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CONSTRAINTS ON THE TOTAL AND KINETIC ENERGY OF GROUND STATES
IN A CLASS OF POTENTIAL MODELS

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ABSTRACT

It is shown that the ground state energy in a central potential is a concave (convex) function of angular momentum ℓ when this potential is a concave (convex) function of r^2 . A result stronger than concavity is obtained when the Laplacian of the potential is negative. New bounds in the kinetic energy of these states are derived in terms of energy differences and for s-states in terms of the wave function at the origin. These bounds can be used to give good estimates of the ground state energies for power law potentials.

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1. - INTRODUCTION

In recent work [1] we have obtained constraints on states bound by a central potential $V(r)$ belonging to a class for which energy-level ordering theorems may be proved. We will consider here in particular the energy $E(0, \ell)$ of the ground state of angular momentum ℓ . In Section 2 we will demonstrate a previous result [2] that $E(0, \ell)$ is a convex (concave) function of ℓ when the potential $V(r)$ is a convex (concave) function of r^2 , and strengthen it when the Laplacian of $V(r)$ is negative for all $r > 0$.

An integrated form of the concavity condition is

$$E(0, \ell+1) - E(0, \ell) < E(0, \ell) - E(0, \ell-1). \quad (1.1)$$

This inequality can also be tightened when $V(r)$ has negative Laplacian, as will be demonstrated in Section 2 using a variational method applied by one of us (A.M.) in an earlier proof [3] of the concavity of $E(0, \ell)$.

Bounds on the kinetic energy $\langle T \rangle_{0, \ell}$ and mean square radii $\langle r^2 \rangle_{0, \ell}$ for the above ground states of angular momentum ℓ , have been obtained in earlier work by one of us (A.M.) in collaboration with Bertlmann [4]. They are in terms of energy differences between adjacent states, and in some cases only hold for integer (physical) values of ℓ as they have been derived using sum rules. In Section 3 we demonstrate how they may be extended to general non-negative ℓ and tightened for certain classes of potentials.

Finally in Section 4, improved upper and lower bounds on the wave function at the origin of the S-wave ground state are obtained which depend only on the expectation value of the kinetic energy for this state. As demonstrated by one of us (A.K.C.) previously [5], this type of bound can be useful in determining quark mass differences using experimental estimates of the above value of the wave function from the leptonic decay rates of quarkonium via the Van Royen-Weisskopf formula [6].

There are several reasons why it is of interest to study the above types of constraints. Firstly they enable one to obtain a general impression of the distribution of energy levels for given classes of potentials and vice versa, e.g., as discussed in Ref. [2], the distribution of the lowest energy levels indicate that the quark-antiquark potential is not a convex function of r^2 . Also for specific potentials such as simple powers of r , precise estimates can be given for $E(0, \ell)$ without detailed numerical evaluation. Some results were presented in Ref. [1] and some improved estimates are given in Section 3.

Finally, the bounds we have obtained have the merit of being rigorous. We feel that they should be published so that future investigations of potential models may have them to hand.

2. - THE CONVEXITY AND CONCAVITY OF $E(0, \ell)$

In a previous work [1] we considered the two following classes of potentials.

Set A: $Vr > 0$, one of the following conditions hold:

- i) $D_{\alpha} V(r) > 0$, $1 < \alpha < 2$; $V(r) > 0$,
- ii) $D_{\alpha} V(r) > 0$, $\alpha < 1$; $V(r) < 0$,
- iii) $[r^2 \frac{d^2}{dr^2} + (3-2\alpha) \frac{d}{dr}] V(r) > 0$, $1 < \alpha < 2$; $\frac{dV}{dr} > 0$,

where

$$D_{\alpha} V(r) \equiv \frac{d^2 V}{dr^2} + (5-3\alpha) \frac{1}{r} \frac{dV}{dr} + 2(1-\alpha)(2-\alpha)V(r)/r^2$$

(the special cases $\alpha = 1$, $\alpha = 2$ correspond to potentials convex in $1/r$ and r^2 respectively.)

Set B: $Vr > 0$, one of the following conditions hold:

- i) $D_{\alpha} V(r) < 0$, $\alpha > 2$ or $\alpha < 1$; $V(r) > 0$,
- ii) $D_{\alpha} V(r) < 0$, $1 < \alpha < 2$; $V(r) < 0$,
- iii) $[r^2 \frac{d^2}{dr^2} + (3-2\alpha) \frac{d}{dr}] V(r) < 0$, $\alpha > 2$.

We showed that if $V(r)$ belongs to set $\begin{bmatrix} A \\ B \end{bmatrix}$ for $\alpha = \beta$, then for $\ell > 0$ and $n > k$ such that all integrals concerned exist,

$$\begin{aligned} & [2\ell + 1 + \beta + k\beta] \left\langle r^{2(\beta-1)+n\beta} \right\rangle_{0,\ell} < \left\langle r^{2(\beta-1)+(k-1)\beta} \right\rangle_{0,\ell} \\ & \sum \left[2\ell + 1 + \beta + n\beta \right] \left\langle r^{2(\beta-1)+k\beta} \right\rangle_{0,\ell} < \left\langle r^{2(\beta-1)+(n-1)\beta} \right\rangle_{0,\ell}. \end{aligned} \quad (2.1)$$

where

$$\langle r^k \rangle_{0,l} = \int_0^\infty u_{0,l}^2(r) r^k dr,$$

and $u_{0,l}(r)$ is the reduced wave function for the ground state of angular momentum l .

