Refining the comparison theorem of quantum mechanics

1992 J. Phys. A: Math. Gen. 25 4459

(http://iopscience.iop.org/0305-4470/25/16/021)

J. Phys. A: Math. Gen. 25 (1992) 4459-4469. Printed in the UK

Refining the comparison theorem of quantum mechanics

Richard L Hall

Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Blvd W, Montreal, Quebec, Canada H3G 1M8

Received 17 January 1992

Abstract. If two potentials $V_1(x)$ and $V_2(x)$ are ordered $V_1 < V_2$, then the comparison theorem tells us that the corresponding Schrödinger eigenvalues are ordered $E_1 < E_2$. We present some simple conditions which allow us to predict such spectral ordering for the ground state, even when the graphs of the potentials cross over. As illustrations, the truncated quartic oscillator and the Yukawa potential are studied. By allowing Coulomb 'tangents' to cross over the Yukawa in various ways, we are able to improve earlier energy upper bounds which we had obtained by representing the Yukawa potential as a smooth transformation of the Coulomb potential, and also to augment these results with lower bounds.

1. Introduction

We consider a single particle which obeys non-relativistic quantum mechanics and moves in the attractive symmetric potential $V(x)$. In suitable units the Hamiltonian H of this problem is given by

$$H = K + V(x) \tag{1.1}$$

where $K = -\Delta$ is the kinetic-energy operator. It is a well known consequence of the min-max characterization [1-3] of Schrödinger eigenvalues that, if we compare two potentials $V_1(x)$ and $V_2(x)$, and if $V_1 < V_2$, then all the respective pairs of eigenvalues are similarly ordered $E_1 < E_2$. This result is often called the comparison theorem of quantum mechanics.

If the graphs of two potentials cross over, then there seems little reason to hope that any simple spectral relationship could exist. For example, the power-law potentials $|x|$, x^2, and x^4 shown in figure 1 cross over at $|x| = 1$, and the (ground-state) Schrödinger eigenvalues (in one dimension) are respectively $E_1 = 1.018\,79$, $E_2 = 1$ and $E_4 = 1.060\,36$. In a previous paper [4] we studied the eigenvalues E_q corresponding to the potentials $|x|^q$ by representing one power potential as a transformation of another; in this way we could claim that the rather complicated function E_q was, in a sense, 'understood'. However, the pure power laws are a very particular family of potentials and we should like to explore the possibility of more general results.

If we were to truncate the above three power-law potentials so that $V(x) = 1$ for $|x| > 1$, then the potentials would be clearly ordered $V_4 < V_2 < V_1$ and the comparison theorem would immediately tell us that $E_4 < E_2 < E_1$. In figure 2 we show the graphs of these same three power-law potentials truncated now at $V(x) = 1.75$ so that the potentials cross over at $|x| = 1$. It turns out that the eigenvalues become respectively $E_4 = 0.830\,67$, $E_2 = 0.903\,76$ and $E_1 = 0.992\,77$. On the basis of some very simple tests,

0305-4470/92/164459+11$04.50

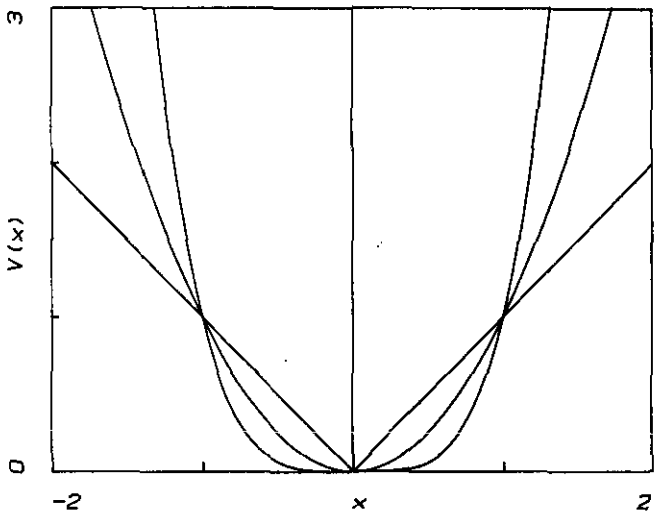

Figure 1. Three power-law potentials $|x|$, x^2, and x^4 which cross over at $|x|=1$. It is not easy to predict that the corresponding ground-state eigenvalues E_1, E_2, and E_4 are ordered $E_2<E_1<E_4$.

