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ORDER OF LEVELS IN POTENTIAL MODELS

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A B S T R A C T

Various extensions of a previous derived theorem on the order of levels of quantum mechanical systems are discussed. Local conditions on the potential are given, such that the n -th level of angular momentum l lies above (or below) the $(n-1)$ -th level with angular momentum $l + \alpha$. Some improved versions are formulated as conjectures and are shown to be true in certain limiting situations. As possible applications, we discuss besides heavy quark systems the level order in atomic physics.

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I. Introduction

Although nonrelativistic quantum mechanics is well established since a long time, general results on the distribution of energy eigenvalues are not known. Recently there has been increasing interest in such questions. One motivation comes from heavy quark spectroscopy, since both the ψ and the T system allow a nonrelativistic treatment. Since an ultimate calculation of the interquark force from QCD including quark loops (on a lattice) is still remote, phenomenologically motivated potentials might be adjusted and levels and decay properties determined. (For a review see [1].) A different approach has been advocated by two of us (A.M. and H.G.). The main idea concerns the determination of general features of potential models, like level ordering, relations between decay quantities and the like. Our early results [2] were restricted to low lying levels, but recently a general result concerning the order of all levels has been derived [3].

Starting from the reduced radial Schrödinger equation with rotational symmetric potential ($\hbar = 2m = 1$)

$$H_{\ell} u_{n,\ell}(r) = E_{n,\ell} u_{n,\ell}(r) , \quad H_{\ell} = - \frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r) , \quad (1.1)$$

where the wave function $u_{n,\ell}$ and energy levels $E_{n,\ell}$ are labelled by the number of nodes n of the former within $(0, \infty)$ and the angular momentum ℓ , we intend to find relations between $E_{n,\ell}$ and $E_{n-1,\ell+\alpha}$ for certain values of α (notice the change of notations with respect to ref. [3]).

Our previous result concerns the case $\alpha = 1$ and says that the sign of the Laplacian of $V(r)$ determines the relative order of levels which would be degenerate for the Coulomb case; more precisely

$$\Delta V(r) \gtrless 0 \quad \forall r \neq 0 \quad \Rightarrow \quad E_{n,\ell} \gtrless E_{n-1,\ell+1} \quad \forall n, \ell \quad (1.2)$$

(1.2) was first shown within the WKB approximation [4], then perturbatively [5] and finally the general result was obtained [3]. Let us mention that various applications have been discussed already [6,7]

and a further application will be given in part IV. The classical analog to (1.2), that the Laplacian of V controls the perihelion motion has been discussed as well [8].

Our main concern here is to generalize (1.2) in various ways. Since one knows that the n -th level of angular momentum ℓ for the harmonic oscillator is degenerate with the $(n-1)$ -th level of angular momentum $\ell+2$, it is natural to ask for a generalization of (1.2), which yields an optimal answer in that case. Such a generalization is known to hold perturbatively [5].

There exists even a more general result: We found local conditions on the potential such that the n -th level to angular momentum ℓ lies above (or below) the $(n-1)$ -th level of angular momentum $\ell + \alpha$ for any α . One of these results says that for a positive potential with

$$D_{\alpha} V(r) > 0 \quad 1 < \alpha < 2 \quad \Rightarrow \quad E_{n,\ell} > E_{n-1,\ell+\alpha} \quad (1.3)$$

$$D_{\alpha} V(r) < 0 \quad 2 < \alpha \text{ or } \alpha < 1 \quad \Rightarrow \quad E_{n,\ell} < E_{n-1,\ell+\alpha}$$

where the second order differential operator D_{α} is defined by

$$D_{\alpha} = \frac{d^2}{dr^2} + (5 - 3\alpha) \frac{1}{r} \frac{d}{dr} + 2(1 - \alpha)(2 - \alpha) \frac{1}{r^2} . \quad (1.4)$$

Let us especially mention the case $\alpha = 2$. Convexity (respectively concavity) of the potential in r^2 implies relations between energy levels

$$\left(\frac{d}{dr^2}\right)^2 V(r) \gtrless 0 \quad \Rightarrow \quad E_{n,\ell} \gtrless E_{n-1,\ell+2} . \quad (1.5)$$

Note that equality for the energy levels on the r.h.s. of (1.5) for all n and ℓ is obtained for the harmonic oscillator. (1.5) is a generalization of our previous result concerning perturbations around the harmonic oscillator. The well-known transformation from the Coulomb problem to the harmonic oscillator is actually at the origin of our new results.