In the following we will need to use a limiting form of (2.1) obtained by setting $n = k + \delta$ and letting $\delta \rightarrow 0_+$. This gives,

$$\frac{\langle r^{2(\beta-1)+k\beta} \log r \rangle_{0,l}}{\langle r^{2(\beta-1)+k\beta} \rangle_{0,l}} \leq \frac{\langle r^{2(\beta-1)+(k-1)\beta} \log r \rangle_{0,l}}{\langle r^{2(\beta-1)+(k-1)\beta} \rangle_{0,l}} + [2l+1+\beta+k\beta] \quad (2.2)$$

when $V(r)$ is in set $[B^A]$ for $\alpha = \beta$. The moment inequalities follow from the inequalities [7],

$$-\left[\frac{w'_{0,\lambda}(z)}{w_{0,\lambda}(z)} \right]' \geq \frac{\lambda+1}{z^2}, \quad (2.3)$$

which hold for $V(r)$ in set $[B^A]$ where $z \equiv r^\alpha$, $\lambda \equiv (2l-\alpha+1)/2\alpha$ and $w_{0,\lambda}(z) \equiv [r^{\alpha-1}]^{\frac{1}{2}} u_{0,l}(r)$. In the original variables, (2.3) takes the form,

$$-\left[\frac{u'_{0,l}(r)}{r^{\alpha-1} u_{0,l}(r)} \right]' \geq \frac{(l+1)\alpha}{r^{1+\alpha}}, \quad (2.4)$$

when $V(r)$ is in set $[B^A]$ for a given value for α .

The inequalities (2.4) hold for all $r, l \geq 0$ and will now be used to prove a lemma to the main theorem of this paper:

Lemma (2.1)

If $V(r)$ is in set $[B^A]$ for a given value of $\alpha > 1$, then

$$J(\alpha) \geq - \frac{2l+3-\alpha}{\alpha-1} \int_0^\infty u_{0,l}(r) \frac{\partial u_{0,l}(r)}{\partial l} \frac{dr}{r^\alpha}, \quad (2.5)$$

where

$$J(\alpha) = \frac{1}{\alpha-1} \int_0^\infty r^{1-\alpha} \int_0^r \left[\frac{2\ell+1}{r'^2} - \frac{\partial E(0,\ell)}{\partial \ell} \right] u_{0,\ell}^2(r') dr' dr. \quad (2.6)$$

Proof The reduced wave function satisfies,

$$-u_{0,\ell}'' + \frac{\ell(\ell+1)}{r^2} u_{0,\ell} + V(r) u_{0,\ell} = E(0,\ell) u_{0,\ell}. \quad (2.7)$$

Taking the limit of the Wronskian of two solutions of (2.7) for neighbouring values of ℓ ,

$$u_{0,\ell}(r) \frac{\partial u_{0,\ell+1}(r)}{\partial \ell} - u_{0,\ell+1}(r) \frac{\partial u_{0,\ell}(r)}{\partial \ell} = \int_0^r \left[\frac{2\ell+1}{r'^2} - \frac{\partial E(0,\ell)}{\partial \ell} \right] u_{0,\ell}^2(r') dr'. \quad (2.8)$$

Since the right-hand side is positive, $[(\partial u_{0,\ell}(r)/\partial \ell)/u_{0,\ell}(r)]$ is an increasing function of r and has one zero in $(0,\infty)$. As

$$\int_0^\infty u_{0,\ell}(r) \frac{\partial u_{0,\ell}}{\partial \ell}(r) dr = 0,$$

therefore

$$\int_0^r u_{0,\ell}(r') \frac{\partial u_{0,\ell}(r')}{\partial \ell} dr' < 0 ; \quad r > 0. \quad (2.9)$$

Using (2.4),

$$\begin{aligned} - \int_0^\infty u_{0,\ell}'(r) \frac{\partial u_{0,\ell}(r)}{\partial \ell} \frac{dr}{r^{\alpha-1}} &= \int_0^\infty \frac{d}{dr} \left[\frac{u_{0,\ell}'(r)}{r^{\alpha-1} u_{0,\ell}(r)} \right] \left[\int_0^r u_{0,\ell}(r') \frac{\partial u_{0,\ell}(r')}{\partial \ell} dr' \right] dr \\ &\geq - \int_0^\infty \frac{(\ell+1)\alpha}{r^{1+\alpha}} \left[\int_0^r u_{0,\ell}(r') \frac{\partial u_{0,\ell}(r')}{\partial \ell} dr' \right] dr \\ &= -(\ell+1) \int_0^\infty u_{0,\ell}(r) \frac{\partial u_{0,\ell}(r)}{\partial \ell} \frac{dr}{r^\alpha} \end{aligned} \quad (2.10)$$

for potentials $V(r)$ in set $[A_B]$ for given α . Using (2.8) after integrating by parts,

$$\int_0^\infty u_{0,\ell}(r) \frac{\partial u_{0,\ell}(r)}{\partial \ell} \frac{dr}{r^\alpha} = \frac{2}{\alpha-1} \int_0^\infty u_{0,\ell}'(r) \frac{\partial u_{0,\ell}(r)}{\partial \ell} \frac{dr}{r^{\alpha-1}} + J(\alpha), \quad (2.11)$$

where $\alpha > 1$ and $J(\alpha)$ is defined in (2.5). Using (2.10) in (2.11) gives immediately the required result.