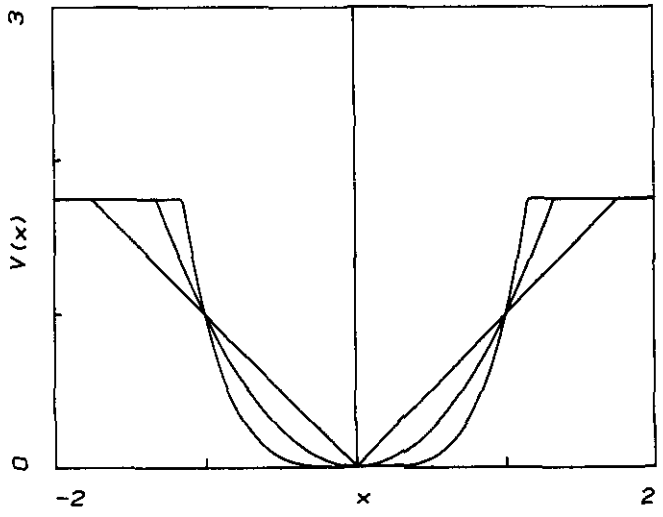

Figure 2. Three power-law potentials $|x|$, x^2, and x^4, truncated so that $V(x)\leqslant 1.75$. Even though these potentials cross over at $|x|=1$, the new comparison theory predicts the correct spectral ordering $E_4<E_2<E_1$.

the theory which we develop in this paper allows us to predict such spectral ordering, at least for the ground-state energy. Consequently, many of the comparison approximations which we commonly use in quantum mechanics can immediately be improved.

There is one central idea that generates all the new energy bounds: we replace the condition $V_1<V_2$ with the weaker condition $U_1<U_2$, where $U(x)=\int_0^x V(t)\rho(t)\,\mathrm{d}t$, and ρ is a suitable positive non-increasing function. In section 2 we discuss some general assumptions and results for problems in one dimension, and we use the choices $\rho=1$, and also $\rho=\psi_i$, where ψ_i is the ground state corresponding to V_i. In section 4 we extend these results to problems in three dimensions.

In sections 3 and 5 we consider two examples, the truncated quartic oscillator, and the Yukawa potential. Upper and lower energy bounds for the truncated quartic oscillator are found by comparing it with the soluble square-well potential. In a previous paper [5] we expressed the Yukawa potential as a smooth concave transformation of the Coulomb potential, and we used this 'envelope representation' to estimate the Yukawa eigenvalues. Since we can now allow the Coulomb 'tangents' to cross over the Yukawa potential in various ways, this leads to improved upper energy bounds and also to some new lower bounds.

2. Assumptions and basic general results in one dimension

We consider the problem in one spatial dimension and we assume that the real potential $V(x)$ is (i) finite, (ii) symmetric about $x=0$, and (iii) attractive, that is to say, monotone increasing on $[0,\infty)$. The ground-state ψ satisfies Schrödinger's equation:

$$-\psi''(x)+V(x)\psi(x)=E\psi(x). \tag{2.1}$$

Since V is real and we are considering only bound states, we may assume that the wavefunctions are real. Because the ground state has no nodes, we may assume without loss of generality that the (otherwise un-normalized) ground state satisfies $\psi(0)=1$. Consequently $\psi(x)>0$, for all x. Since, by symmetry, the solutions are either even or odd, the positive ground state ψ must be even. We may therefore conclude that $\psi'(0)=0$. We have assumed that $V(x)$ is finite in order to avoid the (interesting) pathologies [6, 7] of potentials like $-|x|^{-1}$. Our results now hinge on various kinds of monotone behaviour.

