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SOME PROPERTIES OF BOUND STATES IN POTENTIALS

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A B S T R A C T

We summarize the most important theorems on the order of energy levels in central potentials. Then we present new results on spacing between energy levels. Finally we present some results of V. Glaser on the wave function at the origin and subsequent developments.

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1. - INTRODUCTION

I was very pleased to be invited by Professor Mitter to lecture at the 26th Session of the Schlading School, which is dedicated to Walter Thirring on the occasion of his 60th birthday. As a member of CERN, I remember the period when Walter was a member of the CERN Directorate. This was a very critical period. European nations could not agree on the choice of a site for the future SPS, and finally, the Directorate decided to follow the proposal of John Adams to study the possibility of building the SPS on the very site of CERN. This study was done in complete secrecy for it was expected that not everybody would agree with this idea. Indeed when the project was ready, it was presented to the Council and for a short time there were strong oppositions to it. However, very quickly, the tempest quieted down, the opponents understood that the project was in fact very clever, and you all know what followed: the SPS was built, and so well built that it could be transformed into a collider, producing the sensational results which gave to Europe the leadership in particle physics.

Of course, the main reasons of my admiration for Walter are that he is a great (mathematical) physicist and a great teacher. I had a great pleasure collaborating with him, for instance participating to the preliminary investigations on the problem of stability of matter, which was finally solved by Lieb and Thirring. I have an immense debt to him because I collaborated and still collaborate with his remarkable students, like Harald Grosse and, to some extent, Bernard Baumgartner, and also the students of his students like Reinhold Bertlmann, who was a student of Herbert Pietschmann.

What I shall speak about is work which was precisely started in a collaboration with H. Grosse in 1977 and later R. Bertlmann, with a decisive contribution of B. Baumgartner in 1984. This is the part on the order of levels. More recently we have studied the question of the spacing between energy levels, and in this collaboration, Jean-Marc Richard, Pierre Taxil and Alan Common contributed. Finally, I shall describe the work of Vladimir Glaser on the wave function at the origin and some developments of mine. Certainly, V. Glaser would have been present to this celebration. We are all very sad that he is not with us any more.

2. - THE PROBLEM OF THE ORDER OF LEVELS

The reason why I got interested in the order of levels in central potentials was that potentials were used to describe quarkonia, i.e., mesons made of a heavy quark-antiquark pair and one question, raised by M.A.B. Bég, was to know what would lead to the lowest excitation energy: radial excitation or orbital excitation? We have been able to find an answer to this question and found many more results. Naturally the results we get can be applied to any domain of physics when the Schrödinger equation holds: atomic physics, etc.

The radial Schrödinger equation can be written as

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V(r) - E(n, l) \right] u_{n, l}(r) = 0. \quad (1)$$

The energy E depends in general on two quantum numbers, n , the number of nodes of the radial wave function, l the orbital angular momentum.

For a completely general potential, two properties are well known:

i) the energy increases with the number of nodes:

$$E(n+1, l) > E(n, l), \quad (2)$$

this is the standard Sturm-Liouville theory of second-order differential equations;

ii) the energy increases with angular momentum:

$$E(n, l+1) > E(n, l). \quad (3)$$

This comes from the fact that the coefficient of the centrifugal term increases with l . The set of energy levels with the same n and different l 's constitute what is called since 1959 a "Regge trajectory". It was pointed out by Regge that l , in the radial equation (1), need not be integer or even real! For l real $> -\frac{1}{2}$ we have

$$E(n, l+\delta) > E(n, l), \quad \forall \delta > 0.$$

What we really want is more subtle than that. We want to be able to compare pairs (n, l) , (n', l') . There are two well-known special cases of exceptional degeneracy:

- i) The Coulomb potential $V = -1/r$, then the energies depend only on the principal quantum number $N = n + l + 1$, and we have a level structure:

(the dotted lines are Regge trajectories). So $E(n+1, l) = E(n, l+1)$

- ii) The harmonic oscillator potential, $V = r^2$: then the energies depend only on the combination $n + l/2$, and $E(n+1, l) = E(n, l+2)$, and we have the diagram:

Among other things, we want to compare the order of levels of a given potential with the Coulomb case and the harmonic oscillator case. However, we shall get other results as well. We give below a series of theorems on the order of levels. Later we shall give indications on the proofs.

Theorem 1¹⁾

$$E(n+1, l) \geq E(n, l+1)$$

$$\text{if } \Delta V \equiv \frac{1}{r^2} \frac{d}{dr} r^2 \frac{dV}{dr} \geq 0 \quad \forall r > 0.$$

Naturally, in the Coulomb case, $\Delta V = 0$ outside the origin. This means that this theorem is in its optimal form.

A slight refinement is that

$$E(n+1, l) \leq E(n, l+1)$$

if

$$\Delta V(r) \leq 0 \quad \text{or} \quad \frac{dV}{dr} \leq 0 \quad \forall r > 0.$$

Theorem 2²⁾

$$E(n+1, l) \geq E(n, l+2),$$

$$\text{if } Y(r) = \frac{d}{dr} \frac{1}{r} \frac{dV}{dr} \geq 0 \quad \forall r > 0;$$

clearly $Y = 0$ for a harmonic oscillator.

Y positive means that V is convex in r^2 , Y negative means that V is concave in r^2 .

One has also the analogue of the refinement of Theorem 1.

Now, ΔV , or Y , are, except for common factors, linear combinations of $r(d^2V/dr^2)$ and dV/dr . It turns out to be possible to get other inequalities by using combinations with different coefficients. A subset of these theorems is given here. Others can be found in Ref. 2).

Theorem 3

$$E(n+1, l) \leq E(n, l+\alpha), \quad \alpha \geq 2,$$

$$\text{if } r \frac{d^2V}{dr^2} + (3-2\alpha) \frac{dV}{dr} \leq 0 \quad \forall r > 0.$$

Theorem 4

$$E(n+1, l) \geq E(n, l+\alpha), \quad 1 \leq \alpha \leq 2,$$

$$\text{if } r \frac{d^2V}{dr^2} + (3-2\alpha) \frac{dV}{dr} \geq 0 \quad \text{and} \quad \frac{dV}{dr} \geq 0, \forall r > 0.$$

Theorem 5

$$E(n+1, l) \leq E(n, l+\alpha) \quad 1 \leq \alpha \leq 2$$

$$\text{if } r \frac{d^2V}{dr^2} + (3-\alpha) \frac{dV}{dr} < 0, \forall r > 0.$$

You may remark that, contrary to Theorems 1 and 2, Theorems 3, 4 and 5 take the form of one-sided inequalities. If we had two-sided inequalities, we would have a new case of degeneracy for arbitrary n . We know that it is not so.

