

## THE BERTLMANN-MARTIN INEQUALITIES AND THE UNCERTAINTY PRINCIPLE

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### Abstract

A lower bound to  $\langle r \rangle_{1s}$  is established from the Thomas-Reiche-Kuhn sum rule applied to the reduced equation for the s-states. It is linked to the average value of  $\langle r^2 \rangle_{1s}$ . We discuss, on few examples, how the use of approximate value for  $\langle r^2 \rangle_{1s}$ , derived from the generalized Bertlmann and Martin inequalities, preserves the lower bound character of  $\langle r \rangle_{1s}$ . Finally, by using the uncertainty principle and the uncertainty in the radial position, we derive a low bound to the ground state kinetic energy.

**Keywords:** “Bertlmann-Martin inequalities”, “uncertainty principle”, “ground state kinetic energy”, “low bounds”.

### I- THE LOWER BOUND TO $\langle r \rangle_{1s}$

In two body system, the average of  $r$  yields the mean distance between the two particles. In some respect, this quantity is more useful than the mean square radius ( $\langle r^2 \rangle$ ). However, it is rather difficult to reach experimentally, except in some special cases. One of them is the method used to determine the size of the He dimmer [1], a quasi macroscopic object. Therefore, a bound to  $\langle r \rangle$  is a valuable piece of information in many areas of the few body physics. It plays an important role in the determination of the central ground state density from its moments [2, 3].

In  $D = 3$ , the reduced s-states wave function

$$U_{n0}(r) = r R_{n0}(r)$$

satisfies a differential equation similar to the  $D = 1$  Schrödinger equation; the solutions are restricted to the right half plane.

It is possible to apply the original Bertlmann- Martin inequality [BMI] in 1 dimension [4] to the s-state spectrum with the appropriate modifications. We, briefly, recall the derivation of the BMI from the Thomas-Reiche-Kuhn dipole sum rule in the case of the s-states.

$$2 \sum_n (E_{n0} - E_{10}) |\langle n0|r|10 \rangle|^2 = 1 \quad (1)$$

where  $E_{n0}$  is the energy of the  $n^{\text{th}}$   $s$  state  $|n0\rangle$ . We use  $\hbar = m = 1$

By replacing  $(E_{n0} - E_{10})$  by  $(E_{20} - E_{10})$ , we obtain:

$$2(E_{20} - E_{10}) \sum_n |\langle n0|r|10 \rangle|^2 \leq 1 \quad (2)$$

Then, by using the closure approximation and taking into account that  $\langle 10|r|10 \rangle = \langle r \rangle_{1s} \neq 0$ , we get:

$$2(E_{20} - E_{10})(\langle r^2 \rangle_{1s} - \langle r \rangle_{1s}^2) \leq 1 \quad (3)$$

Here,  $\langle r^2 \rangle_{1s}$  represents  $\langle 10|r^2|10 \rangle$ . Consequently, an absolute lower bound to  $\langle r \rangle$  is derived:

$$\langle r \rangle_{1s} \geq \sqrt{\langle r^2 \rangle_{1s} - \frac{1}{2(E_{20} - E_{10})}} \quad (4)$$

This bound is valid for any local potential having at least one bound excited state. The radial excitation energy and  $\langle r^2 \rangle_{1s}$  are needed to fix the lower bound (4). Since it is not easy to measure  $\langle r^2 \rangle_{1s}$ , it is useful to have an estimation of it. The corrected Bertlmann-Martin relationships provide us with good approximate value of  $\langle r^2 \rangle$  for a wide class of potentials [5, 6]. However, although this approximate value is often accurate to the 1% level or better, there is no guarantee that it ensures a strict low bound when inserted in (4). Therefore, our task is to investigate for which kind of potentials its use still yields a lower bound.

## II-ESTIMATION OF $\langle r^2 \rangle_{1s}$

In few and many-body systems, the average value of  $r^2$ , the mean square radius, is usually interpreted as a measure of the system size. As we noticed it previously, the knowledge of  $\langle r^2 \rangle$  is required when we establish a lower bound to  $\langle r \rangle$ .

