2 for the eigenvalues corresponding to the Coulomb-plus-linear potential $V(r) = -a/r + br$, where $a$ and $b$ are positive coupling parameters. For the upper bound we use as a comparison potential the shifted linear potential $h(r) = -\alpha + \beta r$, where $\alpha$ and $\beta > 0$. We allow the potentials $V(r)$ and $h(r)$ to cross over exactly twice, as illustrated in figure 2. Let $A$ and $B$ represent the absolute values of the areas (or of the $\psi$-weighted areas) between the potentials. We vary $\alpha$ and $\beta$ so that $A = B$, and thereafter theorems 5 and 6 imply $E^V \leqslant E^h$. For simplicity of derivation of the upper-bound formula, we will use theorem 7 (with no use of the wavefunction $\psi$). Thus we have two equations to solve in this case,

$$-\frac{a}{r} + br = -\alpha + \beta r \qquad \int_0^r \left[-\frac{a}{t} + bt + \alpha - \beta t\right] t^{N-1}\,\mathrm{d}t = 0$$

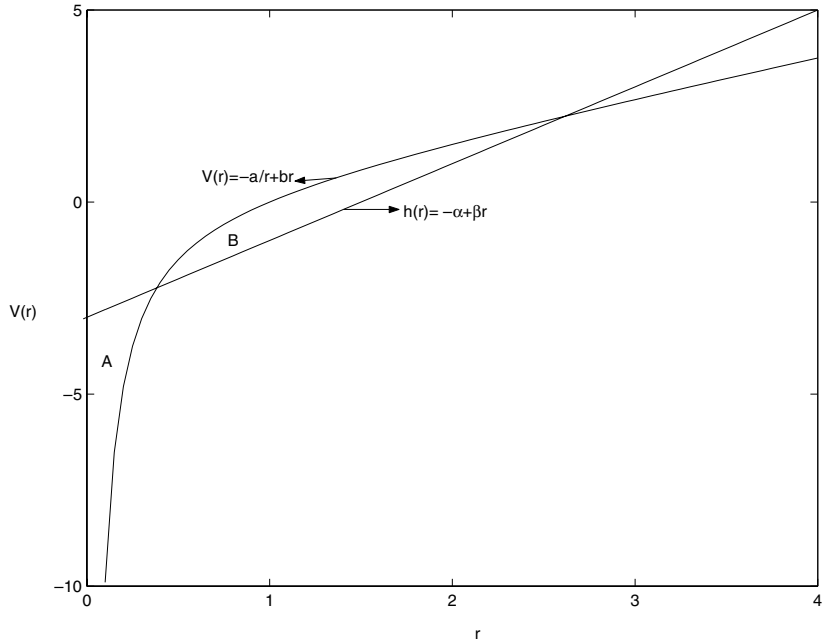


**Figure 2.** The linear potential $h(r) = \alpha r + \beta$ used to estimate an upper bound for the eigenvalues of the Coulomb-plus-linear potential $V(r) = -a/r + br$. $A$ and $B$ are the absolute values of the inter-potential areas (or $\psi$-weighted areas). We vary $\alpha$ and $\beta$ so that $A = B$, and thereafter theorems 5 and 6 imply $E^V \leqslant E^h$.

where $r = r_2$ is the second crossing point. These reduce to the quadratic equations

$$(\beta - b)r^2 - \alpha r + a = 0 \qquad N(N-1)(b-\beta)r^2 + \alpha(N-1)(N+1)r - aN(N+1) = 0$$

with the simultaneous solution $r = \frac{2aN}{\alpha(N-1)}$. Now the best upper bound is obtained after minimizing with respect to $r$, giving

$$E^U = \min_{r>0}\left\{-\left(\frac{2aN}{(N-1)r}\right) + \left(\frac{(N+1)a}{(N-1)r^2} + b\right)^{\frac{2}{3}} \mathcal{E}^N(1)\right\}. \tag{5.1}$$

At the expense of further complication, the use of $\psi_1(r)$ (the Airy function) would lower this upper bound.

