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Preservation of Logarithmic Concavity by the Mellin Transform and Applications to the Schrödinger Equation for Certain Classes of Potentials

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Abstract. We prove that the Mellin transform of a function log-concave (convex) is, after division by $\Gamma(\nu+1)$, where ν is the argument of the transform, itself log-concave (convex) in ν. This theorem is first applied to the moments of the ground state wave function of the Schrödinger equation where the Laplacian of the central potential has a given sign, and generalized to other situations. This is used to derive inequalities linking the ℓ^{th} derivative of the ground state wave function at the origin for angular momentum ℓ and the expectation value of the kinetic energy, and applied to quarkonium physics. A generalization to higher radial excitations is shown to be plausible by using the WKB approximation. Finally, new bounds on ground-state energies in power potentials are obtained.

1. Physical Motivation

In 1984, Baumgartner, Grosse and Martin [1] proved that if, in the Schrödinger equation, the central potential has a Laplacian with a given sign, the order of levels corresponding to what would be a degenerate multiplet for the Coulomb potential is known. Specifically the multiplet is characterized by $N=\ell+n+1=\text{const}$, ℓ being the angular momentum and n the number of nodes of the radial wave function. Then if $\Delta V>0$, the energies decrease when ℓ increases for fixed N, and if $\Delta V<0$ the energies increase when ℓ increases.

A crucial lemma to prove this theorem is the following:

If $\Delta V \gtrless 0$, $\forall r>0$,

$$-\left(\frac{u_\ell'}{u_\ell}\right)' - \frac{\ell+1}{r^2} \gtrless 0, \quad \forall r>0, \tag{1}$$

where u_ℓ is the reduced ground state wave function with angular momentum ℓ.

It has been noticed by Ashbaugh and Benguria [2], who gave an alternative derivation of (1), that (1) is equivalent to

$$\left(\log\left(\frac{u_\ell}{r^{\ell+1}}\right)\right)'' \gtrless 0 \quad \forall r > 0. \tag{2}$$

More recently, a third derivation of (1) was given by Martin [3]. Initially this lemma was thought to be nothing more than a lemma, but later it was noticed by Common [4] that property (1) leads to interesting inequalities on the expectation values of r^ν – i.e., the moments – in the ground state of the angular momentum ℓ. Specifically, Common proved, by using (1) and making two integrations by parts, that

$$(2\ell + 3 + \alpha)\frac{\langle r^\alpha \rangle}{\langle r^{\alpha+1}\rangle} \gtrless (2\ell + 3 + \beta)\frac{\langle r^\beta \rangle}{\langle r^{\beta+1}\rangle}, \quad \alpha > \beta, \tag{3}$$

where $\langle r^\alpha \rangle = \int_0^\infty r^\alpha u_\ell^2(r) dr$ if $\Delta V \gtrless 0$.

In the special case $\beta = \alpha - 1$, we get

$$\frac{2\ell + 3 + \alpha}{2\ell + 2 + \alpha}(\langle r^\alpha \rangle)^2 \gtrless \langle r^{\alpha+1}\rangle \langle r^{\alpha-1}\rangle \tag{4}$$

if $\Delta V \gtrless 0$, so that if $\Delta V > 0$ we get an inequality going in the *opposite* direction to the Schwarz inequality, while if $\Delta V < 0$ we get a "reinforced" Schwarz inequality. Equation (4) can be rewritten as

$$\left(\frac{\langle r^\alpha \rangle}{\Gamma(2\ell + 3 + \alpha)}\right)^2 \gtrless \frac{\langle r^{\alpha+1}\rangle}{\Gamma(2\ell + 4 + \alpha)} \frac{\langle r^{\alpha-1}\rangle}{\Gamma(2\ell + 2 + \alpha)} \tag{5}$$

if $\Delta V \gtrless 0$. Equation (5) then looks like a kind of concavity (convexity) property in α for

$$\log\left[\frac{\langle r^\alpha \rangle}{\Gamma(2\ell + 3 + \alpha)}\right], \tag{6}$$

except for the fact that the variable has to jump by integers.

In using these types of properties to get inequalities linking the kinetic energy and the wave function at the origin, for situations where the potential V belongs to a different class [5, 6], such as

$$\frac{d}{dr}\frac{1}{r}\frac{dV}{dr} \gtrless 0 \quad \forall r > 0, \tag{7}$$

we met the need to prove that the quantity (6) is really concave or convex in α if the Laplacian of the potential is correspondingly positive or negative.