Since these theorems are not very transparent, we shall give illustrations with power-like potentials:

- $V = r^4$ (three-dimensional anharmonic oscillator)

$$E(n, l+2) \underset{\text{(Theorem 2)}}{<} E(n+1, l) \underset{\text{(Theorem 3)}}{<} E(n, l+3) \quad (4)$$

- $V = r$ (linear potential)

$$E(n, l+3/2) \underset{\text{(Theorem 4)}}{<} E(n+1, l) \underset{\text{(Theorem 2)}}{<} E(n, l+2) \quad (5)$$

- $V = -r^{-1/2}$

$$E(n, l+1) \underset{\text{(Theorem 1)}}{<} E(n+1, l) \underset{\text{(Theorem 5)}}{<} E(n, l+3/2) \quad (6)$$

Now we would like to give indications on the method of proof. All these theorems can be deduced from Theorem 1 by changes of variables plus some elementary operations. In fact, Theorem 1 is the most important because of its applications in particle physics, atomic physics and even solid state physics.

Historically, in 1977, conditions much stronger than those of Theorem 1 were used to derive a weaker result, applying only to $n = 0$ and $n = 1$. However, Feldman, Fulton and Devoto³⁾ "proved" Theorem 1 in the WKB limit, i.e., $n \gg l \gg 1$. They found that the relevant quantity was $d/dr \ r^2 \ dV/dr$ without noticing its proportionality to the Laplacian. However, the difference between the WKB approximation and the exact levels is very hard to control theoretically, even though, in practice, WKB is often very good. H. Grosse and I⁴⁾ decided to look at the case of perturbations around the Coulomb potential:

$$V = -\frac{1}{r} + \lambda v \quad (7)$$

Then, to compare $E(n+1, l)$ and $E(n, l+1)$ in the limit of $\lambda \rightarrow 0$, we have to find the sign of the quantity:

$$\delta = \int_0^\infty v(r) \left[(u_{n+1,l}(r))^2 - (u_{n,l+1}(r))^2 \right] dr, \quad (8)$$

where the u 's are Coulomb wave functions, i.e., Laguerre polynomials times exponentials. As it is, the integrand oscillates tremendously if n is large. However, H. Grosse noticed that $u_{n+1,l}$ and $u_{n,l+1}$ are obtained from one another by using raising and lowering operators, because the Coulomb degeneracy is tied to an O_4 symmetry. These raising and lowering operators are simple first-order differential operators:

$$\begin{aligned} u_{n,l+1} &= \text{const. } A_+ u_{n,l} \\ u_{n+1,l} &= \text{const. } A_- u_{n,l+1} \\ A_\pm &= \pm \frac{d}{dr} - \frac{l+1}{r} + \frac{1}{l+1} \end{aligned} \quad (9)$$

All one has to do is to replace $u_{n+1,l}$ by $\text{const. } A_- u_{n,l+1}$ and integrate twice by parts. In that way one gets

$$\delta = \int \left(\frac{d}{dr} r^2 \frac{dv}{dr} \right) [\text{positive bracket}] dr, \quad (10)$$

and hence, δ is positive (negative) if the Laplacian of v is positive (negative).

The problem is then to get a non-perturbative proof. The idea, due to Baumgartner, was to generalize the notion of raising operator. The final version, obtained by Baumgartner, Grosse and I¹⁾ is the following.

If $u_{n,l}$ is the solution of

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + v(r) - E \right] u_{n,l} = 0 \quad (11)$$

define

$$\tilde{u} = A_+ u_{n,l}$$

where

$$A_+ = \frac{d}{dr} - \frac{u'_{0,l}}{u_{0,l}},$$

$u_{0,l}$ being the solution of (11) with $n = 0$ (ground state). Then $\tilde{u}$ is the solution of:

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + 2 \frac{d}{dr} \left(-\frac{u'_{0,e}}{u_{0,e}} \right) + V - E \right] \tilde{u} = 0. \quad (12)$$

This transformation, that we reinvented, was, as K. Chadan pointed it to us, in the work of Marchenko in 1945, and goes back in fact to the French mathematician Darboux. If V is regular at the origin, i.e., less singular than $1/r^2$, u behaves like r^{l+1} and one can easily show that $\tilde{u}$ behaves like r^{l+2} . One can also show that $\tilde{u}$ has one node less than u .

Under these circumstances, one can interpret $\tilde{u}$ as a state with angular momentum $l+1$, and $n-1$ nodes, and rewrite (12) as

$$\left[-\frac{d^2}{dr^2} + \frac{(l+1)(l+2)}{r^2} + \tilde{V}(r) - E \right] \tilde{u} = 0 \quad (13)$$

with

$$\tilde{V} = V + 2 \left[\frac{d}{dr} \left(-\frac{u'_{0,e}}{u_{0,e}} \right) - \frac{l+1}{r^2} \right]. \quad (14)$$

Here comes a crucial lemma:

$$\text{if } \Delta V(r) \geq 0 \quad \left(\text{i.e. } V \begin{array}{c} \text{CONVEX} \\ \text{CONCAVE} \end{array} \text{ in } \frac{1}{r} \right) \quad \forall r > 0$$

$$\frac{d}{dr} \left(-\frac{u'}{u} \right) - \frac{l+1}{r^2} \geq 0 \quad (u \equiv u_{0,e}). \quad (15)$$

and in fact

$$\text{if } \Delta V(r) < 0 \quad \text{or} \quad \frac{dV}{dr} < 0 \quad \forall r > 0,$$

$$\frac{d}{dr} \left(-\frac{u'}{u} \right) - \frac{l+1}{r^2} < 0. \quad (16)$$

To prove these inequalities, one has to compare the solution u with the potential V with a comparison solution u_c with a Coulomb potential V_c , such that $E - V(r) = E_c - V_c(r)$. Then because V is, say, convex in $1/r$, $E - V$ and $E_c - V_c$ do not intersect, either in $0-r$ or in $r-\infty$. This allows us to write an inequality for the Wronskian of u and u_c which gives the result. A little care is needed, but all the steps are simple calculations.