By minoring the Thomas-Reiche-Kuhn dipole sum rule, Bertlmann and Martin derived inequality relating the ground state average value of  $r^2$  to the lowest dipole excitation energy [4]. In the framework of 3 dimensions, they obtained:

$$\langle r^2 \rangle_{1s} \leq \frac{3\hbar^2}{2m} \frac{1}{E_{11} - E_{10}} \quad (5)$$

Here,  $E_{11}$  is the lowest  $p$ -state energy. For a particle in a central, spherically symmetric potential,  $m$  is the particle mass, which is replaced by the reduced mass in a two-body problem.

We recall that the exact value of  $\langle r^2 \rangle_{1s}$  is defined by:

$$\langle r^2 \rangle_{1s} = \int_0^{\infty} |R_{10}(r)|^2 r^4 dr \quad (6)$$

Note that the angular part of the wave function has been factorized and normalized separately. Eq. (5) turns to equality in the case of the harmonic oscillator, but is off by about 25% for the Coulomb potential. Bertlmann and Martin proposed a phenomenological correction factor which transforms Eq. (5) into equality for the case of the Coulomb force.

On the other hand, it has been shown that an empirical generalized correction factor turns inequality (5) into equality for a wide class of potentials [5, 6]. It gives:

$$\langle r^2 \rangle_{1s} \cong \frac{3}{2} \frac{1}{E_{11} - E_{10}} \left(1 - \frac{1}{4} C(1)\right) \quad (7)$$

$$C(1) = \left( \frac{E_{20} + E_{10} - 2E_{11}}{E_{20} - E_{10}} \right)^2 \quad (8)$$

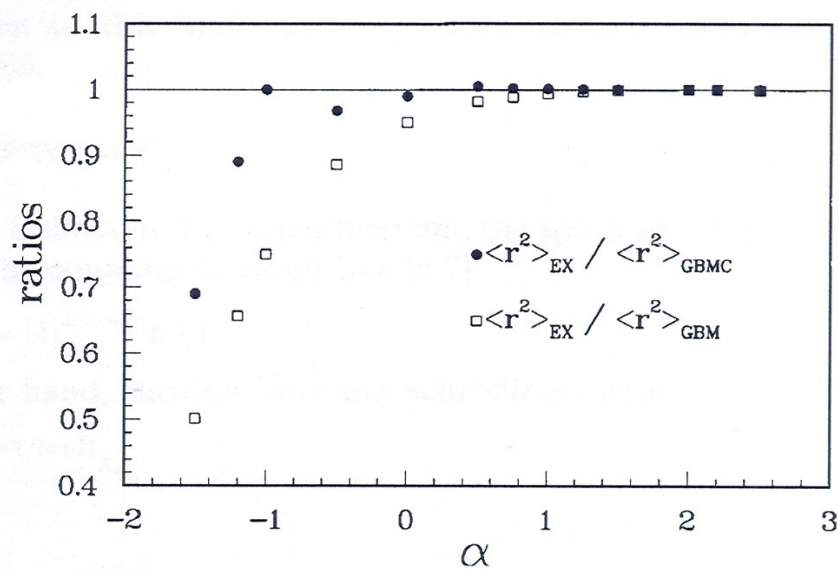
To illustrate the usefulness of (8), exact values of  $\langle r^2 \rangle$  have been compared to the predictions of Eq. (7), for power-law potentials [6] defined by:

$$V(r) = \text{sgn}(\alpha) \cdot \lambda r^\alpha \quad -1.5 < \alpha < 2.5 \quad (9)$$

The results are displayed in Fig. 1 as the ratios  $\langle r^2 \rangle_{EX} / \langle r^2 \rangle_{GBM}$  and  $\langle r^2 \rangle_{EX} / \langle r^2 \rangle_{GBMC}$  where  $E_X$  means exact value, GBM and GBMC, the predictions of Eq.(7) without and with the correction factor  $C(1)$ , respectively.

In this context, "exact" means analytical or accurate numerical value.