With the reinterpretation of inequalities (1) by Ashbaugh and Benguria [2], and after a redefinition of the variables and the functions, the problem is reduced to studying the concavity or convexity of

$$\log\left(\frac{\int_0^\infty r^\nu w(r) dr}{\Gamma(\nu + 1)}\right)$$

when $\log w(r)$ has a given concavity. In the physical case, w represents $(u_\ell/r^{\ell+1})^2$. However, the property we shall obtain transcends the particular physical problem which motivated it and belongs to pure mathematics.

2. The Theorem

Let $w(r)$ be a positive continuous function, defined on $\mathbb{R}_0^+$, such that all moments

$$\{r^\nu\} = \int_0^\infty r^\nu w(r) dr \tag{8}$$

exist for $\nu > \nu_0 > -1$.

If $\log w(r)$ *is convex (concave) in r, then*

$$\log\left(\frac{\{r^\nu\}}{\Gamma(\nu+1)}\right)$$

is convex (concave) in ν for all $\nu > \nu_0$.

Proof. Here, for simplicity, we shall assume strict convexity or concavity, but it is easy to see that it is an unnecessary assumption. First we remind the reader of the property (or definition!)

$$\Gamma(\nu+1)\lambda^{-\nu-1} = \int_0^\infty r^\nu e^{-\lambda r} dr. \tag{9}$$

i) *The Convex Case.* For $\nu > \nu_0$, $\varepsilon > 0$ such that $\nu - \varepsilon > \nu_0$, with three parameters $\lambda > 0$, $\sigma > 0$, $\mu \in \mathbb{R}$, we construct the following quantity

$$I = \int_0^\infty \left[\frac{2r^\nu}{\Gamma(\nu+1)} - \frac{\lambda^\varepsilon r^{\nu+\varepsilon}}{\Gamma(\nu+1+\varepsilon)} - \frac{\lambda^{-\varepsilon} r^{\nu-\varepsilon}}{\Gamma(\nu+1-\varepsilon)}\right][e^{\phi(r)} - e^{-\lambda\sigma r+\mu}]dr, \tag{10}$$

where we have replaced w by e^ϕ with ϕ strictly convex. The strategy will be, first of all, to choose the parameters σ and μ such that the integrand is non-negative for any given λ.

The change of variable $t = \lambda r$ will give

$$I = \lambda^{-\nu-1} \int_0^\infty \left[\frac{2t^\nu}{\Gamma(\nu+1)} - \frac{t^{\nu+\varepsilon}}{\Gamma(\nu+1+\varepsilon)} - \frac{t^{\nu-\varepsilon}}{\Gamma(\nu+1-\varepsilon)}\right][e^{\phi(t/\lambda)} - e^{-\sigma t+\mu}]dt. \tag{11}$$

If we look at the first bracket we see that it is negative for $t \to 0$ and $t \to \infty$.

After factoring out $t^{\nu-\varepsilon}$ we see that it is a second-degree polynomial in $x = t^\varepsilon$. The discriminant of this polynomial is

$$\Delta' = [\Gamma(\nu+1)]^{-2} - [\Gamma(\nu+1+\varepsilon)\Gamma(\nu+1-\varepsilon)]^{-1},$$

which is positive in view of the logarithmic convexity of the Γ function. Therefore we find two distinct roots $t_2 > t_1 > 0$. As a consequence, the first bracket is positive between the roots, negative outside.

Now let us look at the second bracket. It vanishes when $\phi(t/\lambda) = -\sigma t + \mu$, and since ϕ is strictly convex it vanishes at most twice. For any $\lambda > 0$ we define σ by

$$\sigma = \frac{\phi\left(\frac{t_1}{\lambda}\right) - \phi\left(\frac{t_2}{\lambda}\right)}{t_2 - t_1}, \tag{12}$$

and μ by

$$\mu = \frac{t_2\phi\left(\frac{t_1}{\lambda}\right) - t_1\phi\left(\frac{t_2}{\lambda}\right)}{t_2 - t_1}. \tag{13}$$

Then the second bracket vanishes at t_1 and t_2. Furthermore it is negative between the zeros and positive outside implying that I is negative.

Therefore, for any $\lambda > 0$, we have

$$\frac{2\{r^\nu\}}{\Gamma(\nu+1)} - \lambda^\varepsilon \frac{\{r^{\nu+\varepsilon}\}}{\Gamma(\nu+1+\varepsilon)} - \lambda^{-\varepsilon} \frac{\{r^{\nu-\varepsilon}\}}{\Gamma(\nu+1-\varepsilon)}$$
$$\leqq e^\mu(\lambda\sigma)^{-\nu-1}[2 - \sigma^{-\varepsilon} - \sigma^\varepsilon] \leqq 0, \tag{14}$$

with μ and σ defined as above.