We are now in position to prove the following:

Theorem (2.1)

(a) If
$$\frac{d}{dr} \left[\frac{1}{r} \frac{dV}{dr} \right] \geq 0, \quad \forall r > 0,$$

then

$$\frac{\partial^2 E(0, l)}{\partial l^2} \geq 0, \quad l \geq -\frac{1}{2}. \quad (2.12)$$

(b) If
$$\frac{d}{dr} \left[r^2 \frac{dV}{dr} \right] \leq 0, \quad \frac{dV}{dr} \geq 0, \quad \forall r > 0,$$

then

$$\frac{\partial^2 E(0, l)}{\partial l^2} + \frac{1}{l+1} \frac{\partial E(0, l)}{\partial l} \leq 0, \quad l \geq 0. \quad (2.13)$$

Proof Integrating the definition of $J(2)$ in (2.6) by parts,

$$J(2) = -(2l+1) \left[\langle r^{-2} \log r \rangle_{0, l} \langle 1 \rangle_{0, l} - \langle r^{-2} \rangle_{0, l} \langle \log r \rangle_{0, l} \right] \quad (2.14)$$

The potentials satisfying the conditions (a) in set $\left[\frac{A}{B} \right]$ for $\alpha = 2$. Therefore from (2.5),

$$(2l+1) \int_0^\infty u_{0, l}(r) \frac{\partial u_{0, l}(r)}{\partial l} \frac{dr}{r^2} \geq -J(2) \geq -\langle r^{-2} \rangle_{0, l}. \quad (2.15)$$

The right-hand inequality follows from (2.14) and (2.2) with $\beta = 2$, $k = -1$.

However,

$$\frac{\partial^2 E(0, l)}{\partial l^2} = 2 \int_0^\infty u_{0, l}^2(r) \frac{dr}{r^2} + 2(2l+1) \int_0^\infty u_{0, l}(r) \frac{\partial u_{0, l}(r)}{\partial l} \frac{dr}{r^2}. \quad (2.16)$$

The result (2.12) then follows on using (2.15) in (2.16).

The potentials satisfying the conditions in (b) are in set B for $\alpha = 2$ and $\alpha = 1$. Now (2.2) may be used twice with $\beta = 1$ and first $k = 0$ and then $k = -1$ to give,

$$J(2) \geq \langle r^{-2} \rangle_{0,l} \left[1 + \frac{2l+1}{2l+2} \right] \quad (2.17)$$

In this case, using (2.16)

$$\frac{\partial^2 E(0,l)}{\partial l^2} \leq 2 \langle r^{-2} \rangle_{0,l} - 2 J(2) \leq -\frac{2l+1}{l+1} \langle r^{-2} \rangle_{0,l} = -\frac{1}{l+1} \frac{\partial E(0,l)}{\partial l},$$

and the result (2.13) follows.

The inequalities (2.12) are equivalent to the convexity (concavity) of $E(0,l)$ for potentials $V(r)$ which are convex (concave) in r^2 . They cannot be improved for the class of potentials considered in (a) since the inequalities are saturated by the harmonic oscillator potential for which $d/dr[(1/r)(dV/dr)] = 0$, $\forall r > 0$. The Coulomb potential $V(r) = -1/r$ satisfies the conditions for case (b) and we know for this potential that,

$$\frac{\partial^2 E(0,l)}{\partial l^2} + \frac{3}{2(l+1)} \frac{\partial E(0,l)}{\partial l} = 0. \quad (2.18)$$

Therefore (2.13) is not saturated and there may be still scope for improvement in case (b).

An integrated form of concavity of $E(0,l)$ in l is given in (1.1) and holds for potentials which are concave in r^2 . We now modify a previous argument [3] to show that (1.1) can be improved for potentials with negative Laplacian:

Theorem (2.3)

If
$$\frac{d}{dr} \left[r^2 \frac{dV}{dr} \right] \leq 0, \quad \forall r > 0,$$

then

$$[E(0, l+1) - E(0, l)] \leq \left[\frac{l}{l+2} \right] [E(0, l) - E(0, l-1)]. \quad (2.19)$$

Proof Following the discussion in Ref. [3], we use [7] $v(r) = r u_{0,l}(r)$ as a trial wave function in the variational estimate of $E(0, l+1)$ and obtain the inequality

$$\begin{aligned}
 E(0, l+1) &\leq \int_0^\infty [r'^2 + (l+1)(l+2)r^2/r^2 + V(r)r^2] dr / \int_0^\infty r^2 dr \\
 &= \int_0^\infty [r^2 u_{0,l}'^2 + (l+1)(l+2) u_{0,l}^2 + V(r) r^2 u_{0,l}^2] dr / \langle r^2 \rangle_{0,l} \\
 &= \left\{ \int_0^\infty r^2 u_{0,l} \left[-u_{0,l}'' + \frac{l(l+1)}{r^2} u_{0,l} + V(r) u_{0,l} \right] dr + (2l+3) \int_0^\infty u_{0,l}^2 dr \right\} / \langle r^2 \rangle_{0,l} \\
 &= E(0, l) + (2l+3) / \langle r^2 \rangle_{0,l}.
 \end{aligned} \tag{2.20}$$

Notice that this inequality is valid for arbitrary potentials. Similarly by taking $v = u_{0,l}(r)/r$ as a trial wave function to estimate $E_{0,l}$ we obtain the inequality,

$$E(0, l-1) \leq E(0, l) - (2l-1) \frac{\langle r^{-4} \rangle_{0,l}}{\langle r^{-2} \rangle_{0,l}} \tag{2.21}$$

Previously the lower inequality (2.1) with $\beta = 2$ was used to prove from (2.20) and (2.21) that (1.1) holds if $V(r)$ is concave in r^2 . However, if $d/dr[r^2(dv/dr)] < 0$, $Vr > 0$, the lower moment inequalities (2.1) can be used with $\beta = 1$. Take this value of β and $n = 2$, $k = -3$, then this lower inequality gives,

$$\langle r^2 \rangle_{0,l} \langle r^{-4} \rangle_{0,l} \geq \langle r \rangle_{0,l} \langle r^{-3} \rangle_{0,l} \frac{2l+4}{2l-1}, \tag{2.22}$$

while with $n = 1$, $k = -2$

$$\langle r \rangle_{0,l} \langle r^{-3} \rangle_{0,l} \geq \langle 1 \rangle_{0,l} \langle r^{-2} \rangle_{0,l} \frac{2l+3}{2l} \tag{2.23}$$