Similarly, to improve our lower bound, we allow the Coulomb-plus-linear potential to intersect twice with the hydrogenic potential $h(r) = -\frac{\alpha}{r} + \beta$, with the exact wavefunction solution $\psi = \mathrm{e}^{-\alpha r/(N-1)}$ and the exact energy $E^h = \beta - \alpha^2/(N-1)^2$, where $\alpha$ and $\beta$ are positive parameters. Again, let $A$ and $B$ represent the absolute values of the areas (or of the $\psi$-weighted areas) between the potentials. We vary $\alpha$ and $\beta$ so that $A = B$, as illustrated in figure 3, and thereafter theorems 5 and 6 imply $E^h \leqslant E^V$. Subsequently, we obtain the lower bound (without $\psi$) by solving the following three equations:

$$\frac{-a}{t} + bt = -\frac{\alpha}{t} + \beta \qquad \int_0^t \left[\frac{-a}{r} + br + \frac{\alpha}{r} - \beta\right] r^{N-1}\,\mathrm{d}r = 0$$

$$E^L = \min_{t>0}\{\beta - (\alpha/(N-1))^2\}. \tag{5.2}$$

For the case $a = 1$ and $b = 1$, we compare in figure 4 the upper and lower bounds obtained by means of the classical envelope method and by the comparison theorems introduced in

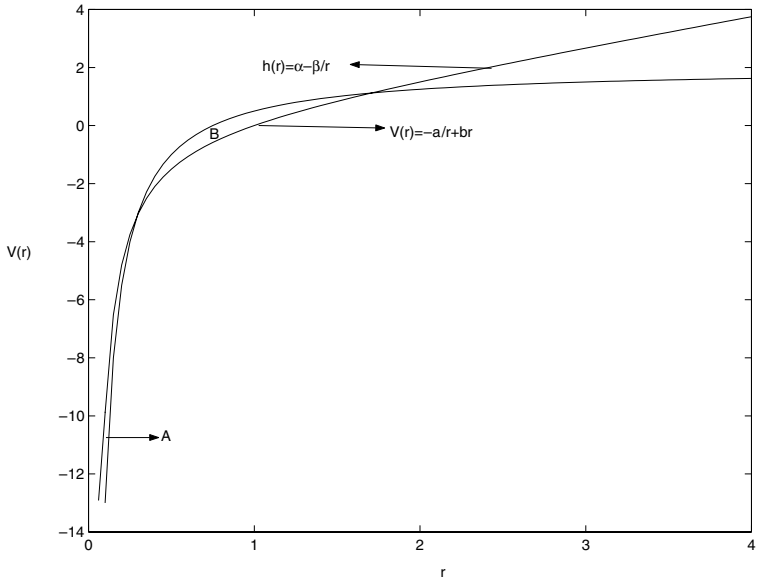


**Figure 3.** The hydrogenic potential $h(r) = -\alpha/r + \beta$ used to estimate a lower bound for the eigenvalues of the Coulomb-plus-linear potential $V(r) = -a/r + br$. $A$ and $B$ are the absolute values of the inter-potential areas (or $\psi$-weighted areas). We vary $\alpha$ and $\beta$ so that $A = B$, and thereafter theorems 5 and 6 imply $E^h \leqslant E^V$.

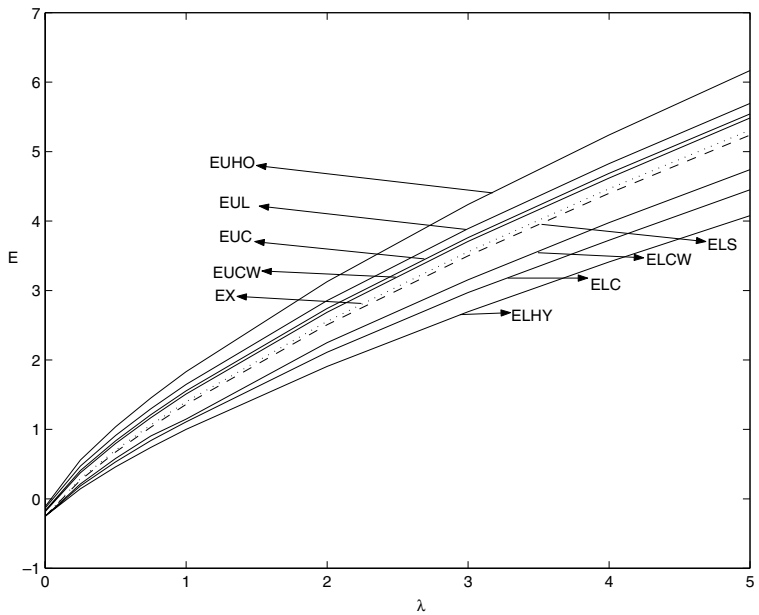


**Figure 4.** We compare the bounds for $E(\lambda)$, where $E(\lambda)$ is the ground-state eigenvalue $(n = 1, \ell = 0)$ of the Hamiltonian $H = -\Delta - 1/r + \lambda r$. The upper bounds (full lines) are by harmonic-oscillator tangents EUHO, linear tangents EUL, linear chords EUC and linear chords with the wavefunction EUCW. The lower bounds (lower full lines) are by hydrogenic tangents ELHY, hydrogenic chords ELC and hydrogenic chords with the wavefunction ELCW. The dashed curve ELS represents the lower bound given by the sum approximation. Accurate numerical data (dotted curve) EX are shown for comparison.