Choosing

$$\lambda = \left(\frac{\{r^{\nu-\varepsilon}\}\Gamma(\nu+1+\varepsilon)}{\{r^{\nu+\varepsilon}\}\Gamma(\nu+1-\varepsilon)}\right)^{1/2\varepsilon}$$

yields

$$\frac{\{r^\nu\}}{\Gamma(\nu+1)} \leqq \left[\frac{\{r^{\nu-\varepsilon}\}}{\Gamma(\nu+1-\varepsilon)} \frac{\{\Gamma^{\nu+\varepsilon}\}}{\Gamma(\nu+1+\varepsilon)}\right]^{1/2}, \tag{15}$$

which is the desired result.

ii) *The Concave Case.* The proof will follow the same lines and each step will give the reversed inequality. However, the reversed version of (13) is only useful if $\sigma = 1$.

Then we would have:

$$\frac{2\{r^\nu\}}{\Gamma(\nu+1)} \geqq \lambda^\varepsilon \frac{\{r^{\nu+\varepsilon}\}}{\Gamma(\nu+1+\varepsilon)} + \lambda^{-\varepsilon} \frac{\{r^{\nu-\varepsilon}\}}{\Gamma(\nu+1-\varepsilon)}, \tag{16}$$

and the theorem would follow from the arithmetic-geometric-mean inequality.

Therefore it remains to show the existence of $\lambda > 0$ such that equality (12) is satisfied with $\sigma = 1$. To do so, we prove the existence of a fixed point of the continuous mapping

$$\lambda_{n+1} = g(\lambda_n) \tag{17}$$

with g defined by

$$g(\lambda) = \frac{\phi\left(\frac{t_1}{\lambda}\right) - \phi\left(\frac{t_2}{\lambda}\right)}{\frac{t_2 - t_1}{\lambda}}. \tag{18}$$

First of all, we claim that $g(\lambda)$ is monotone non-increasing in λ. To prove this we need the following lemma that we state without proof.

Lemma. *Let $\phi:\mathbb{R}\to\mathbb{R}$ be a continuous (strictly) concave function. Then, for any a, b, c, d such that*

$$a < b, \quad c < d,$$

$$\frac{\phi(c)-\phi(a)}{c-a} \geqq \frac{\phi(d)-\phi(b)}{d-b}. \tag{19}$$

The monotonicity of $g(\lambda)$ is derived as follows. For $\lambda' < \lambda$ we take

$$a = \frac{t_1}{\lambda}, \quad c = \frac{t_2}{\lambda}, \quad b = \frac{t_1}{\lambda'}, \quad d = \frac{t_2}{\lambda'} \tag{20}$$

and apply the lemma.

From the monotonicity of $g(\lambda)$ it follows that either $g(\lambda)$ tends to $+\infty$ for $\lambda\to 0$, or has a limit. In the former case the mapping has necessarily a unique fixed point since $\lambda - g(\lambda)$ increases from $-\infty$ to $+\infty$ as λ varies from 0 to ∞. If $g(\lambda)$ has a limit for $\lambda\to 0$ let us show that this limit is necessarily strictly positive.

Assume $g(0) = \lim_{\lambda\to 0} g(\lambda) \leqq 0$. Then, from monotonicity, $g(\lambda) < 0$, $\lambda > 0$. Then given any x and $\delta > 0$, the previous lemma gives

$$\phi(x+\delta) - \phi(x) \geqq \frac{\delta\lambda}{t_2 - t_1}\left[\phi\left(\frac{t_2}{\lambda}\right) - \phi\left(\frac{t_1}{\lambda}\right)\right] > 0, \tag{21}$$

provided λ is sufficiently small so that $t_2/\lambda > x + \delta$ and $t_1/\lambda > x$. Therefore ϕ would be non-decreasing and the integral defining $\{r^\nu\}$ would diverge for $\nu > -1$, contrary to the assumption.

Hence $g(0) > 0$ and $\lambda - g(\lambda)$ increases monotonously from $-g(0) < 0$ to $+\infty$ and takes the value zero once and only once.

Therefore, in the *concave* case, there exists a unique value λ such that $\sigma = 1$ in Eq. (11). Hence, inequality (16) holds for this particular value of λ and since $A^2 + B^2 > 2AB$, we get

$$\frac{\{r^\nu\}}{\Gamma(\nu+1)} > \left[\frac{\{r^{\nu+\varepsilon}\}}{\Gamma(\nu+1-\varepsilon)}\frac{\{r^{\nu-\varepsilon}\}}{\Gamma(\nu+1-\varepsilon)}\right]^{1/2}, \tag{22}$$

which establishes the theorem for the concave case.

Except for the factor $\Gamma(\nu+1)$ dividing $\{r^\nu\}$ we see that the theorem implies the preservation of logarithmic concavity by the direct Mellin transform.