Due to the fact that the results are independent on the strength  $\lambda$  for  $\alpha \geq -2$  [6], the calculations have been made for  $\lambda=1$ .



**Fig.1:** The ratios  $\langle r^2 \rangle_{EX} / \langle r^2 \rangle_{GBM}$  and  $\langle r^2 \rangle_{EX} / \langle r^2 \rangle_{GBMC}$  in the case of power-law potentials.

As noticed in [6], the results show the regular variation of the bound to  $\langle r^2 \rangle_{1s}$  with respect to  $\alpha$  and its increasing saturation as  $\alpha$  approaches 2. For  $\alpha \geq -1$ , the correction factor (8) has a sensible effect and we have a good agreement with the exact value. For  $\alpha = -0.5$ , we found the worst discrepancy which reaches about 2%. Below  $\alpha = -1$ , the correction improves the saturation but it is not sufficient; it underlines that the universal character of the correction factor is by no means obvious.

It is tempting to check how the lower bound (4) is close from the exact  $\langle r \rangle$  value when calculations are performed with Eq. (7) for  $\langle r^2 \rangle$ .

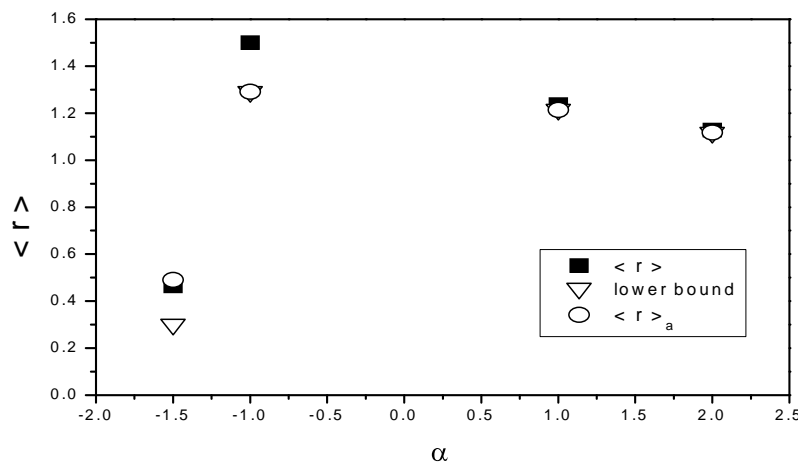
### III- ILLUSTRATIVE EXAMPLES

3 kinds of potentials are considered: the power-law potentials, the modified Pöschl-Teller and the Hulthén potentials. The power-law potentials have retained a lot of interest as confining potentials for the non-relativistic description of heavy quark systems [7]. The Hulthén and Pöschl-Teller potentials have been widely studied, respectively, by Aguilera-Navarro and *al* [8] and Nieto [9].

#### III.1. Power-law Potentials

These potentials are defined by Eq. (9). Calculations have been made with a strength  $\lambda = 1$ , for  $\alpha = -1.5, -1.0$  (Coulomb potential), 1.0 (linear potential) and 2.0 (harmonic oscillator).

Testing Eq. (4) is achieved by comparing the exact value  $\langle r \rangle$  to the Bertlmann-Martin (B.M) bound (4),  $\langle r \rangle_{BM}$ , calculated with the exact value of  $\langle r^2 \rangle$ , and to this bound  $\langle r \rangle_a$ , using the approximate expression (7) of  $\langle r^2 \rangle$ . The results are displayed in Fig.2 for the four values of  $\alpha$ .



**Fig.2:** The exact value  $\langle r \rangle$  is compared to the Bertlmann-Martin (B.M) bound (4),  $\langle r \rangle_{BM}$ , calculated with the exact value of  $\langle r^2 \rangle$ , and to this bound  $\langle r \rangle_a$ , using the approximate expression (7) of  $\langle r^2 \rangle$ .