We take λ to be a positive parameter to be adjusted later and use (2.20) to (2.23) to prove the sequence of inequalities,

$$\begin{aligned}
 &[E(0, l-1) - E(0, l)] + \lambda [E(0, l+1) - E(0, l)] \\
 &\leq -(2l-1) \langle r^{-4} \rangle_{0,l} / \langle r^{-2} \rangle_{0,l} + \lambda (2l+3) \langle 1 \rangle_{0,l} / \langle r^2 \rangle_{0,l} \\
 &\leq \frac{\langle 1 \rangle_{0,l}}{\langle r^2 \rangle_{0,l}} \left\{ -(2l-1) \frac{2l+4}{2l-1} \frac{2l+3}{2l} + \lambda (2l+3) \right\}
 \end{aligned} \tag{2.24}$$

By appropriate choice of λ , the right-hand side can be put equal to zero and (2.19) follows.

Inequality (2.19) is an appreciable improvement on (1.1) especially for small λ . However, (2.19) is again not "saturated" for the Coulomb potential where for example when $\lambda = 1$ the ratio of the left-hand side to right-hand side is 5/9. Here again there is the possibility for improvement.

3. - BOUNDS ON $\langle T \rangle_{0,\lambda}$ and $\langle r^2 \rangle_{0,\lambda}$

In a previous work one of us (A.M.) and Bertlmann [4] obtained the following lower bounds on the average value of the kinetic energy for the ground state S and P waves:

$$\langle T \rangle_{0,0} \geq \frac{3}{4} [E(0,1) - E(0,0)] \quad (3.1a)$$

$$\langle T \rangle_{0,1} \geq \frac{5}{4} [E(0,2) - E(0,1)] \quad (3.1b)$$

These inequalities hold for general central potentials. The method used to derive them involved sum rules over physical states therefore could not be generalized to non-integer values of λ . We demonstrate now how they can indeed be generalized to all $\lambda > 0$.

Theorem (3.1)

For general potentials $V(r)$ and all $\lambda > 0$

$$\langle T \rangle_{0,\lambda} \geq \frac{2\lambda+3}{4} [E(0,\lambda+1) - E(0,\lambda)] \quad (3.2)$$

Proof We have with the usual normalization $\int_0^\infty u_{0,\lambda}^2 dr = 1$,

$$\begin{aligned} \langle T \rangle_{0,\lambda} &= \int_0^\infty \left[u_{0,\lambda}'^2 + \frac{\lambda(\lambda+1)}{r^2} u_{0,\lambda}^2 \right] dr \\ &= \int_0^\infty \left[u_{0,\lambda}' - \frac{\lambda+1}{r} u_{0,\lambda} \right]^2 dr \end{aligned} \quad (3.3)$$

Consider now

$$\begin{aligned} I(\lambda) &= \int_0^\infty \left[u_{0,\lambda}' - (\lambda+1) \frac{u_{0,\lambda}}{r} - \lambda r u_{0,\lambda} \right]^2 dr = \\ &= \int_0^\infty \left[u_{0,\lambda}' - (\lambda+1) \frac{u_{0,\lambda}}{r} \right]^2 dr - 2\lambda \int_0^\infty \left[r u_{0,\lambda}' u_{0,\lambda}' - (\lambda+1) u_{0,\lambda}^2 \right] dr + \lambda^2 \int_0^\infty r^2 u_{0,\lambda}^2 dr \end{aligned} \quad (3.4)$$

$$= \langle T \rangle_{0,l} + \lambda (2l+3) + \lambda^2 \langle r^2 \rangle_{0,l}. \quad (3.5)$$

Since $I(\lambda) \geq 0$ for all real λ ,

$$4\langle T \rangle_{0,l} \langle r^2 \rangle_{0,l} \geq (2l+3)^2. \quad (3.6)$$

Then using (2.20) in the form,

$$E(0, l+1) - E(0, l) < (2l+3) / \langle r^2 \rangle_{0,l} \quad (3.7)$$

we obtain the required inequality. It cannot be improved for general potentials since it becomes an equality for the harmonic oscillator potential.

Corresponding upper bounds to $\langle T \rangle_{0,l}$ in terms of energy differences can be obtained for certain classes of potentials as the following:

Theorem (3.2)

If

$$\frac{d}{dr} \left[\frac{1}{r} \frac{dW}{dr} \right] < 0, \quad \forall r > 0,$$

then, for all $l \geq 1$,

$$\langle T \rangle_{0,l} \leq \frac{2l+3}{4} [E(0, l) - E(0, l-1)]. \quad (3.8)$$

Proof The above class of potentials are in Set B defined in Section 2 for $\alpha = 2$. Therefore from inequality (3.6) of Ref. [1]

$$\langle T \rangle_{0,l} \leq \frac{2l+3}{4} \frac{\partial E(0, l)}{\partial l} \quad (3.9)$$

$$\leq \frac{2l+3}{4} [E(0, l) - E(0, l-1)] \quad (3.10)$$

where in the last step we have used the concavity of $E(0, l)$.