3. Implications for the Moments of the Schrödinger Wave Function for a Given Class of Potentials

In the introduction we have seen that if, in the Schrödinger equation

$$-u_\ell'' + \frac{\ell(\ell+1)}{r^2}u_\ell + (V-E)u_\ell = 0, \tag{23}$$

the potential has the property $\Delta V \gtrless 0$, then $\log(u_\ell/r^{\ell+1})$ is $\begin{cases}\text{concave}\\ \text{convex}\end{cases}$, where u_ℓ is the ground state wave function. Hence

$$\log\left(\frac{\int_0^\infty \left(\frac{u_\ell}{r^{\ell+1}}\right)^2 r^\nu dr}{\Gamma(\nu+1)}\right) \quad \text{is} \quad \begin{cases}\text{concave}\\ \text{convex}\end{cases},$$

or, changing notations,

$$\log\left(\frac{\int_0^\infty u_\ell^2 r^\mu dr}{\Gamma(\mu+2\ell+3)}\right) \quad \text{is} \quad \begin{cases}\text{concave}\\ \text{convex}\end{cases}.$$

It is obvious that Eqs. (3) and (4) in the introduction are consequences of this concavity–convexity property. Notice that u_ℓ^2 can be replaced by the product of two wave functions with different ℓ's.

Now it has already been noticed [5–7] that one can also obtain interesting results for other classes of potentials for which the Laplacian is not of a given sign. A simple way to generate such classes is to make a change of variables

$$\left.\begin{aligned} z &= r^\alpha \\ w_\lambda(z) &= r^{(\alpha-1)/2} u_\ell(r) \end{aligned}\right\}. \tag{24}$$

Then the Schrödinger equation becomes

$$\left.\begin{aligned} &\left[-\frac{d^2}{dz^2}+\frac{\lambda(\lambda+1)}{z^2}+U(z,E)\right]w_\ell(z)=0 \\ &\text{with} \\ &U(z,E)=\frac{V(r)-E}{\alpha^2 z^{2-(2/\alpha)}}, \\ &\lambda=\frac{2\ell+1-\alpha}{2\alpha}. \end{aligned}\right\} \tag{25}$$

Then, if the Laplacian of U in the variable z has a given sign, we get interesting properties on the order of energy levels. For instance, with $\alpha = 2$ the property

$$\frac{d}{dr}\frac{1}{r}\frac{dV}{dr} \gtrless 0 \quad \text{becomes} \quad \Delta_z U \gtrless 0. \tag{26}$$

Notice that the limit case of (26) is the harmonic oscillator. For *positive* energy levels, the change of variable (24) shows that if

$$D_\alpha V(r) = \frac{d^2V}{dr^2} + (5-3\alpha)\frac{1}{r}\frac{dV}{dr} + 2(1-\alpha)(2-\alpha)\frac{V(r)}{r^2} > 0, \tag{27}$$

$\Delta_z U$ is positive. More generally, we can define two sets A and B of *sufficient* conditions to have $Y = -(w'/w)' - (\lambda+1)/z^2$ of a given sign:

Set A $(Y > 0)$

(i) $D_\alpha V(r) > 0 \quad 1 < \alpha < 2 \quad V(r) > 0,$

(ii) $D_\alpha V(r) > 0 \quad \alpha < 1 \quad V(r) < 0,$ (28)

(iii) $r\dfrac{d^2V}{dr^r} + (3-2\alpha)\dfrac{dV}{dr} > 0, \quad \dfrac{dV}{dr} > 0, \quad 1 < \alpha < 2,$

Set B $(Y < 0)$

(i) $D_\alpha V(r) < 0 \quad \alpha > 2 \quad \text{or} \quad \alpha < 1 \quad V(r) > ($

(ii) $D_\alpha V(r) < 0 \quad 1 < \alpha < 2 \qquad V(r) < ($

(iii) $r\dfrac{d^2V}{dr^2} + (3-2\alpha)\dfrac{dV}{dr} < 0, \quad \alpha > 2.$ (29)

Returning now to our present problem, we notice first that the change of variables, function and angular momentum defined by (24) and (25) leaves $u_\ell(r)/r^{\ell+1}$ "invariant," i.e.,

$$\frac{u_\ell(r)}{r^{\ell+1}} = \text{const.}\frac{w_\lambda(z)}{z^{\lambda+1}}. \tag{30}$$

If $V(r)$ belongs to set (A,α) or (B,α), then

$$\log\left(\frac{\int\left(\frac{w_\lambda(z)}{z^{\lambda+1}}\right)^2 z^\nu dz}{\Gamma(\nu+1)}\right)$$

is concave or, respectively, convex. Translating back in the variable r, we conclude

$$\log\left(\frac{\int_0^\infty (u_\ell(r))^2 r^\mu dr}{\Gamma\left(\frac{\mu+2\ell+3}{\alpha}\right)}\right) \quad \text{is concave or convex} \tag{31}$$

if V belongs respectively to set (A,α) or (B,α).