Now take, say, $\Delta V > 0$. Then we have $\tilde{V} > V$. However, the energies in (11) and (13) are the same so that

$$E(n-1, l+1, \tilde{V}) = E(n, l, V).$$

However, the energies are monotonous in the potential, i.e.,

$$E(n-1, l+1, \tilde{V}) > E(n-1, l+1, V),$$

which proves the desired result. Clearly, the same argument applies in the opposite case.

To get the other theorems all one has to do is to make a change of variables and functions. In particular, to get Theorem 2 we make the change which transforms the Coulomb case into the harmonic oscillator:

$$z = r^2, \quad \mathcal{Q} = \frac{2l-1}{4}, \quad w(z) = r^{1/2} u(r).$$

The other theorems are obtained by a more general change of variables, $z = r^\alpha$, and, in their initial form, one has to know the sign of the energy, but after some manipulations, Theorems 3, 4 and 5 have been obtained with no reference to a particular zero of energies, since the conditions contain only derivatives of V .

Let us indicate now that Theorems 3, 4 and 5 are not optimal. We have a conjecture which is not yet completely established. Theorem 3 should be replaced by

$$E(n+1, l) \leq E(n, l + \sqrt{\nu+2})$$

$$\text{if } r \frac{d^2 V}{dr^2} \leq (\nu-1) \frac{dV}{dr}, \quad \nu \geq 2, \quad (17)$$

so that if $V = r^4$, we expect

$$E(n+1, l) < E(n, l + \sqrt{6}) < E(n, l + 2.45)$$

while Theorem 3 says

$$E(n+1, l) < E(n, l+3).$$

We were led to this conjecture by noticing that for large l one can replace the effective potential $V + (l(l+1)/r^2)$ by a harmonic oscillator. In the special case of power potentials one can write an asymptotic expansion in inverse powers

of $(l(l+1))^{\frac{1}{2}}$. To show how far we are in the proof, let us say that we know that the conjecture is true for $V = r^5$, $n = 0$, $l > 20$. We have also systematic numerical calculations up to $n = 6$, $l = 6$ for $V = r^4$.

3. - COMMON'S INEQUALITIES AND GENERALIZATIONS

We have seen that in the proof of Theorem 1, an essential ingredient is

$$\frac{d}{dr} \left(- \frac{u'_{0,l}}{u_{0,l}} \right) \geq \frac{l+1}{r^2} \quad \text{if} \quad \Delta V(r) \geq 0$$

A.K. Common⁵⁾ has exploited this auxiliary result to derive certain properties of the ground state with angular momentum l . The simplest result concerns the kinetic energy. It is well known that for a general potential the radial kinetic energy satisfies

$$T_2 = \int_0^\infty u'^2 dr > \frac{1}{4} \int_0^\infty \frac{u^2}{r^2} dr. \quad (18)$$

If one knows that $\Delta V(r) > 0$, one can do better than that, using (15):

$$\begin{aligned} \int_0^\infty u'^2 dr &= \int_0^\infty \frac{u'}{u} u u' dr = \frac{u^2}{2} \frac{u'}{u} \Big|_0^\infty - \int_0^\infty \left(\frac{u'}{u} \right)' \frac{u^2}{2} dr \\ &> \frac{l+1}{2} \int_0^\infty \frac{u^2}{r^2} dr. \end{aligned} \quad (19)$$

Conversely, if $\Delta V < 0$ you get the opposite sign in the inequality.

The total kinetic energy, including the angular part, satisfies

$$\begin{aligned} T_l &\geq (l + \frac{1}{2})(l+1) \int \frac{u^2}{r^2} dr = \frac{l+1}{2} \frac{dE}{dl}, \\ &\text{if} \quad \Delta V(r) \geq 0 \quad \forall r > 0. \end{aligned} \quad (20)$$

In the case $\Delta V > 0$ the inequality also holds for excited states.

A.K. Common has also obtained an inequality on moments:

$$\int_0^\infty (u_{0,l}(r))^2 r^\alpha dr = \langle r^\alpha \rangle. \quad (21)$$

Here you have to carry two partial integrations if you want to see the quantity $(u'/u)'$ appearing, but you must eliminate all the integrated terms. So Common combines two moments and gets finally:

$$\begin{aligned} (2l+3+\alpha) \frac{\langle r^\alpha \rangle}{\langle r^{\alpha+1} \rangle} &\geq (2l+3+\beta) \frac{\langle r^\beta \rangle}{\langle r^{\beta+1} \rangle}, \alpha > \beta, \\ \text{if } \Delta V(r) &\geq 0 \quad \forall r > 0. \end{aligned} \quad (22)$$

If you want to see that this means, take $\alpha = 0$, $\beta = -1$. You get, for $\Delta V < 0$ $(2l+3/2l+2) > \langle r \rangle \langle r^{-1} \rangle$, i.e., the opposite of Schwarz inequality in one case and an improved Schwarz inequality in the other case.

What A.K. Common and I realized⁶⁾ is that the same change of variables which leads from Theorem 1 to Theorems 2, 3, 4 and 5 can be used. In this way one gets, for instance,

$$\begin{aligned} T_l &> \frac{1}{2} \left(l + \frac{\alpha+1}{2} \right) \frac{d\epsilon}{dl} \\ \text{if } r \frac{d^2 V}{dr^2} + (3-2\alpha) \frac{dV}{dr} &> 0 \quad \text{and} \quad \frac{dV}{dr} > 0 \\ 1 &\leq \alpha \leq 2 \end{aligned} \quad (23)$$

which can be used to prove the inequality

$$\begin{aligned} \epsilon(0, l) &> \left(\frac{\nu+2}{\nu} \right) \left(\frac{\nu}{2} \right)^{\frac{2}{\nu+2}} \left(l + \frac{\nu+4}{4} \right)^{\frac{2\nu}{\nu+2}} \\ \text{for } V = r^\nu, \quad 0 < \nu < 2. \end{aligned} \quad (24)$$

This inequality turns out to be reasonably tight, when one compares with numerical calculations.