These results together with further generalizations will be discussed in part II. Part III is devoted to conjectures which can be proven in

certain limits. Final remarks and applications are put into part IV.

II. Results on Level Ordering

Since our main steps are motivated by our previous results, let us first mention the ideas leading to (1.2). Using the nodeless wave function $u_{0,\ell}$ to angular momentum ℓ we defined "ladder" operators $A_\ell^\pm$ by

$$A_\ell^\pm = \pm \frac{d}{dr} + g_\ell(r), \quad g_\ell(r) = - \frac{u'_{0,\ell}(r)}{u_{0,\ell}(r)}, \quad (2.1)$$

which are adjoint to each other. A little algebra, using the fact that g_ℓ solves a Riccati equation, shows that on the one hand

$$A_\ell^- A_\ell^+ + E_{0,\ell} = H_\ell, \quad (2.2)$$

and on the other hand that $A_\ell^\pm$ map from one operator H_ℓ to another one $A_\ell^+ A_\ell^- + E_{0,\ell}$ which is "essentially iso-spectral". This terminology means that both operators have the same spectrum except for possible zero energy states and these relations have been extensively discussed by Deift [9]. Properties of $A_\ell^\pm$ can be summarized by

$$[A_\ell^+, A_\ell^-] = 2g'_\ell, \quad [H_\ell, A_\ell^+] = -2g'_\ell A_\ell^+. \quad (2.3)$$

This algebra is also behind the supersymmetric quantum mechanics, but its origin was observed already in the fifties by Crum and Marchenko [10].

The supersymmetry aspect is to add one fermionic degree of freedom (form the tensor product of Hilbert space by C^2) and consider the operators

$$B^+ = \begin{pmatrix} 0 & A_\ell^+ \\ 0 & 0 \end{pmatrix}, \quad B^- = \begin{pmatrix} 0 & 0 \\ A_\ell^- & 0 \end{pmatrix}.$$

B^- is the adjoint to B^+ , as A_ℓ^- is the adjoint to A_ℓ^+ (A_ℓ^+ is defined with Dirichlet boundary conditions at $r = 0$). The Hamiltonian

$$H = B^- B^+ + B^+ B^-$$

has a nondegenerate zero-energy eigenvalue and otherwise a doubly degenerate spectrum.

Our previous results come from application of a

LEMMA 1: If $\Delta V \geq 0$ for all $r \neq 0$, then

$$\frac{d}{dr} g_\ell(r) \geq 2 \frac{\ell+1}{r^2}. \quad (2.4)$$

The proof of Lemma 1 was given in ref. [3]; starting now from a solution $u_{n,\ell}$ of equ. (1.1) to energy $E_{n,\ell}$ one finds first using (2.3) that

$$\phi_\ell(r) = A_\ell^+ u_{n,\ell} = \left(\frac{d}{dr} + g_\ell(r)\right) u_{n,\ell} \quad (2.5)$$

solves a Schrödinger equation with the same energy $E_{n,\ell}$ with a potential $V(r) + 2g'_\ell(r)$. (2.4) then allows to conclude, using the Mini-Max-principle that the true energy levels $E_{n-1,\ell+1}$ for the potential $V(r)$ lie below or above $E_{n,\ell}$. Here and throughout this paper we may define $E_{n-1,\ell+\alpha}$ as the infimum of the essential spectrum of $H_{\ell+\alpha}$, if this operator happens to have less than $n-1$ bound states. Since the conditions on V we will eventually suppose to hold imply that the infimum of the essential spectrum is the same in all ℓ -sectors, the inequality $E_{n,\ell} \geq E_{n-1,\ell+\alpha}$ then actually implies the existence of at least $n-1$ bound states of $H_{\ell+\alpha}$. That the number of nodes of $\phi_\ell(r)$ is one less than the number of nodes of $u_{n,\ell}$ can be deduced easily.