4 Application to Inequalities Between the ℓ^{th} Derivative of the Wave Function at the Origin and the Kinetic Energy (Angular and Total)

In ref. [6] we have obtained inequalities linking the wave function at the origin for $\ell = 0$ states and the expectation value of the kinetic energy. Some of these inequalities were not optimal because we did not know the theorem established in the present paper and the generalization to arbitrary angular momentum was missing. We do this here. $\lim_{r\to 0^+}(u_\ell/r^{\ell+1})$ is proportional to the ℓ^{th} derivative of the wave function at the origin. It is easy to see that

$$\lim_{r\to 0^+}\left(\frac{u_\ell}{r^{\ell+1}}\right)^2 = \alpha \lim_{\mu\to -2\ell-3}\frac{\int_0^\infty (u_\ell(r))^2 r^\mu dr}{\Gamma\left(\frac{\mu+2\ell+3}{\alpha}\right)}. \tag{32}$$

The quantity appearing on the right-hand side of (32) is the same as that appearing in (31). If we call

$$f_\alpha(\mu)=\frac{\int u_\ell^2(r)r^\mu dr}{\Gamma\left(\frac{\mu+2\ell+3}{\alpha}\right)}, \tag{33}$$

we have, if V belongs to sets (A,α), (B,α)

$$\frac{2\log f_\alpha(-2\ell-3)+(2\ell+1)\log f_\alpha(0)}{2\ell+3}\gtrless \log f_\alpha(-2); \tag{34}$$

so

$$\lim_{r\to 0}\left(\frac{u_\ell}{r^{\ell+1}}\right)^2 \gtrless \alpha\left(\frac{\int \frac{u_\ell^2}{r^2}dr}{\Gamma\left(\frac{2\ell+1}{\alpha}\right)}\right)^{\ell+(3/2)} \times\left(\Gamma\left(\frac{2\ell+3}{\alpha}\right)\right)^{\ell+(1/2)}. \tag{35}$$

But we also have [5]

$$\langle T\rangle_{0,\ell}\gtrless(\ell+\tfrac{1}{2})\left(\ell+\frac{\alpha+1}{2}\right)\int\frac{u_\ell^2}{r^2}dr, \tag{36}$$

where $\langle T\rangle_{0,\ell}$ is the expectation value of the kinetic energy in the ground state with angular momentum ℓ, if V belongs to sets (A,α), (B,α) respectively, so that we have

$$\lim_{r\to 0}\left(\frac{u_\ell}{r^{\ell+1}}\right)^2 \lessgtr \alpha\frac{\Gamma\left(\frac{2\ell+3}{\alpha}\right)^{\ell+(1/2)}}{\Gamma\left(\frac{2\ell+1}{\alpha}\right)^{\ell+(3/2)}}\left(\frac{\langle T\rangle_{0,\ell}}{\left(\ell+\frac{1}{2}\right)\left(\ell+\frac{\alpha+1}{2}\right)}\right)^{\ell+(3/2)}. \tag{37}$$

In particular, if $\Delta V\gtrless 0$ ($\alpha=1$, A or B)

$$\lim_{r\to 0}\left(\frac{u_\ell}{r^{\ell+1}}\right)^2 \lessgtr \frac{[4\langle T\rangle_{0,\ell}]^{\ell+(3/2)}}{\Gamma(2\ell+3)}, \tag{38}$$

and if

$$\frac{d}{dr}\frac{1}{r}\frac{dV}{dr}\gtrless 0 \quad (\alpha=2, A \text{ or } B)$$

$$\lim_{r\to 0}\left(\frac{u_\ell}{r^{\ell+1}}\right)^2 \lessgtr \frac{2}{\Gamma(\ell+\frac{3}{2})}\left(\frac{\langle T\rangle_{0,\ell}}{\ell+\frac{3}{2}}\right)^{\ell+(3/2)}. \tag{39}$$