We note that the results reflect the tendency already discussed in section II. For  $\alpha < -1$ , the empirical correction factor (8) is not as efficient as for larger values of  $\alpha$ , so, the Bertlmann-Martin bound is less saturated as  $\alpha$  decreases. Consequently, for  $-2 < \alpha < -1$ ,  $\langle r \rangle_a$  is not necessary a lower bound. For instance, for  $\alpha = -1.5$ ,  $\langle r \rangle_a$  over-passes the exact value by about 5%. However, for  $\alpha \geq -1$ , it is still a low bound.

### III.2. Modified Pöschl-Teller Potential

We follow the notation of Flügge [10]:

$$V(r) = -\frac{1}{2} \frac{\lambda(\lambda-1)}{(\cosh \alpha r)^2} \quad (10)$$

For the sake of simplicity we have chosen  $\alpha = 1$ .

The Pöschl-Teller potential possesses a finite number of bound states depending on the coupling constant  $\lambda$  which must sit above a critical value depending on the angular momentum. Since  $\langle r^2 \rangle_{1s}$  requires  $E_{2s}$ , we have to ensure that the 2s state is bound, which means  $\lambda \geq 4$ .

Calculations have been made for  $\lambda = 5, 6, 9$  and  $12$ ; the results are displayed in Table 1. As before, the exact value  $\langle r \rangle$  is compared to the BM bound (4) and  $\langle r \rangle_a$ .

**Table 1.** Case of Pöschl-Teller potential. The exact value  $\langle r \rangle$  is compared to the lower bound (4) and to this bound using the approximate expression (7) for  $\langle r^2 \rangle$ .

$\lambda$	$\langle r \rangle$	Lower bound	$\langle r \rangle_a$
5	0.662	0.636	0.630
6	0.571	0.559	0.553
9	0.429	0.423	0.422
12	0.358	0.354	0.354

The general tendency is similar to the one observed for power law-potentials (9) with  $\alpha \geq -1$ . For  $\lambda > 12$ , we observe the same situation as for the harmonic oscillator (the correction factor (8) is useless in this case).

### III.3. Hulthén Potential

In this example, we consider the following potential:

$$V(r) = -\lambda \frac{e^{-r/a}}{1 - e^{-r/a}} \quad (11)$$

In order to obtain bound states, we must choose the coupling constant  $\lambda$  above critical values. We display, in Table 2., the results for 3 values of  $\lambda$ . We compare, as for the preceding cases, the exact value  $\langle r \rangle$  to the B.M bound and  $\langle r \rangle_a$ .

**Table 2.** Same as in Table 1. for the Hulthén potential.

$\lambda$	$\langle r \rangle$	Lower bound	$\langle r \rangle_a$
3	0.509	0.426	0.435
5	0.302	0.257	0.259
7	0.215	0.184	0.185

We see that, for deep states, the results are comparable to those obtained for the Coulomb potential.  $\langle r \rangle_a$  is a lower bound for the 3 values of the coupling constant  $\lambda$ .

#### IV- LOWER BOUND FOR GROUND STATE KINETIC ENERGY

The uncertainty in radial position can be obtained as follows:

$$\Delta r = \sqrt{\langle r^2 \rangle - \langle r \rangle^2} \quad (12)$$

Since  $\langle r \rangle_{1s}$  and  $\langle r^2 \rangle_{1s}$  are linked by inequality (4), we get:

$$(\Delta r)_{1s} \leq \frac{1}{\sqrt{2(E_{20} - E_{10})}} \quad (13)$$

Thus, the uncertainty in radial position for the  $s$ -state is directly linked to the inverse of the radial excitation energy. It yields an upper bound (u.b); we compare it to the exact values for the potentials used previously. The results are listed in Table 3.

**Table 3.** Comparison between  $(\Delta r)$  exact and its upper bound (u.b) for power-law potentials (left), Pöschl-Teller potentials (center) and Hulthén potential (right).