Our first claim is that the ground state ψ, like the potential, is monotone on $[0,\infty)$, but decreasing; that is to say,

$$\psi'(x)\leqslant 0 \qquad x\in[0,\infty). \tag{2.2}$$

We show this by the following elementary argument. Since $V(x)$ is monotone increasing on $[0,\infty)$, and E cannot be below $V(0)$, without loss of generality, we may suppose that $V(a)=E$, for some $a>0$. From (2.1) we find that $\psi''(x)\leqslant 0$ on $[0,a)$ and $\psi''(x)\geqslant 0$ on (a,∞). Since we have $\psi'(0)=0$, it follows that $\psi'(x)<0$ on $[0,a]$. Since ψ is square integrable, we know that $\psi'(\infty)=0$. Hence, on the interval $[a,\infty)$, $\psi'(x)$ must increase to zero. Consequently, $\psi'(x)\leqslant 0$ for all $x>0$, as claimed.

We now consider two potentials $V_1(x)$ and $V_2(x)$ both of the type described above. We have two Schrödinger equations for the respective ground states ψ_1 and ψ_2 and the corresponding eigenvalues E_1 and E_2:

$$-\psi_1''(x)+V_1(x)\psi_1(x)=E_1\psi_1(x) \tag{2.3}$$

$$-\psi_2''(x)+V_2(x)\psi_2(x)=E_2\psi_2(x). \tag{2.4}$$

If we multiply (2.3) by ψ_2 and (2.4) by ψ_1, integrate over $[0,\infty)$, and subtract, we find:

$$J=\int_0^\infty [V_1(x)-V_2(x)]\psi_1(x)\psi_2(x)\,dx=[E_1-E_2]\int_0^\infty \psi_1(x)\psi_2(x)\,dx. \tag{2.5}$$

Since $\psi_1(x)$ and $\psi_2(x)$ are positive, the integral on the right is positive. Hence conditions which guarantee that the integral J on the left is (say) negative, imply that $E_1<E_2$.

The two main results of this section are obtained from (2.5) in this way. In fact, we claim the following:

Theorem 1.

$$g(x)=\int_0^x [V_1(t)-V_2(t)]\,dt \leqslant 0 \qquad \forall x \Rightarrow E_1 \leqslant E_2 \tag{2.6}$$

and

Theorem 2.

$$h(x)=\int_0^x [V_1(t)-V_2(t)]\psi_i(t)\,dt \leqslant 0 \qquad \forall x \Rightarrow E_1 \leqslant E_2 \tag{2.7}$$

where $i=1$ or 2.

We shall first prove (2.7). For definiteness we assume that $i=1$; the proof is just the same with the other choice. We study the integral J on the left side of (2.5). Integrating by parts we find

$$J=[h(x)\psi_2(x)]_0^\infty - \int_0^\infty h(x)\psi_2'(x)\,dx. \tag{2.8}$$

Since $h(0)=\psi_2(\infty)=0$, the first term vanishes, and J is therefore equal to the negative of integral on the right side of (2.8). But the integrand of this integral is positive because $h(x)\leqslant 0$, by hypothesis, and we know that $\psi_2'(x)\leqslant 0$ from (2.2). This proves that $J\leqslant 0$. Consequently, by (2.5), we know that $E_1\leqslant E_2$, and this proves (2.7). The proof of (2.6) follows the above proof exactly: we simply replace $\psi_1(x)$ everywhere by the positive decreasing product $\psi_1(x)\psi_2(x)$, and we replace $h(x)$ by $g(x)$, and then all the steps go through similarly.

If the two potentials do not cross over each other in *very* complicated ways, we can greatly simplify the conditions of our main results; such simplifications are useful in applications. For example, suppose that the potentials cross over as is illustrated in figure 3. Let A, B, and C represent the absolute values of the areas (or of the