In the special case $\ell=0$ (38) gives the same result as ref. [6]:

$$|u'(0)|^2\lessgtr 4\langle T\rangle_{0,0}^{3/2}, \tag{40}$$

for $\Delta V\gtrless 0$, while (39) leads to an improvement:

$$|u'(0)|^2\lessgtr\frac{4}{\sqrt{\pi}}(\tfrac{2}{3})^{3/2}\langle T\rangle_{0,0}^{3/2}\cong 1.2284\langle T\rangle_{0,0}^{3/2} \quad \text{for} \quad \frac{d}{dr}\frac{1}{r}\frac{dV}{dr}\gtrless 0 \tag{41}$$

instead of

$$|u'(0)|^2 < \tfrac{4}{3}\langle T\rangle_{0,0}^{3/2} \tag{42}$$

restricted to

$$\frac{d}{dr}\frac{1}{r}\frac{dV}{dr} \geqq 0.$$

For the *linear* potential, which corresponds to class A with $\alpha = 3/2$, we get

$$|u'(0)|^2 < \frac{3}{2}\left(\frac{8}{5}\right)^{3/2} \frac{1}{\Gamma(\frac{2}{3})^{3/2}} \langle T\rangle_{0,0}^{3/2} \cong 1.927\langle T\rangle_{0,0}^{3/2},$$

not too far from the exact answer $(3/E_0)^{3/2} \cong 1.455$, where $-E_0$ is the first zero of the Airy function.

For convex potentials, we do not do as well as with the special trick used in ref. [6].

Before closing this section we want to give an illustration of the possible uses of these inequalities in quarkonium physics. It is known that the $c\bar{c}$ and $b\bar{b}$ systems are well described by potential models [8], but it is interesting to try to obtain results which do not depend on a particular potential, but only on rather general features. An inequality previously derived by Bertlmann and Martin [9] links, for arbitrary potentials, the expectation value of the kinematic energy, appearing already in this section and the ground state and first angular excitation energies. It is

$$\langle T\rangle_{0,0} \geqq \tfrac{3}{4}[E(n=0,\ell=1) - E(n=0,\ell=0)]. \tag{43}$$

This inequality is saturated by an harmonic oscillator potential.

This inequality can be combined with inequality (41), with $d/dr\ 1/r\ dV/dr < 0$, also saturated by the harmonic oscillator potential, to give directly an inequality linking the wave function at the origin and the two energy levels. It happens that the static potential between quarks derived from lattice QCD is monotonous increasing and concave [10], i.e., $V > 0$ and $V'' < 0$. This implies that $d/dr\ 1/r\ dV/dr$ is indeed *negative* in reasonable models.

Then one gets

$$|u'(0)|^2 > \frac{4}{\sqrt{\pi}}\left(\frac{2}{3}\right)^{3/2} [\tfrac{3}{4}(E(\ell=1) - E(\ell=0))]^{3/2}. \tag{44}$$

Reinserting the mass dependence omitted in Eq. (23) and taking into account the angular integration we have

$$|\psi(0)|^2 > \frac{1}{\pi^{3/2}} [\tfrac{1}{2}M_q(E(\ell=1) - E(\ell=0))]^{3/2}, \tag{45}$$

where M_q is the quark mass in the quark–antiquark system.

Now the wave function at the origin enters in the Van Royen–Weisskopf formula for the leptonic width:

$$\Gamma_{e^+e^-} = 16\pi\alpha^2 e_Q^2 \frac{|\psi(0)|^2}{M_V^2}, \tag{46}$$

where M_V is the mass of the quark–antiquark system, e_Q is the charge of the quark, 2/3 for c quarks, $-1/3$ for b quarks, and $\alpha^{-1} \cong 137$, the inverse of the fine structure constant.

Therefore we obtain an inequality between physically accessible quantities (except for the "constituent" quark mass, slightly model-dependent):

$$\Gamma_{e^+e^-} > \frac{16e_Q^2}{\pi^{1/2}} \frac{\alpha^2}{M_V^2} [\tfrac{1}{2}M_q(E(\ell = 1) - E(\ell = 0))]^{3/2}. \tag{47}$$

This can be applied to the $c\bar{c}$ system with [11, 8]

$$\begin{aligned} M(\ell = 1) &= 3.52\,\text{GeV}, \\ M(\ell = 0) \equiv M_V &= 3.10\,\text{GeV}, \\ e_Q &= \tfrac{2}{3}, \\ M_q &= 1.5 \text{ to } 1.8\,\text{GeV}. \end{aligned}$$

This gives

$$\Gamma_{e^+e^-} > 3.9 \text{ to } 5.2\,\text{KeV},$$

to be compared to 4.7 ± 0.35 KeV experimentally [11]. The agreement is almost too good since we know that the $c\bar{c}$ potential is rather far from the harmonic oscillator potential. This is an indication that, as many people think, the Van Royen–Weisskopf formula should be "renormalized."

