CERN-TH.4998/88

SOME COMPARISON THEOREMS ON MOMENTS IN THE GROUND STATE *)
AND IN EXCITED STATES OF A TWO-BODY SYSTEM

A. Martin
CERN - Geneva

ABSTRACT

We prove and extend some conjectures by Dib, Franzini and Gilman on the comparison of expectation values of r^ν in the ground state and the first radial excited state of a two-body system for a given, non-zero angular momentum. One of the by-products is that for usual potentials, the overall splitting of the P states is likely to be smaller for the excited state than for the ground state. We also make comparisons between the ground state and angular excitations and prove that the expectation values of r^ν , $-3 < \nu < 0$, decrease rapidly with the angular momentum for concave potentials, which explains why the fine splitting of quarkonium levels is getting small for large ℓ .

*) This preprint is an enlarged version of CERN-TH.4972/
/88 (1988).

Recently, Dib, Gilman and Franzini [1] have studied the P state splittings by spin-dependent interactions in quarkonium, both for the ground state and for the first radial excited state. On this occasion, they have made interesting numerical observations on the ratios

$$R(\nu) = \frac{\langle r^\nu \rangle_{\text{first radial excited state}}}{\langle r^\nu \rangle_{\text{ground state}}} \quad (1)$$

in particular for $\nu = -1$ and $\nu = -3$. Here we would like to prove these conjectures, made essentially for power potentials, and try also to generalize to larger classes of potentials. We shall also compare the expectation values of r^ν for different angular momenta later on.

The starting point is a sum rule which is based on the well-known formula for the wave function at the origin for the $\ell = 0$ partial wave (we take $2\mu = \hbar = 1$)

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

If we consider now a state with angular momentum $\ell > 0$ (strictly!) we can think of it as an $\ell = 0$ state with an effective potential

$$W(r) = V(r) + \frac{\ell(\ell+1)}{r^2} \quad (3)$$

where V is a "good" potential, such that $\lim_{r \rightarrow 0} r^2 V = 0$, and then, since the reduced wave function behaves as $r^{\ell+1}$, $u'(0) = 0$. Hence we get

$$0 = \int u^2 \left[\frac{dV}{dr} - 2 \frac{\ell(\ell+1)}{r^3} \right] dr \quad (4)$$

This sum rule can be found in a physics report by Grosse and myself [2] and has also recently been rederived independently by Cahn [3].

From the sum rule, one obtains in particular two simple results:

i) for the logarithmic potential, $V = \lambda \log r$ we get, for any state

$$\lambda \left\langle \frac{1}{r} \right\rangle = 2 \ell(\ell+1) \left\langle \frac{1}{r^3} \right\rangle \quad (5)$$

and therefore

$$R(-1) = R(-3) \quad , \quad (6)$$

or, for a given l ,

$$\frac{\langle \frac{1}{r} \rangle}{\langle \frac{1}{r^3} \rangle} = \text{const.},$$

independent of the radial excitation.

ii) For the linear potential, $V = \mu r$

$$R(-3) = R(0) = 1, \quad (7)$$

since the wave function is normalized. So $\langle 1/r^3 \rangle$ is independent of the radial excitation.

We would like to go beyond these simple observations made also independently by R. Cahn [3]. The strategy we shall use follows essentially the techniques developed in Ref. [2]. First we notice that $R(v)$ cannot take three times the same value, i.e., $R = R(v_1) = R(v_2) = R(v_3)$, with $v_1 > v_2 > v_3$, is impossible. Then we would have

$$\int (u_1^2 - R u_0^2) [r^{v_1} + A r^{v_2} + B r^{v_3}] dr = 0, \quad (8)$$

where u_0 is the ground state wave function and u_1 is the first radial excitation. $u_1^2 - R u_0^2$ vanishes at most twice for $0 < r < \infty$. By combining the Schrödinger equations

$$\begin{aligned} -u_1'' + \left(V(r) + \frac{l(l+1)}{r^2} \right) u_1 &= E_1 u_1 \\ -u_0'' + \left(V(r) + \frac{l(l+1)}{r^2} \right) u_0 &= E_0 u_0 \end{aligned}$$

we get

$$-u_0 u_1' + u_1 u_0' = (E_1 - E_0) \int_0^r u_1 u_0 dr' = -(E_1 - E_0) \int_r^\infty u_1 u_0 dr'$$