This upper bound complements the lower bound (3.2) and is again "saturated" by the harmonic oscillator potential. The factor multiplying the energy differences is the same in the upper and lower bounds. By restricting the class of potentials

further, upper and lower bounds with the same energy difference but different multiplying factors may be obtained. An example is given by the following result:

Corollary (3.2)

If $\frac{d}{dr} \left[\frac{1}{r} \frac{dV}{dr} \right] \leq 0$ and $\frac{d}{dr} \left[r^2 \frac{dV}{dr} \right] > 0, \forall r > 0$, then

$$\langle T \rangle_{0,l} \leq \frac{2l+9}{4} [E(0, l+1) - E(0, l)] \quad (3.11)$$

Proof As discussed earlier in Section 2, $\int_0^r \frac{\partial u_{0,l}(r')}{\partial l} u_{0,l}(r') dr' < 0$,

Therefore

$$\begin{aligned} \frac{\partial E(0, l)}{\partial l} + \frac{\partial \langle T \rangle_{0,l}}{\partial l} &= 2 \int_0^\infty \left[r \frac{dV}{dr} + V(r) \right] u_{0,l} \frac{\partial u_{0,l}}{\partial l} dr \\ &= -2 \int_0^\infty \frac{d}{dr} \left[r \frac{dV}{dr} + V(r) \right] \int_0^\infty u_{0,l}(r') \frac{\partial u_{0,l}(r')}{\partial l} dr' \quad (3.12) \\ &\geq 0. \end{aligned}$$

Integrating (3.12) over $(l, l+1)$,

$$\langle T \rangle_{0,l} < E(0, l+1) - E(0, l) + \langle T \rangle_{0, l+1} \quad (3.13)$$

Using (3.8) with $l \rightarrow l+1$ gives immediately (3.11). Unfortunately this inequality is not saturated by the Coulomb potential for small l . An improved inequality may be obtained by further restricting the class of potential.

Corollary (3.2a)

If $\frac{d}{dr} \left[\frac{1}{r} \frac{dV}{dr} \right] < 0$ and $\frac{d}{dr} \left[r \frac{dV}{dr} \right] > 0$,

then

$$\langle T \rangle_{0,l} \leq \frac{2l+5}{4} [E(0, l+1) - E(0, l)] \quad (3.14)$$

The proof is similar to that of the previous corollary.

We now obtain associated bounds on $\langle r^2 \rangle_{0,l}$.

Theorem (3.3)

If

$$\frac{d}{dr} \left[\frac{1}{r} \frac{dV}{dr} \right] < 0, \quad \forall r > 0,$$

then

$$\frac{2l+3}{E(0,l+1)-E(0,l)} \geq \langle r^2 \rangle_{0,l} \geq \frac{2l+3}{E(0,l)-E(0,l-1)} \quad (3.15)$$

and alternatively,

$$\langle r^2 \rangle_{0,l} \geq \frac{(2l+3)^2}{(2l+9)[E(0,l+1)-E(0,l)]}, \quad (3.16)$$

if in addition

$$\frac{d}{dr} r^2 \frac{dV}{dr} \geq 0.$$

These inequalities hold for all $l > 0$ except that in the right-hand inequality in (3.15), $l \geq 1$.

Proof Using (3.6) which holds for all potentials and the upper bounds on $\langle T \rangle_{0,l}$ given by (3.8) and (3.11), the right-hand side of (3.15) and (3.16) are obtained immediately. The left-hand side of (3.15) is just (3.7). The inequalities (3.15) are again "saturated" in the case of the harmonic oscillator potential. As previously, one has upper and lower bounds which differ only by the energy difference used or by the multiplying factor of the inverse of this difference.

In Section 4 of Ref. [1], we used bounds on $\langle T \rangle_{0,l}$ depending on $\partial E(0,l)/\partial l$ to obtain for power law potentials $V(r) = r^\nu$, $\nu > 0$, both upper and lower bounds on $E(0,L)/E(0,l)$ with $L > l > 0$ and also for $E(0,l)$ itself. For $0 < \nu < 2$ we found,

$$\left[(l+5/2)/(l+3/2) \right]^{2\nu/(\nu+2)} \leq E(0,l+1)/E(0,l) \leq \left[\frac{l+1+\frac{\nu+4}{4}}{l+\frac{\nu+4}{4}} \right]^{2\nu/(\nu+2)}, \quad (3.17)$$

while for $\nu \geq 2$ one may similarly prove that

$$\left[\frac{l+1+\frac{\nu+4}{4}}{l+\frac{\nu+4}{4}} \right]^{2\nu/(\nu+2)} \leq \frac{E(0,l+1)}{E(0,l)} \leq \left[\frac{l+5/2}{l+3/2} \right]^{2\nu/(\nu+2)}. \quad (3.18)$$

Then using

$$\lim_{l \rightarrow \infty} \left[E(0,l) / l^{\frac{2\nu}{\nu+2}} \right] = \left(\frac{\nu}{2} \right)^{\frac{2}{\nu+2}} \frac{\nu+2}{\nu},$$

one can obtain from (3.17), (3.18) the following bounds on $E(0, l)$ itself:

$$\left(\frac{\nu+2}{\nu}\right)\left(\frac{\nu}{2}\right)^{\frac{2}{\nu+2}}\left(l+\frac{\nu+4}{4}\right)^{\frac{2\nu}{\nu+2}} \leq E(0, l) \leq \left(\frac{\nu+2}{\nu}\right)\left(\frac{\nu}{2}\right)^{\frac{2}{\nu+2}}\left(l+3\frac{1}{2}\right)^{\frac{2\nu}{\nu+2}} \quad (3.19)$$

and

$$\left(\frac{\nu+2}{\nu}\right)\left(\frac{\nu}{2}\right)^{\frac{2}{\nu+2}}\left(l+3\frac{1}{2}\right)^{\frac{2\nu}{\nu+2}} \leq E(0, l) \leq \left(\frac{\nu+2}{\nu}\right)\left(\frac{\nu}{2}\right)^{\frac{2}{\nu+2}}\left(l+\frac{\nu+4}{4}\right)^{\frac{2\nu}{\nu+2}} \quad (3.20)$$

for $0 \leq \nu \leq 2$,
for $\nu \geq 2$.