For the $b\bar{b}$ system, with [11, 8]

$$\begin{aligned} M(\ell = 1) &= 9.90\,\text{GeV}, \\ M(\ell = 0) &= 9.46\,\text{GeV}, \\ e_Q &= -\tfrac{1}{3}, \\ M_q &= 5.174\,\text{GeV}, \end{aligned}$$

we get

$$\Gamma_{e^+e^-} > 0.7\,\text{KeV},$$

while experiment gives

$$\Gamma_{e^+e^-} \cong 1.34 \pm 0.05\,\text{KeV}.$$

5. A Conjecture on the Wave Function at the Origin for Higher Radial Excitations

For $\Delta V \gtrless 0$ we have seen that we have inequality (40):

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

For $\Delta V = 0$, i.e., $V = -\text{const}/r$, one has, for *all* radial excitations:

$$|u'_{n,0}(0)|^2 = 4\langle T\rangle_{n,0}^{3/2}, \tag{48}$$

where n is the number of nodes of the wave function and, because of the virial theorem, $\langle T\rangle = -E$,

$$|u'_{n,0}(0)|^2 = 4|E_n|^{3/2}. \tag{49}$$

For potentials such that $\Delta V \gtrless 0$ and $V(\infty)=0$, one can integrate

$$2\frac{dV}{dr}+r\frac{d^2V}{dr^2}\gtrless 0, \tag{50}$$

from r to infinity, and get

$$V+\frac{1}{2}r\frac{dV}{dr}+\frac{1}{2}r\frac{dV}{dr}\lesseqgtr 0, \tag{51}$$

and hence, from the virial theorem:

$$\langle T\rangle_n \lesseqgtr |E_n|. \tag{52}$$

Therefore, for $n=0$, from (40):

$$|u_0'(0)|^2 \lesseqgtr 4|E_0|^{3/2}.$$

We want to make the conjecture that this holds for an arbitrary radial excitation n, i.e.,

$$|u_n'(0)|^2 \lesseqgtr 4|E_n|^{3/2}, \tag{53}$$

if $\Delta V \gtrless 0$ and $V(\infty)=0$. We shall make this conjecture plausible in the framework of the WKB approximation. Then for $\ell=0$ we have

$$n-\frac{1}{4}=\frac{1}{\pi}\int_0^{r_T} dr\sqrt{E(n,\ell=0)-V}, \tag{54}$$

where r_T is the turning point. For simplicity, assume $dV/dr>0$ everywhere. Then the turning point is unique ($\Delta V>0$ allows, a priori, *two* turning points). In the WKB framework n can be regarded as continuous as well as ℓ, and the theorem on the level-ordering for $\Delta V \gtrless 0$ can be written in a somewhat generalized form:

$$\frac{\partial E(n,\ell)}{\partial n}-\frac{\partial E(n,\ell)}{\partial \ell}\gtrless 0, \tag{55}$$

and, for $\ell=0$, this means, by differentiating (49),

$$\frac{1}{\dfrac{1}{2\pi}\displaystyle\int_0^{r_T}\frac{dr}{\sqrt{E_n-V}}}-\int_0^{r_T}\frac{u^2\,dr}{r^2}\gtrless 0. \tag{56}$$

The second integral is cut off at r_T because, in the WKB approximation, the rest is negligible. Now, since $(d/dr)r^2(dV/dr)\gtrless 0$, we have

$$V\gtrless V(r_T)+r\frac{dV}{dr_T}-\frac{\left(r^2\dfrac{dV}{dr}\right)_{r_T}}{r}$$

and, remembering that $E_n=V(r_T)$,

$$\frac{1}{2\pi}\int_0^{r_T}\frac{dr}{\sqrt{E_n-V}}\gtrless\frac{1}{2\pi}\frac{1}{\left(r^2\dfrac{dV}{dr}\right)_{r_T}^{1/2}}\int_0^{r_T}\frac{dr}{\sqrt{\dfrac{1}{r}-\dfrac{1}{r_T}}}=\frac{(r_T)^{3/2}}{4\left(r^2\dfrac{dV}{dr}\right)_{r_T}^{1/2}}=\frac{1}{4}\frac{\left(r^2\dfrac{dV}{dr}\right)_{r_T}}{\left(r\dfrac{dV}{dr}\right)_{r_T}^{3/2}}.$$

But, from (51),

$$\left(r\frac{dV}{dr}\right)_{r_T} \lesssim |E_n|,$$

and

$$\frac{1}{2\pi}\int_0^{r_T}\frac{dr}{\sqrt{E_n - V}} \gtrless \frac{1}{4}\frac{\left(r^2\frac{dV}{dr}\right)_{r_T}}{|E_n|^{3/2}},$$

and hence inequality (55), expressing the level ordering, gives

$$4|E_n|^{3/2} \gtrless \left(r^2\frac{dV}{dr}\right)_{r=r_T}\int_0^{r_T}\frac{u^2}{r^2}\,dr, \tag{57}$$

and hence

$$|u_n'(0)|^2 \cong \int_0^{r_T} u_n^2\frac{dV}{dr}\,dr \lessgtr \left(r^2\frac{dV}{dr}\right)_{r_T}\int_0^{r_T}\frac{u^2}{r^2}\,dr \lessgtr 4|E_n|^{3/2}, \tag{58}$$

which is what we wanted to "prove." In the sequence of inequalities (58) the sign of the Laplacian appears again, since we use the fact that $r^2(dV/dr)$ *increases* or *decreases.*