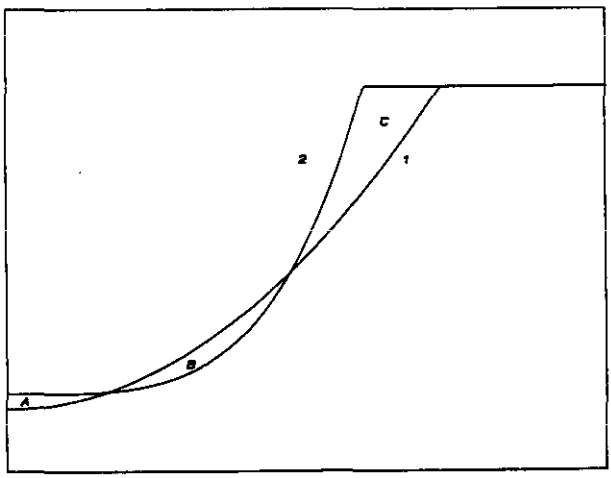

Figure 3. Two attractive symmetric potentials V_1 and V_2 shown for $x>0$. A, B, and C are the absolute values of the inter-potential areas (or ψ_i-weighted areas). If $A\geqslant B$, and $C\geqslant 0$, then, according to theorem 1 (or 2), the potential ordering $V_1<V_2$ on the region A is sufficient to guarantee the spectral ordering $E_1<E_2$.

ψ_i-weighted areas) between the potentials. Then, if $A \geqslant B$, we know that $g(x) < 0, \forall x$ (or $h(x) < 0, \forall x$), and therefore that $E_1 \leqslant E_2$. Intuitively, the situation may be described as follows: if V_1 is beneath V_2 (as soon as they differ), then, because of the monotonicity of the potentials and of the probability density for $x > 0$, min–max favours V_1, provided that the potential cross-over is not too drastic. Of course, the theorems are needed to control the cross-overs so that we can guarantee spectral inequalities. Theorem 2 is stronger than theorem 1 because the condition, albeit requiring knowledge of the exact wavefunction ψ_i, is weaker: this follows because ψ_1 is decreasing on $[0, \infty)$ so that the potentials can cross over 'even more' and still lead to $E_1 \leqslant E_2$.

As an immediate illustration of theorem 1, we return to the three power-law potentials mentioned in the introduction, namely, $V_1(x) = |x|$, $V_2(x) = x^2$, $V_4(x) = x^4$, truncated at $V(x) = 1.75$, and shown in figure 2. Simple calculations show that $\int_0^{1.75} [V_2(x) - V_1(x)]\, dx = -0.012\,105$, and $\int_0^{1.75} [V_4(x) - V_2(x)]\, dx = -0.068\,02$: these negative numbers predict the eigenvalue inequalities $E_2 < E_1$ and $E_4 < E_2$, which indeed are correct. Theorem 1 will be further illustrated in section 3, and the study of the Yukawa potential in section 5 makes very effective use of an extension of theorem 2 to three dimensions which we establish in section 4.

3. The truncated quartic oscillator

We now study the example of the truncated quartic potential defined by

$$V_1(x) = \begin{cases} v(x^4 - 1) & |x| \leqslant 1 \\ 0 & |x| > 1 \end{cases} \tag{3.1}$$

where v is a positive coupling parameter. The comparison potentials are provided by the two-parameter family of square-wells defined by

$$V_2(x) = \begin{cases} -vd & |x| \leqslant a \\ 0 & |x| > a \end{cases} \tag{3.2}$$

where a and d are positive parameters. In order to make the potential comparisons, we use $v = 1$. The idea here is that the soluble square-well problem can be used to estimate the eigenvalue corresponding to the truncated quartic oscillator. We consider the three situations illustrated in figure 4. If we set $a = d = 1$, as shown in figure 4(a), then we immediately get lower bounds ES by the usual comparison theorem. If we

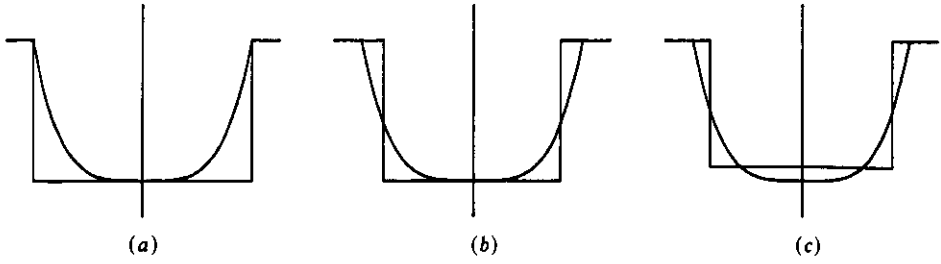

Figure 4. The truncated quartic oscillator with energy E is compared to various square wells with energies $E_\square$. In (a) the usual comparison theorem tells us that $E > E_\square$. In (b) and (c) we have respectively $E > E_\square$ and $E < E_\square$, even though the potentials now cross over.