The generalization which we mentioned in the introduction is formulated in

THEOREM 1: Assume that $V(r)$ is positive and $D_\alpha V(r)$ is positive for $1 < \alpha < 2$ (negative for $\alpha > 2$ or $\alpha < 1$), where D_α has been given in (1.4). Then $E_{n,\ell}$ is greater (smaller) than $E_{n-1,\ell+\alpha}$.

Similarly if $V(r)$ is negative and $D_\alpha V(r)$ is negative for $1 < \alpha < 2$ (positive for $\alpha < 1$) $E_{n,\ell}$ is smaller (greater) than $E_{n-1,\ell+\alpha}$. (The case $D_\alpha V(r) > 0$, $\alpha > 2$, $V(r) < 0$ is empty!)

Proof: The main idea is to transform (1.1) in such a way as to be able to apply the techniques explained before: Starting from (1.1) we make the change of variables from r to z and change of wave function from $u_{n,\ell}$ to $w_{n,\ell}$:

$$z = \int^r dy f(y) , \quad w_{n,\ell}(z) = f^{1/2}(r) u_{n,\ell}(r) , \quad (2.6)$$

where $f(r)$ is assumed to be positive in order to get a bijection from r to z . This transformation gives back a new Schrödinger like equation [11] of the form

$$\frac{d^2}{dz^2} w_{n,\ell}(z) = \left\{ (W(z) + \frac{\ell(\ell+1)}{r^2} - E_{n,\ell}) \gamma^4(r) - \gamma^3(r) \gamma_{rr}(r) \right\} w_{n,\ell}(z) , \quad (2.7)$$

$$r = r(z) ,$$

where $\gamma^2(r) = 1/f(r)$ and $W(z) = V(r)$. As a special case we choose $z = r^\alpha$, which gives $f(r) = \alpha r^{\alpha-1}$ and finally

$$\frac{d^2}{dz^2} w_{n,\ell}(z) = \left\{ U(z; E_{n,\ell}) + \frac{\lambda(\lambda+1)}{z^2} \right\} w_{n,\ell}(z) , \quad U(z; E) = \frac{W(z) - E}{\alpha^2 z^{2-2/\alpha}} \quad (2.8)$$

where $\lambda = (2\ell - \alpha + 1)/2\alpha$ denotes the new angular momentum. (2.8) can be considered as a Schrödinger equation with angular momentum λ , potential $U(z; E)$ and energy zero. From the assumed positivity of $E_{n,\ell}$ and of $D_\alpha V(r)$ for $1 < \alpha < 2$ we deduce by straightforward computation that $\Delta_z U(z; E) > 0$; therefore there exists a new potential $\hat{U}$ which has a zero energy state of angular momentum $\lambda + 1$ and with a wave function which has one node less than $w_{n,\ell}$. Returning to the initial Schrödinger equation (1.1) one gets a state with angular momentum $\ell + \alpha$ and a potential which is above the old one. The new potential now depends on n and $E_{n,\ell}$ but that does not matter. We deduce using the Mini-Max-principle again, that $E_{n,\ell} > E_{n-1,\ell+\alpha}$. The reversed sign for $\alpha > 2$ or $\alpha < 1$ follows from the assumption that $D_\alpha V(r) < 0$ for $\alpha > 2$ or $\alpha < 1$.