Of course, one might object that this is a very special class of potentials. Still less exciting, a priori, are the moment inequalities. Even I thought so until recently, where we used moment inequalities to prove a concavity property of the energy which had resisted all assaults for many years and which will be described in the last section. For future use, I state the inequality obtained with the change of variables $z = r^2$:

$$(2l+3+\alpha) \frac{\langle r^\alpha \rangle}{\langle r^{\alpha+2} \rangle} \geq (2l+3+\beta) \frac{\langle r^\beta \rangle}{\langle r^{\beta+2} \rangle}, \alpha > \beta, \quad (25)$$

if $\frac{d}{dr} \frac{1}{r} \frac{dV}{dr} \geq 0 \quad \forall r > 0.$

4. - APPLICATION OF THE THEOREMS ON THE ORDER OF LEVELS

So far Theorems 3, 4 and 5 are just mathematical curiosities, but this may change! Theorems 1 and 2, on the other hand, are clearly useful.

In atomic physics, if we take an alkaline atom, its outer electron is submitted to the field of the nucleus, point-like in this approximation, and hence with $\Delta V = 0$, and to the field of the electron cloud, which has $\Delta V < 0$, by Gauss's law. Hence $E(n+1, l) < E(n, l+1)$, in agreement with what we know of the alkaline spectra and of the Mendeleef classification.

Muonic atoms, in which the size of the nucleus is not negligible with respect to the size of the Bohr orbit, have clearly $\Delta V > 0$ and hence the level order is

$$\begin{array}{c} \underline{2S} \\ \underline{1S} \end{array} \quad \underline{2P}$$

which was known long ago⁷⁾ for explicit charge distributions of the nucleus but holds as long as the charge density of the nucleus is everywhere positive.

For quarkonium, we notice that $\Delta V > 0$ means that the force exerted on the quark $-z(r)/r^2$, $z(r)$ being the effective charge, is such that $(dz(r)/dr) > 0$ which is asymptotic freedom. So $E(n+1, l) > E(n, l+1)$. On the other hand, it has been shown that the lattice QCD potential is such that $dV/dr > 0$ and $d^2V/dr^2 < 0$ ⁸⁾. Hence $d/dr \frac{1}{r} dV/dr < 0$. Hence $E(n+1, l) < E(n, l+2)$.

This is tested by the $J\psi$ and T spectra:

$$\begin{array}{ccc} \psi' & & \psi'' \\ \underline{\psi'} & \underline{\chi_c} & \\ \underline{\psi''} & & \\ \underline{J\psi} & & \\ l=0 & l=1 & l=2 \end{array}$$

5. - LEVEL SPACING

5.1. Motivation

Evidently one might wonder why we want to study level spacing in potentials. Why not study more refined quantities like n th order differences between energy levels? There is no reason to stop!

However, let us make two remarks. First, if we can get information on the spacing using only some of the conditions appearing in Section 2 and nothing else, why not? Second, we feel that if we want to undertake an investigation of the order of levels for three-body systems we need to know something about the spacing⁹⁾. If we take two-body harmonic oscillator forces we know that the excited states of the three-body system ABC will be highly degenerated. Excitations can be produced by exciting the two-body subsystem AB or exciting C with respect to AB, or both. To compare these different types of excitation when forces deviate from harmonic oscillator forces, we need to know things about spacing of levels in two-body forces.

In the harmonic oscillator potential, we notice that two properties characterize the spectrum

i)

$$E(n, l) = \frac{1}{2} [E(n, l+1) + E(n, l-1)] \quad (26)$$

In other words, for a given n , E is a linear function of l , or "Regge trajectories" are linear

ii)

$$E(n, l+1) = \frac{1}{2} [E(n, l) + E(n+1, l)] \quad (27)$$

the energy of the state with angular momentum $l+1$ is half way between the energies of the two neighbouring states with angular momentum l .

The properties

iii)

$$E(n, l+2) = E(n+1, l), \quad (28)$$

which is nothing but a limiting case of Theorem 2,

iv)

$$E(n, l) = \frac{1}{2} [E(n-1, l) + E(n+1, l)], \quad (29)$$

which is equal spacing of fixed l levels, are in fact consequences from i) and ii).

First we shall study what happens to (26) and (27) when the potential deviates from the harmonic oscillator. The study of fixed spacing will come later.

5.2. Comparing different angular momenta¹⁰⁾

First we look at the perturbative situation, i.e.,

$$V = \frac{r^2}{4} + \lambda v, \quad \lambda \rightarrow 0. \quad (30)$$

Then, as we did before, we use raising and lowering operators, connecting the various wave functions of the harmonic oscillator, but here we have two kinds of operators:

$$\begin{aligned} B_l^+ u_{n+1, l} &= \gamma_{n, l} u_{n, l+1} \\ B_l^- u_{n, l+1} &= \gamma_{n, l} u_{n+1, l} \\ B_l^\pm &= \pm \frac{d}{dr} - \frac{l+1}{r} + \frac{r}{2} \\ (\gamma_{n, l})^2 &= 2n+2 \end{aligned} \quad (31)$$

$$\begin{aligned}
 C_l^+ u_{n,l} &= \beta_{n,l} u_{n,l+1} \\
 C_l^- u_{n,l+1} &= \beta_{n,l} u_{n,l} \\
 (\beta_{n,l})^2 &= 2n+2l+3
 \end{aligned}
 \quad C_l^\pm = \pm \frac{d}{dr} - \frac{l+1}{r} - \frac{\lambda}{2}
 \tag{32}$$

If we want to study what happens to (26), i.e., what happens to a "Regge trajectory", we have to calculate

$$\int r \left[(u_{n,l-1})^2 + (u_{n,l+1})^2 - 2(u_{n,l})^2 \right] dr
 \tag{33}$$

and use operators $C^\pm$. What one finds is the following: for $n = 0$, in which case the u 's reduce to

$$\text{const. } r^{l+1} \exp -\frac{r^2}{4}$$

one finds that (33) is positive if

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

negative, in the opposite case.

In other words if V is sufficiently close to an harmonic oscillator potential

$$\begin{aligned}
 2 E(0, l) &\geq E(0, l+1) + E(0, l-1) \\
 \text{if } \frac{d}{dr} \frac{1}{r} \frac{dV}{dr} &\geq 0 \quad \forall r > 0
 \end{aligned}
 \tag{34}$$

In fact the proof also holds for

$$2 E(0, l) \geq E(0, l+\delta) + E(0, l-\delta).$$

Therefore, if V is sufficiently close to an harmonic oscillator and is concave (convex) in r^2 , $E(0, l)$ is concave (convex) in l . The concavity statement, as we shall see later, is true in general even outside perturbation theory.