set $d = 1$ and $a = 0.8$, then the potential cross-overs lead to two equal-area inter-potential regions: consequently we know that $EL = E_2 \leqslant E_1$; it is not difficult to show that EL is the best possible lower bound of this type. Finally, if we allow cross-overs as in figure 4(c), and set $d = 1 - a^4/5$, for $a \in [0, 1]$, then the first two inter-potential areas are equal and it follows, again by theorem 1, that $E_1 \leqslant E_2(a)$. The best upper bound EU of this collection is found by minimizing $E_2(a)$ with respect to $a \in [0, 1]$, for each choice of the coupling v. We exhibit our results in table 1, along with accurate values EN found by integrating Schrödinger's equation numerically.

Table 1. Ground-state eigenvalues for the quartic oscillator $V(x) = v(x^4 - 1)$, truncated at $V(x) = 1.75$. The comparison potentials are the square wells shown respectively in figures 4(a, b, c). The corresponding approximations are: ES derived from the usual comparison theorem; lower and upper bounds EL and EU resulting from the new comparison theory; and accurate numerical values EN.

v	ES	EL	EN	EU
5	−3.853	−3.479	−3.373	−3.127
10	−8.593	−8.059	−7.812	−7.298
15	−13.453	−12.824	−12.443	−11.703
20	−18.361	−17.666	−17.160	−16.224
25	−23.293	−22.549	−21.926	−20.817
30	−28.241	−27.458	−26.724	−25.460
35	−33.199	−32.384	−31.545	−30.139
40	−38.164	−37.322	−36.384	−34.847

4. Problems in three dimensions

We work in three spatial dimensions and prove an appropriate extension of theorem 2. The ground state $\psi(r)$ corresponding to a spherically-symmetric potential $V(r)$ in three dimensions satisfies the radial equation:

$$-\psi''(r) + V(r)\psi(r) = E\psi(r). \tag{4.1}$$

The potential V is again assumed to be monotone increasing for $r > 0$ and, in order to avoid complications which may arise with extremely singular potentials, we shall also assume that a number γ exists such that

$$\lim_{r \to 0} rV(r) = \gamma. \tag{4.2}$$

The boundary conditions of the problem may then be written [8, 9]

$$\psi(0) = 0 \qquad \int_0^\infty \psi^2(x)\,dx < \infty. \tag{4.3}$$

It is also convenient to 'normalize' the radial wavefunction by simply setting $\psi'(0) = 1$.

Just as for the problem in one dimension, we shall first need to establish an elementary monotonicity property for the ground state ψ. The result we need in this case is

$$\left(\frac{\psi(r)}{r}\right)' < 0 \qquad r > 0. \tag{4.4}$$

We may establish this result by the following argument. Since V is monotone increasing, we see from (4.1) that ψ has only one turning point, say $r=a$. On the interval $[0, a)$ therefore, ψ'' is negative, and furthermore, ψ' must continue to decrease beneath zero because ψ must eventually vanish. Hence, $\psi'(b)=0$ for some $b<a$. Now consider the interval $[0, b]$: on this interval, ψ is concave and lies therefore below its tangents and above its chords; consequently, $0<\psi'(r)<\psi(r)/r$. Meanwhile, for $r>b$, $\psi'(r)<0$, so, again, $\psi'(r)<\psi(r)/r$, since the ground state ψ, which is node free, is itself positive. This establishes (4.4). We note that it follows from (4.1) and (4.2) that the initial value of $(\psi(r)/r)'$ is $\psi''(0)/2=\gamma/2$.