6. Bounds on the Ground State Energy for Power Potentials

For any potential one has the sum rule, for $\ell > 0$

$$\left\langle\frac{dV}{dr}\right\rangle = 2\ell(\ell+1)\langle r^{-3}\rangle, \tag{59}$$

and for $\ell = 0$

$$\left\langle\frac{dV}{dr}\right\rangle = \lim_{\ell\to 0} 2\ell(\ell+1)\langle r^{-3}\rangle = |u'(0)|^2. \tag{60}$$

In the special case

$$V = r^\nu, \quad \nu > 0, \tag{61}$$

(59) reduces to

$$\nu\langle r^{\nu-1}\rangle = 2\ell(\ell+1)\langle r^{-3}\rangle. \tag{62}$$

On the other hand, the energy of any state is given by the virial theorem

$$E = \left\langle V + \frac{1}{2}r\frac{dV}{dr}\right\rangle = \frac{\nu+2}{2}\langle r^\nu\rangle. \tag{63}$$

If we were using only the general property of convexity of $\log\langle r^\mu\rangle$ in μ (valid for *any* state), we could write

$$\frac{\log\langle r^{\nu-1}\rangle - \log\langle r^{-3}\rangle}{\nu+2} < \frac{\log\langle r^\nu\rangle - \log\langle 1\rangle}{\nu} \tag{64}$$

and, combining with (62) and (63),

$$E > \frac{2}{\nu+2}\left(\frac{2\ell(\ell+1)}{\nu}\right)^{\nu/(\nu+2)}, \tag{65}$$

a not terribly interesting inequality, becoming trivial for $\ell = 0$.

However, noticing that $V = r^\nu$ belongs, for $\nu \geqq 2$, to set A defined in (28), with $\alpha = 2$ and set B with $\alpha = (\nu+2)/2$, we can use instead the convexity or concavity of $\log f_\alpha(\mu)$, defined by (33) and get, for the ground-state energy,

$$E(0,\ell) \lessgtr \left(\frac{\nu+2}{2}\right)\frac{\Gamma\left(\frac{2\ell+3+\nu}{\alpha}\right)}{\Gamma\left(\frac{2\ell+3}{\alpha}\right)}\left[\frac{\Gamma\left(\frac{2\ell}{\alpha}\right)}{\Gamma\left(\frac{2\ell+2+\nu}{\alpha}\right)}\frac{2\ell(\ell+1)}{\nu}\right]^{\nu/(\nu+2)}$$

which leads to

$$E(0,\ell) \leqq \frac{\nu+2}{2}\frac{\Gamma\left(\frac{2\ell+3+\nu}{2}\right)}{\Gamma\left(\frac{2\ell+3}{2}\right)}\left[\frac{2\Gamma(\ell+2)}{\nu\Gamma\left(\frac{2\ell+2+\nu}{2}\right)}\right]^{\nu/(\nu+2)}, \tag{66}$$

$$E(0,\ell) \geqq \frac{\nu+2}{2}\frac{\Gamma\left(2\frac{2\ell+3+\nu}{\nu+2}\right)}{\Gamma\left(2\frac{2\ell+3}{\nu+2}\right)}\left[\frac{\Gamma\left(\frac{4\ell+\nu+2}{\nu+2}\right)}{\Gamma\left(\frac{4\ell+2\nu+4}{\nu+2}\right)}\frac{(\ell+1)(\nu+2)}{2\nu}\right]^{\nu/(\nu+2)} \tag{67}$$

These inequalities have non-trivial limits for $\ell \to 0$. It happens that the upper bound (66) is better, numerically, then the previously obtained upper bound [6], at least for $\nu \geqq 4$:

$$E(0,\ell) \leqq \left(\frac{\nu+2}{\nu}\right)\left(\frac{\nu}{2}\right)^{2/(\nu+2)}\left(\ell+\frac{\nu+4}{4}\right)^{2\nu/(\nu+2)}. \tag{68}$$

7. Concluding Remarks

We have shown various applications to the Schrödinger equation of the main theorem of this paper, including, as an illustration, a comparison with experimental data on quarkonium physics. This list, of course, is not limitative. The fact is, we believe that the theorem, though motivated by some of the applications, transcends them and might later be used in a completely different area of mathematical physics.

Independently, we have come close to the proof of a conjecture on the wave function at the origin for radial excitations. This results, or a similar one, might be relevant in quarkonium physics or in atomic physics, where direct calculations of the wave function at the origin are difficult and unstable.

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