On the other hand, for $n \neq 0$, transforming (33) by two integrations by parts into an expression

$$\int \frac{d}{dr} \frac{1}{r} \frac{dv}{dr} [\dots] dr$$

one can show that the bracket has not a definite sign. So even if $d/dr \frac{1}{r} dv/dr < 0$ one can have situations where $E(n, l) < \frac{1}{2}[E(n, l+1) + E(n, l-1)]$, for $n > 1$.

Let us now discuss what happens to (27), i.e., study the sign of

$$E(n, l+1) - \frac{1}{2} [E(n, l) + E(n+1, l)]$$

Here we have to use the operators B^- and C^- to express the integral

$$\int v \left[2 (u_{n, l+1})^2 - (u_{n, l})^2 - (u_{n+1, l})^2 \right]$$

in terms of $u_{n, l}$ and $u'_{n, l}$. It is straightforward to transform this integral into the form

$$\int \frac{d}{dr} \frac{1}{r} \frac{dv}{dr} [\dots] dr$$

and to show that the bracket is manifestly negative.

Therefore, if V is sufficiently close to r^2 ⁹⁾

$$E(n, l+1) \geq \frac{1}{2} [E(n, l) + E(n+1, l)]$$

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

Let us now discuss the non-perturbative situation. Concerning the Regge trajectory we can only look at the $n = 0$ case, and one can prove that the perturbative statement is in fact true in general. The strategy ¹⁰⁾, invented after a discussion with T. Regge, consists in using a variational approach. We can get an upper bound on $E(0, l+\delta)$ by taking as trial function

$$C_{\text{const}} \times r^\delta u_{0, l}(r) \tag{35}$$

where u is the exact wave function for angular momentum l . Clearly the trial function (34) becomes exact if V is a pure harmonic oscillator potential.

One finds

$$E(0, l+\delta) < E(0, l) + \delta(2l+1+2\delta) \frac{\int \frac{u^2}{r^{2-2\delta}} dr}{\int \frac{u^2}{r^{2\delta}} dr}$$

This applies for positive and negative δ . Hence we get

$$2E(l) - E(l+\delta) - E(l-\delta) > \delta \left[(2l+1-2\delta) \frac{\int \frac{u^2}{r^{2+2\delta}} dr}{\int u^2 r^{-2\delta} dr} - (2l+1+2\delta) \frac{\int \frac{u^2}{r^{2-2\delta}} dr}{\int u^2 r^{2\delta} dr} \right]. \quad (36)$$

Now if we use (32), the generalization of Common's inequalities on moments we see that with $\alpha = 2\delta-2$ and $\beta = -2\delta-2$ the right-hand side of (36) is positive if $d/dr \ 1/r \ dV/dr < 0$.

Hence it is true in general that $E(0, l)$ is a concave function of l if the potential is a concave function of r^2 . The opposite statement holds only in perturbations around r^2 , as far as we know.

Notice that while concavity of $E(0, l)$ with respect to l is non-trivial, concavity of $E(0, l)$ with respect to $l(l+1)$ is trivial. This is because $\lambda = l(l+1)$ enters linearly in the Hamiltonian and by a general theorem that can be found, for instance, in the quantum mechanics course of W. Thirring, the energy is concave in λ .

Concerning the comparison of the level with angular momentum $l+1$ to the neighbouring levels with angular momentum l , let us indicate that there is one case completely solved:

$$E(0, l+1) > \frac{1}{2} [E(0, l) + E(1, l)]$$

if $\frac{d}{dr} \frac{1}{r} \frac{dW}{dr} \leq 0$ (37)

This results from the combination of the concavity property (33) with Theorem 2:

$$2E(0, l+1) > E(0, l+2) + E(0, l) > E(1, l) + E(0, l). \quad (38)$$

Do we believe that

$$E(n, l+1) > \frac{1}{2} [E(n, l) + E(n+1, l)]$$

for $d/dr \ 1/dr \ dV/dr < 0$ in general?

Yes, because, outside the perturbation argument, the result also holds in the limit of $l \rightarrow \infty$. Then, if $V(r)$ is sufficiently smooth one can approximate $V_{\text{eff}} = V(r) + (l(l+1)/r^2)$ by an harmonic oscillator potential near the point where $V'_{\text{eff}} = 0$. In this way we get

$$E(n, l) \simeq V(r_0) + \frac{r_0 V'(r_0)}{2} + (2n+1) \sqrt{\frac{1}{2} \left(V''(r_0) + \frac{3V'(r_0)}{r_0} \right)} \quad (39)$$

where r_0 is a minimum of V_{eff} given by

$$r_0^3 V'(r_0) = 2 l(l+1). \quad (40)$$

Under weak, acceptable conditions, r_0 goes to infinity for $l \rightarrow \infty$. It is also reasonable to assume that $(d/dr)^n V(r) = O(V(r)/r^n)$ for $r \rightarrow \infty$. Hence, the second term in (39) is small if V goes to infinity for $r \rightarrow \infty$.

Now $E(n, l+1)$ is approximately:

$$\begin{aligned} E(n, l+1) &\simeq E(n, l) + \frac{2l+1}{r_0^2} \\ &\simeq E(n, l) + \sqrt{\frac{2V'(r_0)}{r_0}} \end{aligned}$$

Hence

$$2E(n, l+1) - E(n, l) - E(n+1, l) \simeq$$

$$2 \sqrt{\frac{2V'(r_0)}{r_0}} - 2 \sqrt{\frac{1}{2} \left(V''(r_0) + \frac{3V'(r_0)}{r_0} \right)} \quad (40)$$

which is positive if

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

5.3. Spacing of $l = 0$ levels¹¹⁾

For the harmonic oscillator, the levels are equally spaced:

$$2 E(n, l=0) = E(n+1, l=0) + E(n-1, l=0).$$

When we undertook this study (J.-M. Richard, P. Taxil and I) we hoped that the same criterium as before, i.e., the sign of $d/dr \frac{1}{r} dV/dr$ would decide if the levels get closer and closer with increasing n or more and more spaced. This is not true. We have examples of perturbations of $r^2/4$ such that $d/dr \frac{1}{r} dV/dr > 0$ for which, for some n

$$2 E(n, 0) > E(n+1, 0) + E(n-1, 0),$$

while we expected the opposite. In pure power potentials, $V = r^\nu$, the naïve expectation seems true, i.e.,

$$2 E(n, 0) \geq E(n+1, 0) + E(n-1, 0) \text{ for } \nu \leq 2.$$

What we have proved was completely unexpected, though a posteriori it was understood. It is as follows:

$$\text{for } V = \frac{r^2}{4} + \lambda r$$

The levels get more and more spaced with increasing n , if:

$$\lim_{r \rightarrow 0} r^3 \nu = 0$$

$$\text{and } Z(r) = \frac{d}{dr} r^5 \frac{d}{dr} \frac{1}{r} \frac{dV}{dr} > 0 \quad \forall r > 0. \quad (40)$$

If, on the other hand, $Z < 0$ $V(r) > 0$, the levels get closer and closer as n increases.