If we now follow section 2 and write down the two Schrödinger equations, multiply by the respective wavefunctions, and integrate, we find again:

$$I=\int_0^\infty [V_1(r)-V_2(r)]\psi_1(r)\psi_2(r)\,dr=[E_1-E_2]\int_0^\infty \psi_1(r)\psi_2(r)\,dr. \quad (4.5)$$

We may now state our generalization of theorem 2 to three dimensions:

Theorem 3.

$$k(r)=\int_0^r [V_1(t)-V_2(t)]t\psi_i(t)\,dt\leqslant 0 \qquad \forall r\Rightarrow E_1\leqslant E_2 \quad (4.6)$$

where $i=1$ or 2.

We shall now prove (4.6). For definiteness we assume that $i=1$; the proof is just the same with the other choice. We integrate the integral for I in (4.5) by parts to obtain

$$I=\left[k(r)\frac{\psi_2(r)}{r}\right]_0^\infty-\int_0^\infty k(r)\left(\frac{\psi_2(r)}{r}\right)'dr. \quad (4.7)$$

Since $k(0)=\psi_2(\infty)=0$, we see that the first term on the right-side of (4.7) vanishes. Meanwhile, the integrand of the second term is positive: this is so because $k(r)$ is negative, by hypothesis, and the other factor is negative by (4.4). Consequently $I\leqslant 0$. This proves (4.6). We note that (4.6) can be viewed also as a comparison theorem for the eigenvalues corresponding to the first excited state of the problem in one spatial dimension.

As we found in section 2, we can easily obtain simplifications to the negativity condition of this theorem. For example, if V_1 is less than V_2, as soon as they differ, and if the potentials cross over only once, then we have the simpler condition:

$$k(\infty)=\int_0^\infty [V_1(t)-V_2(t)]t\psi_i(t)\,dt\leqslant 0\Rightarrow E_1\leqslant E_2 \quad (4.8)$$

with $i=1$ or 2. Similarly, if V_1 is less than V_2, as soon as they differ, and if the potentials cross over exactly twice, and the second cross-over point is r_2, then we have:

$$k(r_2)=\int_0^{r_2} [V_1(t)-V_2(t)]t\psi_i(t)\,dt\leqslant 0\Rightarrow E_1\leqslant E_2 \quad (4.9)$$

with $i=1$ or 2. These sufficient conditions are, of course, much more convenient to work with in practice than (4.6). If in the first example we set $k(\infty)=0$, say, then (4.8) becomes a constraint on the choice of the comparison potential; and similarly for the second example. We shall employ these ideas to study the Yukawa potential in the next section.

5. The Yukawa and Coulomb potentials

For the familiar (but shifted) hydrogenic atom we have the exact solution to (4.1) given by:

$$V_1(r) = v(\beta - \alpha/r) \qquad \psi_1(r) = r\,e^{-v\alpha r/2} \qquad E_1 = v\beta - (v\alpha)^2/4 \tag{5.1}$$

where v, α, and β are positive parameters. This will be our comparison problem. Our main concern in this section is, however, the Yukawa potential given by

$$V_2(r) = -v\frac{e^{-r}}{r}. \tag{5.2}$$

In our earlier paper [5] we showed that the Yukawa potential is a concave transformation g of $-1/r$. Tangents to g were then shifted Coulomb potentials, like V_1 in (5.1), and, for each v, one of these provided a best upper bound to E_2 via the usual comparison theorem. By using theorem 3, we can now allow the potentials to cross over, and then we can optimize by choosing the best Coulomb potential in the sense that it leads to the best upper energy bound.

We organize the problem in the following way. We let the Coulomb potential start out above the Yukawa (as soon as they differ), we let these potentials cross over twice, and we let $r = x$ be the second intersection point. We use x as a parameter, and then we optimize with respect to x. Note that v cancels from some of the equations but it remains in the Coulomb wavefunction ψ_1. We define the weighted-difference function $d(r) = (V_2(r) - V_1(r))\psi_1(r)r/v$ explicitly as follows:

$$d(r) = \left(-\frac{e^{-r}}{r} - \left(\beta - \frac{\alpha}{r}\right)\right) r^2\,e^{-v\alpha r/2}. \tag{5.3}$$