The proof of the second part of Theorem 1 is similar. $\square$

EXAMPLES: A source of examples is given by pure power potentials $\varepsilon(v)r^v$, where ε is the sign function. Then $D_\alpha V(r)$ reduces to $\varepsilon(v)[v-2(\alpha-1)][v+2-\alpha]r^{\alpha-2}$. In this way, we get for

$$V = r^4 \quad E_{n-1, \ell+2} < E_{n, \ell} < E_{n-1, \ell+3} \quad (2.9)$$

$$V = r \quad E_{n-1, \ell+3/2} < E_{n, \ell} < E_{n-1, \ell+2} \quad (2.10)$$

$$V = -r^{-1/2} \quad E_{n-1, \ell+1} < E_{n, \ell} < E_{n-1, \ell+3/2} \quad (2.11)$$

$$V = -r^{-3/2} \quad E_{n-1, \ell+1/2} < E_{n, \ell} < E_{n-1, \ell+1} \quad (2.12)$$

REMARK: We observe that there are potentials which solve the differential equation $D_\alpha V(r) = 0$ and which are transformed to Coulomb potentials:

THEOREM 2: The potentials

$$V_{\alpha, N, Z}(r) = \alpha^2 \frac{Z^2}{4N^2} r^{2\alpha-2} - \alpha^2 Z r^{\alpha-2}, \quad \alpha > 0, Z > 0, N \geq 1/2, \quad (2.13)$$

have zero energy eigenvalues for angular momentum quantum numbers ℓ which satisfy

$$\lambda = \frac{2\ell - \alpha + 1}{2\alpha} = N - n - 1, \quad n = 0, 1, 2, \dots \quad (2.14)$$

where n denotes the number of nodes of the corresponding eigenfunction.

Proof: With the change of variable from r to $\rho = r^\alpha$, the radial Schrödinger equation with potential $V_{\alpha, N, Z}$, angular momentum ℓ and energy zero is transformed to the Schrödinger equation for the Coulomb potential $-Z/\rho$, angular momentum λ and energy $-Z^2/4N^2$. It remains to remark that the Coulomb quantum number N need not be entire: the algebraic treatment of the Coulomb-problem [12,5] works for general real angular momentum λ .

REMARK: One may also do a direct algebraic treatment for the potentials described in Theorem 2. Define

$$A_{\alpha,Z,\ell}^{\pm} = \pm \frac{1}{\alpha} r^{1-\alpha} \frac{d}{dr} - \frac{\mu_{\pm}(\alpha)}{\alpha r} + \frac{\alpha Z}{2\ell+1+\alpha}, \quad \mu_{+} = \ell+1, \quad \mu_{-} = \ell+\alpha, \quad (2.15)$$

and

$$H_{\alpha,N,Z,\ell} = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V_{\alpha,N,Z}(r) \quad (2.16)$$

with Dirichlet boundary conditions at $r = 0$. One calculates easily on the one hand the product of A^{-} and A^{+}

$$A_{\alpha,Z,\ell}^{-} A_{\alpha,Z,\ell}^{+} = \frac{1}{\alpha^2} r^{2-2\alpha} H_{\alpha,N(\ell),Z,\ell} \quad \text{with} \quad N(\ell) = \frac{2\ell+1-\alpha}{2\alpha} + 1, \quad (2.17)$$

on the other hand the commutator

$$[A_{\alpha,Z,\ell}^{+}, A_{\alpha,Z,\ell}^{-}] = \frac{1}{\alpha^2} r^{2-2\alpha} (H_{\alpha,N,Z,\ell+\alpha} - H_{\alpha,N,Z,\ell}). \quad (2.18)$$

This shows that

$$r^{2-2\alpha} H_{\alpha,N,Z,\ell-\alpha} A_{\alpha,Z,\ell-\alpha}^{-} = A_{\alpha,Z,\ell-\alpha}^{-} r^{2-2\alpha} H_{\alpha,N,Z,\ell}. \quad (2.19)$$

The ground state wave function $u_{0,\ell}$ for $H_{\alpha,N,Z,\ell}$ is the solution of the differential equation $A_{\alpha,Z,\ell}^{+} u_{0,\ell} = 0$ and explicitly given by

$$u_{0,\ell}(r) = r^{\ell+1} e^{-Zr^{\alpha}/2N}. \quad (2.20)$$

Furthermore proceeding inductively we see that

$$u_{n,\ell-n\alpha} = A_{\alpha,Z,\ell-n\alpha}^{-} u_{n-1,\ell-(n-1)\alpha} \quad (2.21)$$

solves

$$H_{\alpha,N,Z,\ell-n\alpha} u_{n,\ell-n\alpha} = 0. \quad \square$$

The case $\alpha = 2$, which is a comparison to the level ordering for the 3-dimensional harmonic oscillator, is special:

COROLLARY 1:

$$\begin{aligned}
&\text{If } D_2 V(r) \geq 0 \quad \text{then} \quad E_{n,\ell} \geq E_{n-1,\ell+2} , \\
&\text{if } D_2 V(r) \leq 0 \quad \text{then} \quad E_{n,\ell} \leq E_{n-1,\ell+2} .
\end{aligned} \tag{2.22}$$

Proof: Since D_2 contains no zero-order term, the conditions $D_2 V(r) \gtrless 0$ are equivalent to $\Delta U \gtrless 0$, when we make the same transformations as in the proof of the foregoing theorem. Therefore both of the inequalities for the levels of U yield the inequalities for the levels of V .

REMARK: One can define a "running elastic force constant" $K(r)$ by $V'(r) = K(r) r$. The conditions $D_2 V(r) > (<) 0$ then are equivalent to monotonicity of K : $K'(r) > (<) 0$. This is analogous to the case $\alpha = 1$, where we can consider a "running "Coulomb force constant" $Z(r)$ by $V'(r) = Z(r)/r^2$. There $\Delta V(r) > (<) 0$ means $Z'(r) > (<) 0$.

REMARK: In Theorem 1 one may avoid the assumption that V is positive and reformulate it in terms of $U(z;E)$; but then the condition is energy dependent. Eliminating the energy dependence in such a condition leads to Theorem 3 and 4:

THEOREM 3: If the potential $V(r)$ fulfills

$$\left(r \frac{d^2}{dr^2} + (3 - 2\alpha) \frac{d}{dr} \right) V(r) \leq 0 \quad \text{for} \quad \alpha \geq 2 \tag{2.23}$$

we deduce that $E_{n,\ell} \leq E_{n-1,\ell+\alpha}$.

Proof: We start from the transformed Schrödinger equation (2.8) in the variable $z = r^\alpha$ and use a refined version of our previously derived theorem [3]. There exists a solution to (2.8) with λ increased by one unit and energy zero and a potential being lower than U if

$$I(z) = \Delta_z U(z;E) < 0 \quad \text{wherever} \quad J(z) = \frac{d}{dz} U(z;E) > 0 . \tag{2.24}$$

$J(z)$ positive means explicitly that

$$z \frac{d}{dz} W(z) > \left(2 - \frac{2}{\alpha} \right) (W(z) - E) . \tag{2.25}$$

Now it is simple to realize that (2.25) together with negativity of

$$K(z) = z \frac{dW}{dz} \left(\frac{2}{\alpha} - 1 \right) + z^2 \frac{d^2}{dz^2} W < 0 \quad (2.26)$$

implies that $I(z)$ is negative for $\alpha > 2$. Note that

$$\alpha z I(z) = \alpha z^{2/\alpha-3} K(z) + (2-\alpha)J(z) . \quad (2.27)$$

Condition (2.25) rewritten in the variable r gives (2.23).

REMARK: For pure power potentials we get nothing new compared to Theorem 2, but condition (2.23) is - as it should be - invariant under a change of origin of energies.

Since we did not find a way to weaken the condition $\Delta U(z;E) > 0$, removing the energy dependence in that case can be done only with the help of an additional assumption:

THEOREM 4: Let $V(r)$ be monotonously increasing $dV/dr > 0$, and assume

$$\left(r \frac{d^2}{dr^2} + (3-2\alpha) \frac{d}{dr} \right) V(r) \geq 0 \quad \text{with} \quad 1 < \alpha < 2 , \quad (2.28)$$

then

$$E_{n,\ell} > E_{n-1,\ell+\alpha} . \quad (2.29)$$

Proof: This time we assume that $K(z)$ is positive, which rewritten in the variable r means (2.28). In order to use again (2.27) and to deduce that $I(z)$ is positive for $\alpha > 2$ we would like to show positivity of $J(z)$. This can be obtained by noting that $E_{n,\ell} > W(0)$ from the monotonicity of the potential, and $W(z) - W(0)$ can be bounded since

$$W(z) - W(0) = \frac{\alpha}{2(\alpha-1)} \left\{ z W' - \int_0^z dy \frac{K(y)}{y} \right\} \quad (2.30)$$

and K is positive. This shows that

$$W(z) - E_{n,\ell} < \frac{\alpha}{2(\alpha-1)} z W'(z) \quad (2.31)$$

and implies positivity of $J(z)$ and $I(z)$.

Finally we formulate

THEOREM 5: Assume that $V(r)$ fulfills

$$r \frac{d^2 V}{dr^2} + (3 - \alpha) \frac{dV}{dr} \leq 0 \quad \text{for} \quad 1 < \alpha < 2 , \quad (2.32)$$

then $E_{n,\ell} < E_{n-1,\ell+\alpha}$.

Proof: This time we observe that

$$E_{n,\ell} - W(z) < \int_z^\infty dy W'(y) = \frac{\alpha}{2-\alpha} \left\{ zW' + \int_z^\infty dy [yW'' + \frac{2}{\alpha} W'] \right\} . \quad (2.33)$$

Assume now that

$$\left(\alpha z \frac{d^2}{dz^2} + 2 \frac{d}{dz} \right) W(z) < 0 , \quad (2.34)$$

which is equivalent to (2.23); this shows that

$$E_{n,\ell} - W(z) < \frac{\alpha}{2-\alpha} z W'(z) ; \quad (2.35)$$

splitting $I(z)$ from (2.13) now in an obvious way as to eliminate the term proportional to $E_{n,\ell} - W(z)$ we deduce that $\Delta_z U(z; E_{n,\ell})$ is negative, by using (2.33) again.

III. Conjectures

Besides the expected result for the comparison with the order of energy levels of the harmonic oscillator we have obtained a series of new and unexpected results illustrated by the examples (2.9), (2.10), (2.11), (2.12). However, when one tests numerically these inequalities one sees that they are not as constraining as one might expect. For instance for the potential $V = \ln r$, which corresponds to $\nu \rightarrow 0$, we do not get anything new, but just $E_{n-1,\ell+1} < E_{n,\ell} < E_{n-1,\ell+2}$. We may ask whether the factors $3 - 2\alpha$ in conditions (2.23) and (2.28) as well as the factor $(3 - \alpha)$ in condition (2.32) are optimal or could be replaced by

different factors. Based on the harmonic oscillator approximation for large angular momenta and on numerical checks we are led to formulate improved versions of Theorem 3 and 4 as conjectures:

CONJECTURE: Assume $V(r)$ fulfills

$$\left(r \frac{d^2}{dr^2} - (\alpha^2 - 3) \frac{d}{dr}\right)V(r) < 0 \quad \text{for} \quad \alpha > 2, \alpha < 1, \quad (3.1)$$

we conjecture that $E_{n,\ell} < E_{n-1,\ell+\alpha}$. If on the other hand

$$\left(r \frac{d^2}{dr^2} - (\alpha^2 - 3) \frac{d}{dr}\right)V(r) > 0 \quad \text{for} \quad 1 < \alpha < 2, \quad (3.2)$$

we conjecture the reversed ordering $E_{n,\ell} > E_{n-1,\ell+\alpha}$.

We have a number of arguments supporting this conjecture:

FIRST ARGUMENT: For smooth potentials and large ℓ , we expect that the effective potential

$$V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + V(r) \quad (3.3)$$

will look near its minimum more and more like an harmonic oscillator.