$\alpha$	$\Delta r$	(u.b)	$\frac{\Delta r}{(u.b)}$	$\lambda$	$\Delta r$	(u.b)	$\frac{\Delta r}{(u.b)}$	$\lambda$	$\Delta r$	(u.b)	$\frac{\Delta r}{(u.b)}$
-1.5	0.307	0.468	0.656	5	0.304	0.355	0.856	3	0.297	0.408	0.728
-1.0	0.866	1.155	0.75	6	0.259	0.282	0.918	5	0.175	0.235	0.745
1.0	0.551	0.596	0.92	9	0.188	0.202	0.931	7	0.124	0.167	0.74
2.0	0.476	0.500	0.95	12	0.155	0.165	0.939				

The ratio between the upper bound (u.b) and the exact value is also displayed. We note that it is approaching 1 as the particle is more confined or more bound.

The expectation value of the squared linear momentum is the sum of the radial momentum part and the orbital momentum part

$$P_{nlm}^2 = p_r^2 + \frac{l(l+1)}{r^2} \hbar^2 \quad (14)$$

For the ground state, we have  $P_{n00}^2 = P_r^2$ ; since  $\langle p_r \rangle = 0$ , it leads to:  $\Delta p_r = \sqrt{\langle p_r^2 \rangle}$

By using the uncertainty principle:

$$\Delta r \cdot \Delta p_r \geq 1/2 \quad \text{and} \quad \langle T \rangle_{1s} = \frac{\langle P_r^2 \rangle_{1s}}{2} \quad (15)$$

we can derive an inequality for the ground state kinetic energy:

$$\langle T \rangle_{1s} \geq \frac{1}{4}(E_{20} - E_{10}) = \langle T \rangle_b \quad (16)$$

To fix ideas, the low bound  $\langle T \rangle_b$  is compared to the one derived by Bertlmann and Martin [4], namely  $\langle T \rangle_{1s} \geq \frac{3}{4}(E_{11} - E_{10}) = \langle T \rangle_{B.M}$  and to the exact value of the ground state kinetic energy  $\langle T \rangle_{EX}$ . For the harmonic oscillator and for Pöschl-Teller potential ( $\lambda = 9$ ), the results are summarized in Table 4.

**Table 4.** Comparison between  $\langle T \rangle_{1s}$  exact and its bounds,  $\langle T \rangle_{B.M}$  and  $\langle T \rangle_b$ , derived respectively from the Bertlmann-Martin inequality and the uncertainty principle.

	$\langle T \rangle_{EX}$	$\langle T \rangle_{B.M}$	$\langle T \rangle_b$
Harmonic oscillator	0.75	0.75	0.25
Pöschl-Teller Potential	5.147	5.122	3.063

We note that the bound,  $\langle T \rangle_b$ , derived from the uncertainty principle and the evaluation of  $\Delta r$ , seems less efficient than the one derived by Bertlmann-Martin,  $\langle T \rangle_{B.M}$ ; however, it is still a lower bound.

#### IV. CONCLUSION

We have investigated the possibility of establishing a strict lower bound to the radial position  $\langle r \rangle$  in terms of the average value of  $r^2$  and the lowest radial excitation energy ( $E_{20} - E_{10}$ ).

We have established inequalities and approximate expressions for the average value  $\langle r^2 \rangle$  and  $\langle r \rangle$  on the ground state. The approach follows a method developed by Bertlmann and Martin [4] in the case of the  $s$ -state.

The calculations have been performed for 3 kinds of potentials. The lower bound to  $\langle r \rangle$  is relatively well saturated, i.e. it falls within  $\cong 10$ -15% of the exact value in most of the studied cases.

We have used for  $\langle r^2 \rangle$ , the corrected Bertlmann-Martin expression (7) [5, 6]. The approximation preserves the lower bound character of the bound (4), except in cases where the correction factor is not efficient like in the case of power-law potentials (9) with  $\alpha = -1.5$ . Finally, we have derived an inequality which yields an upper bound to the uncertainty in the radial position  $\Delta r$  for the ground state. The ratio between the bound and the exact value yields a general trend: it is approaching 1 as the particle is more bound.

We have completed our study by using the uncertainty principle to establish a lower bound to the ground state kinetic energy. This bound seems less efficient than the one derived by Bertlmann-Martin [4]; however, it is still a lower bound.

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