We follow essentially the general example (4.9), with the potential subscripts interchanged. The three equations we have to solve for the upper bound therefore become:

$$e^{-x} + \beta x - \alpha = 0 \tag{5.4}$$

$$\int_0^x d(r)\,dr = 0 \tag{5.5}$$

$$EU = \min_{x>0}\,(v\beta - (v\alpha/2)^2). \tag{5.6}$$

In the case $v = 15$ we find, for example, $\alpha = 0.989\,28$, $\beta = 0.843\,82$ and $x = 0.241\,39$: the corresponding graph of the weighted-difference function $d(r)$ is shown in figure 5. In our previous theory (the potential envelope method [5]) the condition for tangency of the Coulomb and Yukawa potentials was used instead of (5.5). The earlier upper bounds EC are necessarily weaker than EU because the tangential Coulomb potentials are now shifted down to produce the controlled cross-overs. The results which we obtain are shown in table 2, along with accurate values EN which we have found numerically, and a lower bound EL to be discussed below.

We can also use the new theory to find a lower-bound formula. We set $\alpha = 1$, so that the potentials agree at $r = 0$, and we allow only one cross-over, at $r = x$. This forces the Coulomb potential to lie below the Yukawa as soon as they differ, that is to say, on the interval $(0, x)$. We then follow the general example (4.8) and require that

$$\int_0^\infty d(r)\,dr = 0. \tag{5.7}$$

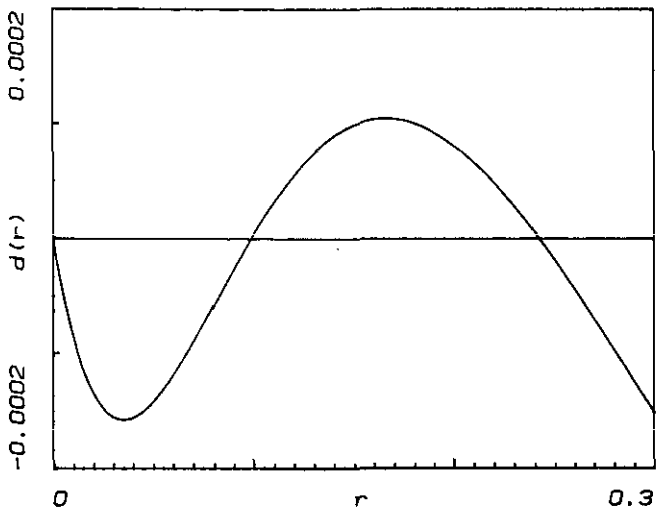

Figure 5. For the Yukawa potential $V_2(r) = -15e^{-r}/r$, the upper Coulomb envelope V_C of the earlier theory [5] is pulled down $V_C \to V_1$ to cross V_2 so that the integral $\int_0^x d(r)\,dr = 0$, where x is the second cross-over point and $d(r) = (V_2(r) - V_1(r))\psi_1(r)r$. According to theorem 3, this is sufficient to guarantee that $E_2 < E_1$, even though the potentials intersect.

Table 2. Ground-state eigenvalues for the Yukawa potential $V(r) = -v\,e^{-r}/r$. *EC* are upper bounds obtained by the envelope method [5], *EL* and *EU* are the lower and upper bounds resulting from the new comparison theory, and *EN* are accurate numerical values. In the new theory, the Yukawa potential is allowed to cross over the Coulomb comparison potential; consequently $EU < EC$.

v	*EL*	*EN*	*EU*	*EC*
15	−43.793	−42.636	−42.394	−42.211
30	−197.754	−196.439	−196.173	−195.979
70	−1157.890	−1156.473	−1156.192	−1155.991

These two conditions immediately yield the relation

$$\beta = \frac{v}{4}[1-(1+2/v)^{-2}] \tag{5.8}$$

and finally, from (5.1), we find:

$$EL = -\frac{v^2}{4}(1+2/v)^{-2}. \tag{5.9}$$

For $v > \sim 31.5$, this lower bound is better than the lower bound of the inequalities

$$-\frac{v^2}{4}(1-2/v)^2 - (0.056)v \leqslant E \leqslant -\frac{v^2}{4}(1-2/v)^2 \tag{5.10}$$

which we found earlier [5, 10]. It may be of interest to generalize the simple formula (5.9) by allowing a range parameter λ in the Yukawa potential. We find

$$-\Delta - v\frac{e^{-\lambda r}}{r} \to E > EL = -\frac{v^2}{4}(1+2\lambda/v)^{-2}. \tag{5.11}$$

In either limits, λ small, or v large, we recover the Coulomb result $-v^2/4$ from this formula.