With r_ℓ being the place of the minimum of $V_\ell(r)$

$$2 \frac{\ell(\ell+1)}{r_\ell^3} = V'(r_\ell), \quad (3.4)$$

we expect that for ℓ going to infinity with n staying finite the energy levels are determined by the harmonic oscillator frequencies around r_ℓ .

$$E_{n,\ell} \approx V_\ell(r_\ell) + (2n+1) \sqrt{V''_\ell(r_\ell)/2}, \quad (3.5)$$

where the curvature is given by

$$V''(r_\ell) = \frac{6\ell(\ell+1)}{r_\ell^4} + V''(r_\ell) = 3 \frac{V'(r_\ell)}{r_\ell} + V''(r_\ell). \quad (3.6)$$

Since one expects for smooth potentials that for $\ell \rightarrow \infty$ and $r_\ell \rightarrow \infty$ [2]

$$V' \approx 0\left(\frac{V}{r_\ell}\right), \quad V'' = 0\left(\frac{V}{r_\ell^2}\right), \quad V_\ell \approx 0\left(\frac{\ell^2}{r_\ell^2}\right), \quad \sqrt{V''} \approx 0\left(\frac{\ell}{r_\ell^2}\right), \quad (3.7)$$

the leading term in (3.5) will be given by V_ℓ . Substituting $\ell + \Delta\ell$ instead of ℓ in (3.5) and using

$$V_\ell(r_{\ell+\Delta\ell}) - V_\ell(r_\ell) \approx (r_{\ell+\Delta\ell} - r_\ell) \frac{d}{dr} V_\ell(r_\ell) = 0 \quad (3.8)$$

which holds at the minimum, gives for the energy difference

$$E_{n,\ell+\Delta\ell} - E_{n,\ell} \approx V_{\ell+\Delta\ell}(r_\ell) - V_\ell(r_\ell) \approx \frac{(2\ell+1)\Delta\ell}{r_\ell^2}. \quad (3.9)$$

One may now ask for which value of $\Delta\ell$, $E_{n,\ell}$ equals $E_{n-1,\ell+\Delta\ell}$. This will be the case if the r.h.s. of (3.9), which can be related to $V'(r_\ell)$ by using (3.4), equals the contribution from changing n to $n-1$ in (3.5). With the help of (3.6) we get

$$2\sqrt{\frac{V'(r_\ell)}{2r_\ell}} \approx \frac{(2\ell+1)\Delta\ell}{r_\ell^2} = 2\sqrt{\frac{3V'(r_\ell) + r_\ell V''(r_\ell)}{r_\ell}}. \quad (3.10)$$

Therefore we deduce the equality of the energy levels in the limit we are considering if

$$r_\ell V''(r_\ell) = [(\Delta\ell)^2 - 3]V'(r_\ell). \quad (3.11)$$

Furthermore if the l.h.s. of (3.11) exceeds the r.h.s. one expects

$E_{n,\ell} > E_{n-1,\ell+\Delta\ell}$ and vice versa for large ℓ . Since for smooth potentials going to infinity for $r \rightarrow \infty$ we expect the WKB approximation to be valid for ℓ finite, $n \rightarrow \infty$, we expect that $E_{n,\ell} \approx E_{n-1,\ell+2}$ [4] and only one of the inequalities will survive for $\Delta\ell > 2$ or $\Delta\ell < 2$ for $n \rightarrow \infty$, ℓ finite and thus we expect (3.1) and (3.2) to hold.

SECOND ARGUMENT: For pure power potentials we found an asymptotic expansion of $E_{n,\ell}$ in decreasing powers of $\Lambda = \ell(\ell+1)$. First we approximate again

$$V_\ell(r) = \frac{\ell(\ell+1)}{r^2} + \varepsilon(v) \cdot r^v, \quad \varepsilon(v) = \begin{cases} +1 & v > 0 \\ -1 & v < 0 \end{cases} \quad (3.12)$$

by an harmonic oscillator and calculate anharmonic corrections. It turns out that (for pure power potentials) the first order perturbation due to the term $V_{\ell}^{IV}(r_{\ell})(r-r_{\ell})^4/4!$ is of the same order as the second order perturbation due to $V_{\ell}^{III}(r_{\ell})(r-r_{\ell})^3/3!$. It is tedious but simple to calculate matrix elements of x^3 and x^4 using the $(a + a^{\dagger})$ representation of x . (A similar expansion can be found in [13].) The final answer is

$$E_{n,\ell} \approx \left(\frac{|v|}{2}\right)^{2/(v+2)} \Lambda^{v/(v+2)} \left\{ \frac{v+2}{v} + \Lambda^{-1/2} (2n+1)\sqrt{v+2} + \right. \\ \left. + \Lambda^{-1} [(2n^2+2n+1)(v-2)(11-v) + \frac{2}{3}(v-5)^2] + \dots \right\} . \quad (3.13)$$