hence, if r_0 is the unique zero of u_1 ,

$$\left| \frac{u_1}{u_0} \right| \quad \text{decreases for } r < r_0$$

$$\left| \frac{u_1}{u_0} \right| \quad \text{increases for } r > r_0$$

If we restrict ourselves to potentials such that $V(r)$ increases to $+\infty$ and $V(r)/r^2 < \text{const.}$, $|u_1/u_0|$ increases from zero to infinity in the interval $r_0 < r < \infty$. Indeed, it can be shown [2] then that the WKB approximation is valid for $r \rightarrow \infty$ and hence

$$\left| \frac{u_1}{u_0} \right| \sim \text{const} \exp \left[\int_c^r \frac{E_1 - E_0}{2\sqrt{V(r')}} dr' \right] \quad (9)$$

The integral under the exponent diverges if $V(r)/r^2$ remains bounded. Therefore, $u_1^2 - Ru_0^2$ has one and only one zero in $r_0 < r < \infty$.

The same result holds if $V(r) \rightarrow 0$, because then

$$\left| \frac{u_1}{u_0} \right| \sim \text{const} \exp \left[r(\sqrt{-E_0} - \sqrt{-E_1}) + \frac{1}{2} \int_c^r V(r') dr' \left[\frac{1}{\sqrt{-E_0}} - \frac{1}{\sqrt{-E_1}} \right] \right] \quad (10)$$

Now the quantity

$$r^{\nu_1} + A r^{\nu_2} + B r^{\nu_3}$$

vanishes at most twice in $0 < r < \infty$. If $u_1^2 - Ru_0^2$ vanishes only once, at $r = r_1$ we can take $B = 0$ and adjust A so that $r_1^{\nu_1} + A r_1^{\nu_2} = 0$. Then

$$\int (u_1^2 - R u_0^2) (r^{\nu_1} + A r^{\nu_2}) dr$$

is positive and therefore

$$R(\nu_1) \neq R(\nu_2)$$

If $u_1^2 - Ru_0^2$ vanishes twice, at $r = r_1$ and $r = r_2$, we can solve for A and B so that

$$r_1^{\nu_1} + A r_1^{\nu_2} + B r_1^{\nu_3} = r_2^{\nu_1} + A r_2^{\nu_2} + B r_2^{\nu_3} = 0.$$

Then we find that the integral (8) is positive. Therefore it is impossible to have

$$R(\nu_1) = R(\nu_2) = R(\nu_3).$$

Assuming $V(r)/r^2$ bounded for $r \rightarrow \infty$, $|u_1/u_0|$ goes to infinity for $r \rightarrow \infty$ and it follows from this that $R(\nu) \rightarrow +\infty$ for $\nu \rightarrow \infty$. Indeed given M arbitrary, we can find R so that $|u_1/u_0|^2 > M$ for $r > R$. Then

$$R(\nu) > \frac{M \int_R^\infty u_0^2 \left(\frac{r}{R}\right)^\nu dr}{\int_0^R u_0^2 \left(\frac{r}{R}\right)^\nu dr + \int_R^\infty u_0^2 \left(\frac{r}{R}\right)^\nu dr}.$$

For $\nu \rightarrow \infty$

$$\int_0^R u_0^2 \left(\frac{r}{R}\right)^\nu dr \rightarrow 0$$

and

$$\int_R^\infty u_0^2 \left(\frac{r}{R}\right)^\nu dr \rightarrow \infty.$$

Hence, given ε , $R(\nu) > M - \varepsilon$ for ν big enough. Since M is as large as we wish we deduce that $R(\nu) \rightarrow +\infty$. $R(\nu)$ is defined for $\nu \geq -(2\ell+3)$ because of the behaviour of u_0 and u_1 at the origin.

From the previous results we deduce that there are only two possibilities

- Either $R(\nu)$ is monotonously increasing from $\nu = -(2\ell+3)$ to $\nu = \infty$
- or $R(\nu)$ has a unique minimum. This means that we have always

$$R(\nu_2) < \sup \{ R(\nu_1), R(\nu_3) \}, \quad (10)$$

if $\nu_1 > \nu_2 > \nu_3$.