However improved upper bounds on $E(0, l+1)/E(0, l)$ and lower bounds on $E(0, l)$ can be obtained from inequality (3.2) as we will now demonstrate. For $V(r) = r^\nu$ we have from the Virial theorem that

$$\langle T \rangle_{0, l} = \frac{\nu}{2+\nu} E(0, l) \quad (3.21)$$

so that inserting in (3.2)

$$\left(\frac{\nu}{2+\nu}\right)E(0, l) \geq \frac{2l+3}{4} [E(0, l+1) - E(0, l)], \quad (3.22)$$

and re-arranging,

$$\frac{E(0, l+1)}{E(0, l)} \leq \frac{(2l+3)/4 + \nu/(2+\nu)}{(2l+3)/4} \quad (3.23)$$

By repeated application of this bound, when $L \geq l$,

$$\frac{E(0, L)}{E(0, l)} \leq \frac{\Gamma(L + 3\frac{1}{2} + \frac{2\nu}{\nu+2}) \Gamma(l + 3\frac{1}{2})}{\Gamma(l + 3\frac{1}{2} + \frac{2\nu}{\nu+2}) \Gamma(L + 3\frac{1}{2})} \quad (3.24)$$

Taking the limit $L \rightarrow \infty$,

$$E(0, l) \geq \left(\frac{\nu}{2}\right)^{\frac{2}{\nu+2}} \left(\frac{\nu+2}{\nu}\right) \frac{\Gamma(l + 3\frac{1}{2} + \frac{2\nu}{\nu+2})}{\Gamma(l + 3\frac{1}{2})} \quad (3.25)$$

We will give now numerical examples which show that (3.24) and (3.25) give better bounds than do (3.17) and (3.20).

Consider the case when $l = 0$. Take $\nu = 4$ in (3.19),

$$1.718 = \left(\frac{3}{2}\right)^{4/3} \leq \frac{E(0,1)}{E(0,0)} \leq \left(\frac{5}{3}\right)^{4/3} \approx 1.975, \quad (3.26)$$

whilst the "new" upper bound (3.23) gives,

$$\frac{E(0,1)}{E(0,0)} \leq \frac{17}{9} \approx 1.778. \quad (3.27)$$

Similarly when $\nu = 1$ in (3.17),

$$1.405 = \left(\frac{5}{3}\right)^{2/3} \leq \frac{E(0,1)}{E(0,0)} \leq \left(\frac{9}{5}\right)^{2/3} = 1.482 \quad (3.28a)$$

and the "new" upper bound gives

$$\frac{E(0,1)}{E(0,0)} \leq \frac{13}{9} \approx 1.444. \quad (3.28b)$$

We see that the "new" upper bound is a substantial improvement for $\nu = 4$ and a small improvement for $\nu = 1$. When it is combined with the "old" lower bound, estimates of the above ratio which are accurate within a few per cent are obtained. Similarly in Ref. [1] we used the lower bounds in (3.18), (3.19) and variational upper bounds to give, for $\nu = 1$

$$2.19301 \leq E(0,0) \approx 2.33810741 \dots \leq 2.380 \quad (3.29a)$$

and for $\nu = 4$,

$$3.24 \leq E(0,0) \approx 3.8 \leq 3.91 \quad (3.29b)$$

Our "new" lower bound (3.26) can be used to give, for $\nu = 1$

$$E(0,0) \geq 2.3079 \quad (3.30a)$$

and for $\nu = 4$

$$E(0,0) \geq 3.6777 \quad (3.30b)$$

which improve on those given in (3.29). The "old" upper bounds with the "new" lower bounds give good estimates for $E(0,0)$ to within a few per cent error.

4. - BOUNDS ON THE WAVE FUNCTION AT THE ORIGIN IN TERMS OF THE KINETIC ENERGY

In Ref. [5] we obtained bounds on $|u'_{0,0}|^2$ in terms of $\langle T \rangle_{0,0}$. $|u'_{0,0}|^2$, for

instance, enters in the expression of leptonic decay rates of quarkonium via the Van Royen-Weisskopf formula [7]. The bounds were given by

$$|u'_{0,0}(0)|^2 > \frac{1}{4} \langle T \rangle_{0,0}^{3/2} \quad \text{if } \frac{dV}{dr} > 0 \quad \forall r > 0 \quad (4.1)$$

$$|u'_{0,0}(0)|^2 < 3 \langle T \rangle_{0,0}^{3/2} \quad \text{if } \frac{d}{dr} r \frac{dV}{dr} \geq 0 \quad \text{and} \quad \frac{dV}{dr} \geq 0, \quad (4.2)$$

The upper and lower bounds are in the ratio 3.73, and so rather weak. Here we shall derive tighter bounds on $u'_{0,0}(0)$ in terms of the kinetic energy and, in some cases these bounds will be valid for $n \neq 0$, i.e., arbitrary radial excitations.

First we derive a series of upper bounds on $|u'(0)|^2$, increasingly tighter, with more and more restricted classes of potentials

Theorem (4.1)

(boundary case Coulomb potential)

$$|u'_{0,0}(0)|^2 \leq 4 \langle T \rangle_{0,0}^{3/2} \quad (4.3)$$

if $\Delta V(r) \geq 0, \forall r > 0$, i.e. $\frac{d}{dr} r^2 \frac{dV}{dr} > 0$.