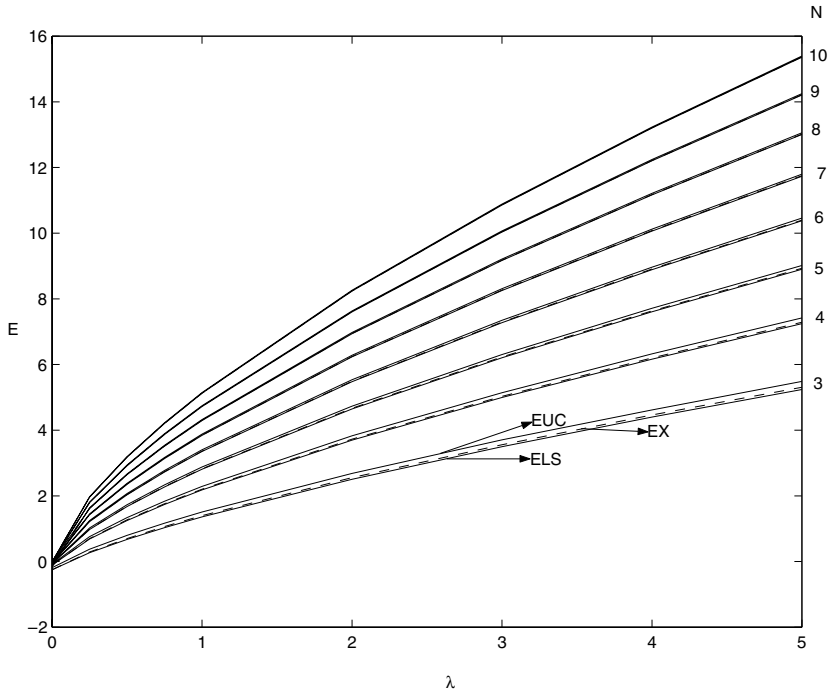


**Figure 5.** Bounds on the eigenvalues $E^N_{10}(\lambda)$ corresponding to the Coulomb-plus-linear potential $V(r) = -1/r + \lambda r$ in $N$ dimensions. Upper bounds EUC by the generalized comparison theorem, lower bounds ELS by the sum approximation and accurate numerical data (dashed line) for $n = 1$, $\ell = 0$ and $N = 3, 4, \ldots, 7$. By theorem 2 we know that the same curves also apply to $\ell > 0$ since $E^N_{1\ell} = E^{N+2\ell}_{10}$.

section 3. Generalizations to cases where there are large numbers of potential crossings are discussed in [37].

## 6. Conclusion

Our proof of the lower bound for the bottom of the spectrum of the operator $H = -\Delta + V^{(1)}(r) + V^{(2)}(r)$, based on kinetic potentials, is more compact and direct than the original proof, and is valid in $N$ dimensions; the principal steps of the earlier proof are repeated because they show that the final result is equivalent to an optimization of the classical theorem of Weyl. The generalized comparison theorem is proved in the present paper for all dimensions $N$, whereas, in its original form, it required two distinct theorems, for $N = 1$ and $N = 3$. Moreover, we are now able to apply the results to the bottom of each angular-momentum subspace since we have proved that this energy is identical to the lowest eigenvalue of a higher-dimensional problem, in $R^{N+2\ell}$. Meanwhile, in order to be practical, weaker sufficient conditions were sought which would guarantee in a simple way that the comparison potentials cross over so as to imply definite spectral ordering. These results greatly clarify the application of the generalized comparison theorem to specific problems.

The Coulomb-plus-linear problem provides a convenient example on which to test the effectiveness of the energy bounds. At the same time it offers an opportunity to sharpen

an earlier energy-bound formula for this problem, and to extend its validity to all $N \geqslant 2$ dimensions. For most of the parameter space of the problem, the energy bounds provided by this formula for the bottom of each angular-momentum subspace ($n = 1$) are accurate to a few per cent and, as we have shown, they become sharper with increasing $N$ or $\ell$. If the sum approximation is capriciously applied also to the higher discrete eigenvalues $n > 1$, the resulting *ad hoc* approximation formula continues to give very accurate estimates, which, however, are no longer bounds. What additional conditions might guarantee bounds from such a formula is an interesting open question.

## Acknowledgment

Partial financial support of this work under grant no GP3438 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

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