If we take the moments considered by Dib, Franzini and Gilman, we have for instance:

$$\frac{\langle \frac{1}{r} \rangle_1}{\langle \frac{1}{r} \rangle_0} < \sup \left\{ 1, \frac{\langle \frac{1}{r^3} \rangle_1}{\langle \frac{1}{r^3} \rangle_0} \right\} \quad (11)$$

Similarly one has

$$R(-1) < \sup \{ 1, R(-2) \} \quad (12)$$

This is amusing for

$$R(-2) = \frac{(2l+1) \int \frac{v_1^2 dr}{r^2}}{(2l+1) \int \frac{v_0^2 dr}{r^2}} = \frac{\frac{dE_1}{dl}}{\frac{dE_0}{dl}} \quad (13)$$

If we look at the upsilon spectrum we have

$$\frac{E(l=1, n=1) - E(l=0, n=1)}{E(l=1, n=0) - E(l=0, n=0)} \cong \frac{220 \text{ MeV}}{440 \text{ MeV}} = 0.5. \quad (14)$$

So it is extremely likely that $R(-2)$ is less than unity and we conclude that for the upsilon P states it is very probable that

$$\frac{\langle \frac{1}{r} \rangle_{n=1}}{\langle \frac{1}{r} \rangle_{n=0}} < 1. \quad (15)$$

Remarkably, we reach this conclusion without knowing the potential.

Now we shall make use of the sum rule (4) and first consider for simplicity attractive power potentials

$$V = \varepsilon(\alpha) r^\alpha, \quad (16)$$

where ε is the sign function. Then we get

$$\alpha \varepsilon(\alpha) \langle r^{\alpha-1} \rangle = 2 l(l+1) \langle r^{-3} \rangle. \quad (17)$$

Hence

$$R(\alpha-1) = R(-3).$$

Then, from property (10), we get by choosing conveniently v_1, v_2, v_3

$$R(v) \leq 1 \quad \text{for } -3 \leq v \leq 0 \quad \text{if } \alpha \leq 1, \quad (18)$$

$$R(-3) > 1 \quad \text{if } \alpha > 1, \quad (19)$$

$$R(-1) > R(-3) \quad \text{if } \alpha < 0, \quad (20)$$

$$R(-1) < R(-3) \quad \text{if } \alpha > 0. \quad (21)$$

Can we say something for non power potentials? Here we shall follow what has been done in the special case of $R(-2)$ in Ref. [2] p. 355.

First we compare $R(-3)$ to 1. Let us prove that if $(d/dr)r^4(d^2V/dr^2)$ has a given sign for all r , $R(-3)$ differs from unity. Assume $R(-3) = 1$ then

$$0 = \int (v_1^2 - v_0^2) \left[\frac{dV}{dr} + \frac{A}{r^3} + B \right] = 0 \quad (22)$$

We can adjust A and B so that $dV/dr + A/r^3 + B$ vanishes at $r = r_1$ and r_2 , the zeros of $u_1^2 - u_0^2$ (if there is only one zero we can take $A = 0$). Then

$$\frac{d}{dr} \left[\frac{dV}{dr} + \frac{A}{r^3} + B \right] = \frac{d^2V}{dr^2} - \frac{3A}{r^4} = \frac{z}{r^4}$$

and

$$z' = \frac{d}{dr} r^4 \frac{d^2V}{dr^2} = r^4 V''' + 4r^3 V''.$$

If z' has a constant sign, z is monotonous and $dV/dr + A/r^3 + B$ vanishes at most twice. Therefore, it vanishes only at $r = r_1$ and $r = r_2$ and the integral has a constant sign, which contradicts (22). To find the sign of $R(-3)-1$ we use the family of potentials

$$V_\lambda = \lambda r^\alpha + (1-\lambda) V(r).$$

$R(-3)$ is a continuous function of λ and for $\lambda = 0$ the sign of $R(-3)$ is known. Choosing conveniently α we get

$$R(-3) > 1 \quad \text{if} \quad rV''' + 4V'' > 0 \quad (23)$$

$$R(\nu) < 1 \quad \text{for} \quad -3 \leq \nu < 0 \quad \text{if} \quad rV''' + 4V'' < 0. \quad (24)$$

(In particular $R(-3) < 1$, $R(-1) < 1$.) If it happens that $u_1^2 - u_0^2$ has a single zero (which could be the case if $V'' < 0$) then it suffices to take $V'' < 0$ to get (24), however, $V'' < 0$ follows from $(d/dr)r^4(d^2V/dr^2) < 0$ by integration.