Proof

$$|u'(0)|^2 = \int u^2 \frac{dV}{dr} dr$$

now if

$$\begin{aligned} & \frac{d}{dr} r^2 \frac{dV}{dr} \geq 0 \\ & \left\langle r \frac{dV}{dr} \right\rangle \left\langle \frac{1}{r^2} \right\rangle - \left\langle \frac{dV}{dr} \right\rangle \left\langle \frac{1}{r} \right\rangle \\ & = \frac{1}{2} \int \frac{dx dy}{x y} u^1(x) u^2(y) [W(x) - W(y)] [x - y] > 0 \end{aligned} \quad (4.4)$$

with

$$W(x) = x^2 \frac{dV}{dx}$$

so

$$|u'_{0,0}(0)|^2 < 2 \langle T \rangle_{0,0} \langle \frac{1}{r^2} \rangle / \langle \frac{1}{r} \rangle, \quad (4.5)$$

but, by using the inequalities of Ref. [1], we have

$$\langle \frac{1}{r^2} \rangle < 2 \left(\langle \frac{1}{r} \rangle \right)^2 \quad (4.6)$$

and

$$\langle \frac{1}{r^2} \rangle < 2 \langle T \rangle_{0,0}, \quad (4.7)$$

if $\Delta V > 0$, which gives (4.3) by substitution in (4.5). Inequality (4.1) is optimal in the sense that it is saturated for the case of a pure Coulomb potential.

Corollary

If $\Delta V > 0$ and if $V(r) \rightarrow 0$ for $r \rightarrow \infty$

$$|u'_{0,0}(0)|^2 < 4 |E(0,0)|^{3/2} \quad (4.8)$$

Proof: if $(d/dr)r^2(dV/dv) > 0$ and if $V(\infty) = 0$, it is easy to get by integration

$$r \frac{dV}{dr} + V(r) < 0 \quad (4.9)$$

and hence

$$2 \langle T \rangle + \langle V \rangle = E + \langle T \rangle < 0.$$

An alternative derivation of this result consists in integrating an inequality recently obtained by Benguria [8]:

$$u'_{0,0} + \sqrt{-E} u_{0,0} - \frac{u_{0,0}}{r} > 0. \quad (4.10)$$

It is possible that theorem 4.1 or at least the corollary applies to radial excitations, but we have no proof of this.

Theorem 4.2

(boundary case, logr potential). If

$$\frac{d}{dr} r \frac{dV}{dr} > 0,$$

$$|u'_{n,0}(0)|^2 < 2 \langle T \rangle_{n,0}^{3/2}. \quad (4.11)$$

Here the inequality holds for any radial excitations.

Proof: following the same technique as in (4.4), we have

$$\langle r \frac{dV}{dr} \rangle \langle \frac{1}{r} \rangle - \langle \frac{dV}{dr} \rangle \langle r \rangle \geq 0$$

if

$$\frac{d}{dr} r \frac{dV}{dr} \geq 0$$

Hence

$$|u'_{n,0}(0)|^2 < 2 \langle T \rangle_{n,0} \frac{\int \frac{u^2}{r} dr}{\int u^2 dr}. \quad (4.12)$$

However, consider the quantity

$$X = \frac{\int u'^2 dr \int u^2 dr}{\left(\int \frac{u^2}{r} dr \right)^2} \quad (4.13)$$

we have, for arbitrary $Z > 0$

$$\int u'^2 dr - Z \int \frac{u^2}{r} dr > - \frac{Z^2}{4} \int u^2 dr,$$

by application of the variational principle to the Hamiltonian

$$- \frac{d^2}{dr^2} - \frac{Z}{r}. \quad (4.14)$$

Hence

$$X \geq \frac{1}{\chi^2} \left(Z \chi - \frac{Z^2}{4} \right), \quad \forall Z > 0$$

where

$$\chi = \int \frac{u^2}{r} dr / \int u^2 dr$$

and choosing $z = 2x$, we get $\chi > 1$. For $n = 0$ the inequality is almost, but not exactly saturated:

$$|u'(0)|^2 / \langle T \rangle^{3/2} = 1.9513... \text{ for } V = \log r.$$

This is because the wave function of (4.14) is not that of a logarithmic potential.

Theorem 4.3

(boundary case linear potential). If $V'' > 0$

$$|u'_{n,0}(0)|^2 < \left(\frac{3}{E_0}\right)^{3/2} \langle T \rangle_{n,0}^{3/2} < 1.455 \langle T \rangle_{n,0}^{3/2} \quad (4.15)$$

where E_0 is the first zero of the Airy function.

Proof Using the same the same technique

$$\left\langle r \frac{dV}{dr} \right\rangle \langle 1 \rangle - \left\langle \frac{dV}{dr} \right\rangle \langle r \rangle > 0$$

and

$$|u'_{n,0}(0)|^2 < 2 \langle T \rangle_{n,0} \frac{\int u^2 dr}{\int r u^2 dr}$$

Now we look for the minimum of

$$\chi' = \frac{\int u'^2 dr \left(\int r u^2 dr \right)^2}{\left(\int u^2 \right)^3}$$

using the same type of variational argument, we get

$$\int u'^2 dr + \mu^3 \int r u^2 dr > E_0 \mu^2 \int u^2 dr$$

where E_0 is the ground state energy of the Hamiltonian

$$-\frac{d^2}{dr^2} + r$$

$$E_0 \cong 2.3381 \dots$$

After optimization with respect to μ , (4.15) follows trivially. For $n = 0$ the inequality is saturated in the case of a linear potential. For $n > 0$ it is obviously not saturated since the wave function at the origin is independent of the excitation.