However, this is not always true outside the perturbation regime, as we shall see.

Now, why this condition? Z is a third order differential operator in v . There are two obvious v 's which make Z equal to zero. These are

$$v = \text{const.}, \quad v = r^2.$$

However, $Z \equiv 0$ admits another solution which is

$$v = \frac{1}{r^2},$$

and this is perfectly normal. Adding $v = C/r^2$ to the harmonic oscillator potential is equivalent to shifting the angular momentum by a fixed amount, and since the Regge trajectories of the oscillator are linear and parallel, i.e., $d/d\lambda(E(n, \lambda))$ is constant, independent of n , all levels are shifted by the same amount and equal spacing is preserved. Naturally, we could invent other criteria, for the knowledge of all $\lambda = 0$ levels does not fix the potential as all experts on the inverse problem know. There is an infinite-dimensional family of potentials with equal spacing of $\lambda = 0$ levels, the parameters being the wave functions at the origin, but we believe that we have here the simplest criterium.

The proof uses again the technique of raising and lowering operators. We want to calculate

$$\Delta = \delta E_{N+1} + \delta E_{N-1} - 2\delta E_N,$$

where $E_N = E(N, \lambda=0)$. If $V = r^2/4 + \lambda v$, then

$$\Delta = \int_0^\infty v \left[u_{N+1}^2 + u_{N-1}^2 - 2u_N^2 \right] dr. \quad (41)$$

u_{N-1} and u_{N+1} are obtained from u_N by using raising or lowering operators:

$$\begin{aligned} \left(2N+2 - \frac{r^2}{2} + r \frac{d}{dr} \right) u_N &= \sqrt{(2N+2)(2N+3)} u_{N+1} \\ \left(2N+3 - \frac{r^2}{2} - r \frac{d}{dr} \right) u_{N+1} &= \sqrt{(2N+2)(2N+3)} u_N. \end{aligned} \quad (42)$$

One carries a series of integrations by parts:

$$\Delta = \lim_{r \rightarrow 0} I(r) r(r) + \int_0^{\infty} I(r) \frac{dv}{dr} dr, \quad (43)$$

where

$$I(r) = \int_r^{\infty} (U_{N+1}^2 + U_{N-1}^2 - 2U_N^2) dr'. \quad (44)$$

However, $I(0) = 0$ since $v = \text{const.}$ should give $\Delta = 0$. Hence

$$I(r) = - \int_0^r (U_{N+1}^2 + U_{N-1}^2 - 2U_N^2) dr'$$

for $r \rightarrow 0$, if $\lim r^3 v = 0$, we can drop the all integrated terms. We repeat the operation, introducing

$$J(r) = \int_r^{\infty} r' I(r') dr' \quad (45)$$

then

$$\Delta = \lim_{r \rightarrow 0} \left(J(r) \frac{1}{r} \frac{dv}{dr} \right) + \int_0^{\infty} J(r) \left(\frac{d}{dr} \frac{1}{r} \frac{dv}{dr} \right) dr;$$

again $J(0) = 0$ for a potential $v = r^2$ should make $\Delta = 0$. Then J behaves like r^5 and if $\lim r^3 v = 0$ there is a sequence of r_n going to zero for which

$$\lim_{n \rightarrow \infty} J(r_n) \frac{1}{r_n} \frac{dv}{dr_n} = 0.$$

In that sense, the integrated term goes away. It is at this stage that, with explicit wave functions, we produced counter examples to the conjecture that the sign of $d/dr \frac{1}{r} dv/dr$ determines the sign of Δ . Now comes the last step, in which $Z(r)$ will appear. Define

$$K(r) = \int_r^{\infty} \frac{J(r') dr'}{r'^5} \quad (46)$$

Then

$$\begin{aligned} \Delta = & \lim_{r \rightarrow 0} K(r) \left[r^5 \frac{d}{dr} \frac{1}{r} \frac{dv}{dr} \right] \\ & + \int_0^{\infty} K(r) \left(\frac{d}{dr} r^5 \frac{d}{dr} \frac{1}{r} \frac{dv}{dr} \right) dr. \end{aligned}$$

However, since $\Delta = 0$ for $v = 1/r^2$ we see that $K(0) = 0$ and, in fact, $K(r) \sim r$ for $r \rightarrow 0$. So the integrated term goes away if $\lim r^3 v = 0$ and if we choose carefully a sequence of r approaching zero. Then

$$\Delta = \int_0^{\infty} K(r) \left(\frac{d}{dr} \left[r^5 \frac{d}{dr} \frac{1}{r} \frac{dv}{dr} \right] \right) dr. \quad (47)$$

$K(r)$ can be calculated explicitly in terms of u_N and u'_N by using equations (42) to express u_{N+1} and u_{N-1} in terms of u_N and u'_N and carrying the successive integrations (44), (45) and (46). By multiplying to the left the Schrödinger equation

$$-u'' + \left(\frac{n^2}{4} - E \right) u = 0$$

by $r^k u$ and $r^{k'} u'$, and making clever combinations, it is tedious, but straightforward to obtain:

$$\begin{aligned} 2N(2N+1)(2N+2)(2N+3) K(r) = & \\ u_N'^2 \left[\frac{3}{2r^3} + \frac{E}{2r} \right] & \\ + u_N^2 \left[-\frac{3E}{4r^3} - \frac{3}{16r} + \frac{E^2}{2r} - \frac{Er}{8} \right] & \\ + u_N u_N' \left[-\frac{3}{4r^4} + \frac{E}{2r^2} \right]. & \end{aligned} \quad (48)$$

This is a quadratic form in u and u' , which has a negative discriminant in most of the "classical region", the most dangerous one where u and u' oscillate. Near the origin, and near and beyond the turning point it is easy to show that (48) is positive. So $K(r)$ is positive for all r and we conclude that the sign of Δ is given by the sign of $Z(r)$ if the latter is the same everywhere.