Most existing potential models of quarkonium satisfy condition (24). For instance, this is the case of power superpositions with $\alpha \leq 1$. In physical terms the meaning of (24) is that, except for miraculous sign arrangements, we expect the overall P state splittings to shrink when one goes from the ground state to the first radial excitation, since in practically all potential models the quantities controlling the fine splittings are expectation values of r^ν , $-3 < \nu < 0$, or superpositions. The special case $\nu = -2$ in (24) was already treated in Ref. [2]. However, the condition found was slightly different:

$$R(-2) = \frac{\frac{dE_1}{d\epsilon}}{\frac{dE_0}{d\epsilon}} < 1 \quad \text{if} \quad 3V'' + rV''' < 0.$$

In reality, a subtlety was overlooked: sometimes $u_1^2 - u_0^2$ has only one zero and then one must make sure that the quantity multiplying it has only one zero. By multiplying $3V'' + rV'''$ by r^2 and integrating, one gets $V'' < 0$ which is sufficient, provided $\lim_{r \rightarrow 0} r^3 V'' = 0$. This is not the case if the potential is singular like $1/r$ or worse. So condition $4V'' + rV''' < 0$ is much better, because it suffices for all cases such that $\lim_{r \rightarrow 0} r^2 V'' = 0$. Almost all potentials used for quarkonium satisfy this condition and by integration we get

$$E(n=1, l=1) - E(n=1, l=0) < E(n=0, l=1) - E(n=0, l=0)$$

which is true for the upsilon system as seen in (14).

One would be tempted to believe that (24) would hold under the weaker condition $V'' < 0$. This does not seem to be the case. Indeed, from (4) one can get, by integration by parts

$$2 \ell(\ell+1) \int \frac{u_1^2 - u_0^2}{r^3} dr = \int_0^\infty V''(r) I(r) dr \quad (25)$$

where

$$I(r) = \int_r^\infty (u_1^2 - u_0^2) dr' = - \int_r^\infty (u_1^4 - u_0^4) dr'$$

In the limit case $V(r) = r$, $u_1^2 - u_0^2$ vanishes twice for ℓ strictly positive. Otherwise one would get a contradiction with the sum rule (4). Then $I(r)$ is not positive definite and this will also be the case for potentials close to the linear potential like

$$V = r - \varepsilon \theta(r-R),$$

for ε sufficiently small. Then one can get an arbitrary sign for (25) by choosing R conveniently.

The other result to generalize to non power potential concerns the comparison of $R(-1)$ and $R(-3)$. Again we assume that $R(-1) = R(-3) = R$ and get

$$\int (u_1^2 - R u_0^2) \left[\frac{dV}{dr} + \frac{A}{r^3} + \frac{B}{r} \right] dr = 0$$

We adjust A and B in the bracket so that it vanishes at $r = r_1$ and r_2 the zeros of $u_1^2 - R u_0^2$ and invent a sufficient condition to make sure that it does not vanish anywhere else. Clearly this condition is

$$\frac{d}{dr} r^3 \frac{d}{dr} r \frac{dV}{dr}$$

of constant sign. Then, using again the trick of the auxiliary power potential we get

$$R(-1) > R(-3) \quad \text{if} \quad \frac{d}{dr} r^3 \frac{d}{dr} r \frac{dV}{dr} < 0$$

(26)

$$R(-1) < R(-3) \quad \text{if} \quad \frac{d}{dr} r^3 \frac{d}{dr} r \frac{dV}{dr} > 0.$$

Now we turn to the comparison of the expectation values of r^v , $-3 < v < 0$, for fixed n (mostly $n = 0$) and variable angular momentum ℓ .

The reduced wave function for $n = 0$ has no nodes and by an argument analogous to the one presented at the beginning of this paper, it is easy to prove that

$$\frac{d}{dr} \left[u_{n=0,L}(r) / u_{n=0,\ell}(r) \right] > 0 \quad \text{for } L > \ell \quad (27)$$

From this it follows that:

$$\begin{aligned} \langle r^v \rangle_{n=0,\ell} & \text{ increases with } \ell & \text{for } v > 0 \\ \langle r^v \rangle_{n=0,\ell} & \text{ decreases with } \ell & \text{for } v < 0 \end{aligned} \quad (28)$$

To prove this, it is sufficient to look at the sign of

$$\langle r^v \rangle_L - \langle r^v \rangle_\ell = \int_0^\infty (u_L^2 - u_\ell^2) (r^v - r_0^v) dr, \quad (29)$$

where r_0 is the unique zero of $u_L - u_\ell$.