Finally, we give:

Theorem 4.4

(limit case, harmonic oscillator). If

$$\frac{d}{dr} \frac{1}{r} \frac{dV}{dr} \geq 0$$

$$|u'_{n,0}(0)|^2 < \frac{4}{3} \langle T \rangle_{n,0}^{3/2} \quad (4.16)$$

Proof: by the same kind of argument

$$|u'_{n,0}(0)|^2 < 2 \langle T \rangle_{n,0} \frac{\int r u^2 dr}{\int r^2 u^2 dr} \quad (4.17)$$

and by Schwarz inequality

$$|u'_{n,0}(0)|^2 < 2 \langle T \rangle_{n,0} \left(\frac{\int u^2 dr}{\int r^2 u^2 dr} \right)^{1/2}.$$

Then

$$X'' = \frac{\int u'^2 dr \int r^2 u^2 dr}{(\int u^2 dr)^2}$$

is minimized by an harmonic oscillator wave function and we get

$$|u'_{n,0}(0)|^2 < \frac{4}{3} \langle T \rangle_{n,0}^{3/2} \quad (4.18)$$

In the special case of $n = 0$, this can be slightly improved by noticing, as was done some years ago by one of us (A.K.C.) [5], that

$$f_k = k \int r^{k+3} u^2 dr$$

form a Stieljes sequence if $dV/dr > 0$, i.e.,

$$f_k \leq (f_{k+1} f_{k-1})^{1/2} \text{ etc...}$$

This allows us to improve the Schwarz inequality. So, if

$$\frac{d}{dr} \frac{1}{r} \frac{dV}{dr} > 0$$

and

$$\frac{dV}{dr} > 0$$

$$|u'_{0,0}(0)|^2 < \sqrt{\frac{5}{3}} \langle T \rangle_{0,0}^{3/2} \quad (4.19)$$

For a pure harmonic oscillator

$$|u'_{0,0}(0)|^2 / \langle T \rangle_{0,0}^{3/2} = \frac{4}{\sqrt{\pi}} \left(\frac{2}{3} \right)^{3/2} = 1.257,$$

while (4.19) gives 1.291, very close indeed.

We could continue this game with tighter and tighter conditions, but it is only for some specific cases, like the Coulomb potential and linear potential that we can get optimal results for the ground state wave function.

We turn now to lower bounds of $u'_{0,0}(0)$, i.e., to improvements of (4.1). We have obtained

Theorem 4.5

If $dV/dr > 0$ and if $V(r)$ is in set B for $\alpha = \beta_1$

$$|u'_{0,0}(0)|^2 \geq \frac{8}{\sqrt{3}(1+\beta_1)^{3/2}} \langle T \rangle_{0,0}^{3/2} \quad (4.20)$$

In the special case $V = r^2$ we can take $\beta_1 = 2$ so that the coefficient in (4.20) becomes $8/9 \approx 0.889$ not too far from the upper bound.

Proof We already said that the

$$f_k = k \int r^{k-3} u^2 dr$$

form a Stieljes sequence. Now

$$\int_0^\infty \frac{u^2 dr}{r^{3-\varepsilon}} \approx \frac{1}{\varepsilon} |u'(0)|^2 \quad \text{for } \varepsilon \rightarrow 0$$

so that

$$f_0 = |u'(0)|^2$$

So [9]

$$\langle r^{-2} \rangle_{0,0} = f_1 \langle f_3 \rangle^{1/3} \langle f_0 \rangle^{2/3} = (3)^{1/3} |u'_{0,0}(0)|^{4/3}, \quad (4.21)$$

but from Ref. [1]

$$\langle T \rangle_{0,0} \leq \frac{1}{4} (1+\beta_1) \langle r^{-2} \rangle_{0,0} \quad (4.22)$$

Combining (4.21) and (4.22) we get (4.20).

Theorem 4.6

The lower bound (4.1) can easily be generalized to arbitrary radial excitations in the form

$$|u'_{n,0}(0)|^2 \geq \frac{1}{4(n+1)} \langle T \rangle_{n,0}^{3/2} \text{ if } \frac{dV}{dr} \geq 0. \quad (4.23)$$

Proof The proof is a carbon copy of the one given in Ref. [5]. We notice that if $dV/dr > 0$ it is still true that

$$|u'_{n,0}(r)|^2 < |u'_{n,0}(0)|^2 \quad (4.24)$$

because $u'^2 + (E-V)u^2$ is decreasing and hence $u'^2(r)$ is less than $u'^2(0)$ as long as $E-V$ is positive, and, for $(E-V) < 0$, $|u'|$ decreases. Therefore, calling $r_1, \dots, r_n$ the zeros of $u_{n,0}$ and $R_1, \dots, R_{n+1}$ the maxima of $|u_{n,0}|$, we have

$$\begin{aligned} \int_{r_p}^{R_{p+1}} u'^2 dr &< |u'(0)| \int_{r_p}^{R_{p+1}} u' dr = |u'(0)| \left[\int_{r_p}^{R_{p+1}} 2|u u'| dr \right]^{1/2} \\ &< \sqrt{2} |u'(0)| \left(\int_{r_p}^{R_{p+1}} u'^2 dr \right)^{1/4} \left(\int_{r_p}^{R_{p+1}} u^2 dr \right)^{1/4} \end{aligned} \quad (4.25)$$

Hence

$$\left(\int_0^{R_1} u'^2 dr \right)^3 + \left(\int_{R_1}^{r_1} u'^2 dr \right)^3 + \dots + \left(\int_{R_{n+1}}^{\infty} u'^2 dr \right)^3 < 4 |u'(0)|^2 \int_0^{\infty} u'^2 dr \quad (4.26)$$

then using the fact that for positive a 's,

$$a_1^3 + a_2^3 + \dots + a_p^3 > \frac{1}{p^2} (a_1 + a_2 + \dots + a_p)^3$$

we easily get (4.23).

Notice that for positive power potentials this lower bound has the correct qualitative behaviour for large n . For instance, for a linear potential $E(n,0) \sim \langle T \rangle_{n,0} \sim n^{2/3}$, so that the lower bound is a positive constant for large n .

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