We obtain a more physical illustration if, following McEnnan *et al* [11], we choose a set of Yukawa parameters suitable for atoms with atomic number Z by the assignments:

$$\lambda = \lambda_0 \alpha_0 Z^{1/3} \qquad v = 2Z^{2/3}/\lambda_0 \tag{5.12}$$

where $\lambda_0 = 1.13$, $\alpha_0 = (137.037)^{-1}$, and the energy in keV is given by the relation: Energy $= (255.4846)E\lambda^2$. Some results which we have obtained using the methods described above are shown in table 3, along with numerical values *EN* from [11]. The improvement of *EU* over the earlier Coulomb-envelope approximations *EC* is evident from this data.

Table 3. Ground-state eigenvalues in keV for the Yukawa potential applied to the outer electrons of atoms with atomic number Z. The approximations *EC*, *EL*, and *EU* are as in table 2; the numerical values *EN* are from McEnnan *et al* [11].

Z	*EL*	*EN*	*EU*	*EC*
13	−1.585	−1.488	−1.466	−1.450
36	−14.476	−14.24	−14.196	−14.16
79	−75.371	−74.95	−74.861	−74.80

6. Conclusion

We have shown in this paper that the condition $V_1 < V_2$, which implies the spectral inequality $E_1 < E_2$, can be replaced with the weaker condition $U_1 < U_2$, where $U_i(x) = \int_0^x V_i(t)\rho(t)\,dt$, $i = 1, 2$, and ρ is a suitable positive non-increasing function. The Yukawa-Coulomb illustration demonstrates that our results apply to the first two eigenvalues of the corresponding problem in one dimension. By suitably choosing the comparison potentials for a given problem, we can generate both lower and upper energy bounds, and we can also optimize the bounds over classes of comparison potentials that meet the sufficient condition $U_1 < U_2$. Because these results depend on monotonic behaviour inherited by the wavefunctions from the potentials, we suspect that the generalization of these methods to higher eigenvalues, beyond the first two, may not easily be achieved.

It has become so comfortable today to solve problems numerically that a strong selection pressure is now applied on analytical methods: if they are very complicated, then we may run out of patience with them and turn instead to the computer. The analytical approach remains particularly valuable if it leads to results which are either very general, or very simple. We believe that the results of this paper have both these aspects. They supply new general conditions for the relation between a potential and the Schrödinger spectrum it generates, and they provide some simple ways in which the spectrum may be approximated in terms of the spectra associated with suitable soluble comparison potentials.

Acknowledgment

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

References

[1] Reed M and Simon B 1981 *Methods of Modern Mathematical Physics IV: Analysis of Operators* (New York: Academic) p 76
[2] Thirring W 1981 *A Course in Mathematical Physics 3: Quantum Mechanics of Atoms and Molecules* (Berlin: Springer) p 152
[3] Epstein B 1970 *Linear Functional Analysis: Introduction to Lebesgue Integration and Infinite-Dimensional Problems* (Philadelphia, PA: Saunders)
[4] Hall R L 1989 *Phys. Rev.* A **39** 5500
[5] Hall R L 1985 *Phys. Rev.* A **32** 14
[6] Boya L J, Kmiecik M and Bohm A 1988 *Phys. Rev.* A **37** 3567
[7] Núñez Yépez H N, Vargas C A and Salas Brito A L 1989 *Phys. Rev.* A **39** 4306
[8] Messiah A 1961 *Quantum Mechanics* vol I (Amsterdam: North-Holland) p 350
[9] Armstrong B H and Power E A 1963 *Am. J. Phys.* **31** 262
[10] Hall R L 1992 *J. Phys. A: Math. Gen.* **25** 1373
[11] McEnnan J, Kissel L and Pratt R H 1976 *Phys. Rev.* A **13** 532