Since fine splittings of quarkonium are usually controlled by $\langle r^v \rangle$, $-3 < v < 1$, we see that these splittings decrease with ℓ .

For concave potentials which are the only acceptable quark-antiquark potential according to lattice QCD [4] (at least for infinitely heavy quarks), we get from the sum rule (4):

$$\begin{aligned} 2L(L+1) \langle r^{-3} \rangle_{n=0,L} - 2\ell(\ell+1) \langle r^{-3} \rangle_{n=0,\ell} = \\ \int (u_L^2 - u_\ell^2) \left(\frac{dV(r)}{dr} - \frac{dV(r_0)}{dr} \right) dr < 0. \end{aligned} \quad (30)$$

Hence

$$2\ell(\ell+1) \langle r^{-3} \rangle_{n=0,\ell}$$

is decreasing with ℓ if V'' is negative.

The other moments are also expected to decrease from Hölder's inequalities obtained by Common and myself [5,6] for potentials such that

$$V'' - rV' \leq 0 \quad (31)$$

a condition always satisfied by concave potentials, to get

$$\begin{aligned} \langle r^{-2} \rangle_{n=0, l \geq 1} &< \left(\frac{2}{l(l+1)} \right)^{2/3} \left(\frac{2l}{2l+1} \right)^{1/3} \langle r^{-3} \rangle_{n=0, l=1}^{2/3} \\ \langle r^{-1} \rangle_{n=0, l \geq 1} &< \left(\frac{2}{l(l+1)} \right)^{1/3} \left(\frac{2l}{2l+1} \right)^{1/3} \langle r^{-3} \rangle_{n=0, l=1}^{1/3}. \end{aligned} \quad (32)$$

For the specific potential

$$V = -\frac{a}{r} + br + c \quad (33)$$

we have even better. For arbitrary n we get from (4), using Hölder's inequality:

$$2l(l+1) \langle r^{-3} \rangle < a \langle r^{-3} \rangle^{2/3} + b. \quad (34)$$

This third degree inequality becomes asymptotically an equality for large l because the wave function becomes localized at the minimum of the effective potential and

$$\langle r^{-3} \rangle \sim b/[2(l+1)a]. \quad (35)$$

This can be made quantitative in the case $n = 0$ by using Common's inequalities [6,7], for potentials with positive Laplacian:

$$\begin{aligned} a \langle r^{-3} \rangle^{2/3} \left(\frac{4l^2}{(2l+1)(2l+2)} \right)^{1/3} + b &< 2l(l+1) \langle r^{-3} \rangle \\ &< a \langle r^{-3} \rangle^{2/3} \left(\frac{2l}{2l+1} \right)^{1/3} + b. \end{aligned} \quad (36)$$

Finally we notice that (31) implies that $n = 0$ energy levels are concave in l [8]. Therefore

$$(2l+1) \langle r^{-2} \rangle_{n=0, l}$$

decreases with l .

These inequalities give a qualitative and semi-quantitative understanding of that the fine splittings of the D states are much smaller than those of the P states as indicated, for instance, by the explicit calculations of Kwong, Rosner and Quigg [9].

ACKNOWLEDGEMENTS

I would like to thank Paula Franzini and Juliet Lee-Franzini for stimulating discussions. I also warmly thank G. Bellettini and M. Greco for their hospitality at La Thuile where some results of this paper were obtained.

REFERENCES

- [1] C.O. Dib, F.J. Gilman and P.J. Franzini, preprint CERN-TH.4847/87, SLAC-PUB-4402 (1987).
- [2] H. Grosse and A. Martin, Physics Reports 60 (1980) 341.
- [3] R. Cahn, manuscript communicated by P. Franzini.
- [4] E. Seiler, Phys. Rev. D18 (1978) 482.
- [5] A.K. Common and A. Martin, J. Phys. A20 (1987) 4247.
- [6] A. Martin, in "Recent Developments in Mathematical Physics", Editors. H. Mitter and L. Pittner, Springer Verlag, Berlin, Heidelberg (1987), p.53.
- [7] A.K. Common, J. Phys. A18 (1985) 2219.
- [8] A.K. Common and A. Martin, Europhys. Lett. 4 (1987) 1349.
- [9] W. Kwong, J.L. Rosner and C. Quigg, Ann. Rev. Nucl. Part. Sci. 37 (1987) 325.