This is, in a way, a miracle, and we were hoping that it could be generalized for $\ell = 0$. This is not the case. For $\ell > \frac{1}{2}$, $K(r)$, for some values of N , has not a definite sign. Examination of the first few values of N indicates that $K(r)$ has a definite positive sign for $-\frac{1}{2} < \ell < +\frac{1}{2}$.

The fact that $K(r)$ has not a definite sign for $\ell > \frac{1}{2}$ indicates that the $\ell = 0$ result does not apply for too large perturbations: if we take a potential

$$V = \frac{r^2}{4} + \frac{2}{r^2} + v(r),$$

with

$$\frac{d}{dr} r^5 \frac{d}{dr} \frac{1}{r} \frac{dv}{dr} > 0,$$

we know that by choosing $v(r)$ cleverly we can have an irregular spacing of the levels since $l = 1$. However, if we think of $2/r^2 + v(r)$ as the "perturbation" we also have

$$\frac{d}{dr} r^5 \frac{d}{dr} \frac{1}{r} \frac{d}{dr} \left[\frac{2}{r^2} + v \right] > 0.$$

This is not the only indication that the property breaks down for too strong perturbations. If we take a potential

$$V = \lambda (r^3 - r^2),$$

for which $Z(r)$ is positive, we find, numerically, that for large enough λ the negative energy levels get closer and closer as N increases and, when one reaches positive energies, they get more and more spaced as N increases. It was pointed out to me by A. Voros that this could be understood in a semi-classical approach.

The question now is how big can the perturbation be to $V = r^2/4$ before the theorem breaks down? We have an unproved conjecture, which is:

$$\begin{aligned} \text{if } \frac{d}{dr} r^5 \frac{d}{dr} \frac{1}{r} \frac{dV}{dr} \geq 0 \quad \forall r > 0 \text{ and } \lim_{r \rightarrow \infty} r^3 V = 0 \\ \text{and } \frac{dV}{dr} > 0 \quad \forall r \geq 0, \\ E_{N+1} + E_{N-1} - 2E_N \geq 0. \end{aligned}$$

This is based on the remark that no counter example has a monotonous potential.

It may take some time before proving this conjecture. In the meantime we shall try to get another criterium, based on the WKB approximation. Then, for a monotonous potential, E can be considered as a continuous function of N , defined by

$$N - \frac{1}{4} = \frac{1}{\pi} \int_0^{\infty} \sqrt{(E - V)_+} \, dr \quad (49)$$

(Here the ground state is given by $N = 1$, not $N = 0$!) Then the spacing is given by dE/dN , and levels get closer with increasing N if

$$\frac{d}{dN} \left(\frac{dE}{dN} \right) < 0, \quad (49)$$

i.e., exchanging function and variable:

$$\frac{d^2 N}{dE^2} > 0. \quad (50)$$

We have, differentiating under the integral sign

$$\frac{dN}{dE} = \frac{1}{2\pi} \int_0^{r_t} \frac{dr}{\sqrt{E-V}}, \quad (51)$$

where r_t is the turning point. We cannot differentiate again, because we would get a divergence at r_t . So we assume $V'(r) > 0 \forall r > 0$, and integrate (51) by parts

$$\begin{aligned} \frac{dN}{dE} &= \frac{1}{2\pi} \int \frac{1}{V'} \frac{V' dr}{\sqrt{E-V}} = \\ &= \frac{1}{\pi} \frac{\sqrt{E-V(0)}}{V'(0)} - \frac{1}{\pi} \int_0^{r_t} \frac{V''}{V'^2} \sqrt{E-V} dr. \end{aligned} \quad (52)$$

Hence

$$\frac{d^2 N}{dE^2} = \frac{1}{2\pi} \frac{1}{V'(0)\sqrt{E-V(0)}} - \frac{1}{2\pi} \int_0^{r_t} \frac{V''}{V'^2 \sqrt{E-V}} dr. \quad (53)$$

A sufficient condition for this to be positive is

$$V'' < 0; \quad (54)$$

however, notice that $d^2 N/dE^2$ does not vanish for $V'' \rightarrow 0$, since the first term survives and cannot be zero since $V'(0)$ is not infinite.

If we believe that the exact solution is sufficiently close to WKB, we conclude that the level spacing decreases with increasing N if V is concave. Numerical experiments indicate that indeed WKB is very good for power potentials $V = r^v$, $0 < v < 1$. We tend to believe that it is good for potentials with second derivative of a constant sign and, since Eq. (53) contains a safety factor which is the integrated term, at least if $V'(0) \neq \infty$, we tend to believe that this result is true in general. The class of potentials concave is rather far away from the harmonic oscillator, but the quarkonium potentials deduced from lattice

QCD are precisely concave⁸⁾. In this way we understand that

$$\begin{aligned} M_{\gamma''} - M_{\gamma'} &< M_{\gamma'} - M_{\gamma} \\ M_{\gamma'''} - M_{\gamma''} &< M_{\gamma''} - M_{\gamma'} \\ M_{\psi'''} - M_{\psi'} &< M_{\psi'} - M_{J\psi} . \end{aligned} \quad (55)$$

However, the last observed level of the $b\bar{b}$ system, called T^{IV} is such that¹²⁾

$$M_{\gamma^{IV}} - M_{\gamma'''} > M_{\gamma'''} - M_{\gamma''}$$

We have therefore an indication that the naïve one-channel potential model breaks down. However, it is high above the $B\bar{B}$ threshold,

$$M_{\gamma^{IV}} \simeq 10.85 \text{ GeV} \gg 10.55 \text{ GeV} ,$$

and coupled channel effects and/or glue contributions may be important¹³⁾.

6. - THE WAVE FUNCTION AT THE ORIGIN (AND ELSEWHERE)

6.1. Introduction

In quarkonium physics, not only the energy levels are important but also (not uniquely) the wave function at the origin which controls the annihilation of quark-antiquark pairs, and therefore the leptonic width and the total width of quarkonium. It is particularly appropriate to speak about it here since there is a formula for the leptonic width, called the Van Royen-Weisskopf formula, which was in fact first discovered by H. Pietschmann and W. Thirring, and also others like M. Krammer.

What I want to say is contained in a Physics Reports dedicated to the memory of V. Glaser¹⁴⁾, and the first part is due to V. Glaser himself, who was stimulated by the interest that people around him, like R. Bertlmann, H. Grosse, and myself, had for the wave function at the origin.

6.2. Glaser's unpublished work

Glaser used the notion of positivity preserving operator. A positivity preserving operator is such that, if it acts on a state with positive wave function in x space, it produces a state with positive wave function. If its matrix elements in x space exist, then

$$\langle x|A|y\rangle > 0, \quad \forall x, \forall y. \quad (56)$$

For such an operator, we write the symbolic inequality

$$A \succ 0. \quad (57)$$

Then $A \succ B$ means

$$A - B \succ 0 \quad (58)$$

and if $A \succ 0$ and $B \succ 0$,

$$AB \succ 0. \quad (59)$$

Consider now the evolution operator for imaginary time

$$e^{-Ht}, \quad \text{where } H = H_0 + V = p^2 + V(x). \quad (60)$$

According to the Trotter formula

$$e^{-Ht} = \lim_{N \rightarrow \infty} \left(e^{-\frac{p^2 t}{N}} e^{-\frac{Vt}{N}} \right)^N \quad (61)$$

Clearly $e^{-Vt/N} \succ 0$ because V is diagonal in x . On the other hand,

$$\langle x|e^{-p^2 t}|y\rangle = (4\pi t)^{-\frac{n}{2}} \exp -\frac{(x-y)^2}{4t} \quad (62)$$

(n is the number of dimensions) hence $e^{-p^2 t} \succ 0$ and, therefore

$$e^{-Ht} \succ 0. \quad (63)$$

Glaser assumes that $V(x)$ is positive. Then, from the Trotter formula (61), it is clear that

$$e^{-Ht} < e^{-H_0 t},$$

and so, in particular

$$\langle x | e^{-Ht} | x \rangle < (4\pi t)^{-\frac{n}{2}}, \quad (63)$$

or, expanding over the complete set of energy levels (assume for simplicity that the spectrum is discrete, the potential confining):

$$\sum_i |\psi_i(x)|^2 e^{-E_i t} < (4\pi t)^{-\frac{n}{2}}, \quad (64)$$

and, hence $E_1 < E_2 < \dots < E_N < \dots$

$$\sum_{i=1}^N |\psi_i(x)|^2 < e^{E_N t} (4\pi t)^{-\frac{n}{2}} \quad (65)$$

t can be chosen arbitrarily, and one can minimize with respect to t:

$$\sum_{i=1}^N |\psi_i(x)|^2 < (E_N)^{\frac{n}{2}} \left(\frac{e}{2\pi n} \right)^{\frac{n}{2}} \quad (66)$$

In particular, in three dimensions, we get

$$\sum_{i=1}^N |\psi_i(x)|^2 < (E_N)^{\frac{3}{2}} \left(\frac{e}{6\pi} \right)^{\frac{3}{2}}. \quad (67)$$

This is to be compared with the semi-classical limit¹⁵⁾

$$\sum_{i=1}^N |\psi_i(x)|^2 \simeq \frac{1}{6\pi^2} (E_N)^{\frac{3}{2}}. \quad (68)$$

The functional form is the same, but the coefficient is different. However, the coefficient of the strict inequality (67) is almost optimal. Taking $N = 1$ and a square well, one finds that the ratio of the left-hand side and right-hand side of (67) deviates from unity by less than 10%.

6.3. The small t behaviour

We can prove that

$$\lim_{t \rightarrow 0} \frac{\langle x | e^{-Ht} | y \rangle}{\langle x | e^{-H_0 t} | y \rangle} - 1 = 0 \quad (69)$$

i) For positive potentials. Then one uses the equation

$$e^{-Ht} = e^{-H_0 t} - \int_0^t e^{-H_0 \tau} V e^{-H(t-\tau)} d\tau. \quad (70)$$

Assume

$$V < A + B r^\nu, \quad (71)$$

and use $e^{-Ht} = e^{-H_0 t} - \int_0^t e^{-H_0 \tau} V e^{-H(t-\tau)} d\tau$, then one can calculate an upper bound on the matrix elements of the integral and prove the desired result.

ii) For lower-bounded potentials, $V > -B$ we have $e^{-Ht} = e^{-H_0 t} e^{Bt}$ and, therefore nothing is changed. However, by working harder, one can find a bound on

$$\langle x | e^{-Ht} - e^{-H_0 t} | y \rangle$$

independent of B, provided the negative part of the potential, V_- is such that

$$\int (V_-)^{\frac{3}{2} + \varepsilon} d^3 x \quad (72)$$

converges for some $\varepsilon > 0$ (we believe that by being more careful one could reach $\varepsilon=0$).

iii) One can then take a sequence of potentials

$$V_B(x) = V(x) \text{ if } V(x) \geq -B, = -B \text{ if } V(x) < -B,$$

for which e^{-Ht} has monotonicity properties and take the limit $B \rightarrow \infty$, provided (72) converges.

7. - THE SEMI-CLASSICAL LIMIT

The previous result implies, if we use diagonal matrix elements,

$$\lim_{t \rightarrow 0} \left[(4\pi t)^{3/2} \sum_{k=1}^{\infty} |\psi_k(x)|^2 e^{-E_k t} \right] = 1, \quad (73)$$

and then one can use a Tauberian theorem of Karamata¹⁶⁾, of which a proof by M. Aizenmann is presented in one of the books of Barry Simon, and conclude:

$$\lim_{N \rightarrow \infty} \frac{\sum_{k=1}^N |\psi_k(x)|^2}{E_N^{3/2}} = \frac{1}{6\pi^2}. \quad (74)$$

If we compare with the result of Quigg and Rosner¹⁵⁾, using the WKB approximation for spherically symmetric potentials

$$|\psi_N(0)|^2 \sim \frac{1}{4\pi^2} E_N^{1/2} \frac{dE_N}{dN} \quad (75)$$

we see that (74) is more vague, but more rigorous, and does not assume spherical symmetry.

In fact one can go a little further than (74). If one imposes a Lipschitz condition on the potential, at least locally

$$|V(x) - V(y)| < C |x - y| \quad (76)$$

one can prove that if the quantity

$$\frac{\sum_{k=1}^N |\psi_k(x)|^2 - \frac{[E_N - V(x)]^{3/2}}{6\pi^2}}{E_N^{1/2}} \quad (77)$$

has a limit, this limit is zero. This shows the validity of the Thomas Fermi approximation for the density when one fills a confining potential with independent fermions.

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