From this expression one gets

$$E_{n,\ell+\sqrt{2+v}} - E_{n+1,\ell} \approx \left(\frac{|v|}{2}\right)^{2/(v+2)} \Lambda^{-2/(v+2)} \frac{n+1}{12} (v-2)(v+1) + \dots . \quad (3.14)$$

This again supports the conjecture that

$$E_{n,\ell+\sqrt{2+v}} > E_{n+1,\ell} \quad \text{for } v > 2 \quad (\text{or } v < -1) \\ \text{but} \\ E_{n,\ell+\sqrt{2+v}} < E_{n+1,\ell} \quad \text{for } -1 < v < 2 . \quad (3.15)$$

THIRD ARGUMENT: A numerical evaluation of energy levels for example for the potential $V(r) = r^4$ gives values for energy levels listed in Table 1. It is seen that all values calculated for $0 \leq n \leq 7$ and $0 \leq \ell \leq 5$ support the conjecture that $E_{n,\ell} < E_{n-1,\ell+\sqrt{6}}$; no violation has been found. A similar test has been made for $V = \ln r$.

FOURTH ARGUMENT: We start with a potential r^{β} and study perturbations around it. We compare (as we did in our early work on level ordering) a 2S level with energy $E_{1,0}$ and wave function $u(r)$ to a level with angular momentum α without nodes, energy $E_{0,\alpha}$ and wave function $v(r)$; we choose α such that $E_{1,0} = E_{0,\alpha}$. Our early work shows that $u^2 - v^2$ vanishes at most twice and is positive near r equal zero.

We perturb now around the pure power potential and treat energy levels $E_{n,\ell}$ for $r^\beta + \lambda V(r)$; we would like to determine the sign of

$$\left. \frac{\partial}{\partial \lambda} (E_{1,0} - E_{0,\alpha}) (\lambda) \right|_{\lambda=0} = \int_0^\infty dr V(r) (u^2(r) - v^2(r)) . \quad (3.16)$$

The virial theorem for the potential r^β and the normalization of $u(r)$ and $v(r)$ proves that for all c_1, c_2

$$\int_0^\infty dr (u^2(r) - v^2(r)) (c_1 r^\beta + c_2) = 0 . \quad (3.17)$$

If we now assume that

$$\left(\frac{d}{dz} \right)^2 V(r) \gtrless 0 , \quad z = r^\beta \quad \forall r \neq 0 , \quad (3.18)$$

we deduce that there are constants c_1, c_2 such that

$$\int_0^\infty dr (u^2(r) - v^2(r)) (V(r) - c_1 r^\beta + c_2) \gtrless 0 . \quad (3.19)$$

The constants are adjusted such that $V(r) - c_1 r^\beta + c_2$ vanishes exactly at the zeros of $u^2 - v^2$, which is always possible. From (3.16) to (3.19) we conclude that if $E_{1,0} = E_{0,\alpha}$ for $\lambda = 0$, then within first order perturbation theory we get $E_{1,0}(\lambda) \gtrless E_{0,\alpha}(\lambda)$ for perturbations around r^β which fulfill

$$r \frac{d^2}{dr^2} V(r) + (1-\beta) \frac{d}{dr} V(r) \gtrless 0 \quad \forall r \neq 0 . \quad (3.20)$$

FIFTH ARGUMENT: A special case of the first part of our conjecture with $n = 1$ and $\ell = 0$ is included in the following theorem, where only monotonicity is required.

THEOREM 5: All monotonous potentials fulfill $E_{1,0} < E_{0,6}$ (in fact we can show that $E_{1,0} < E_{0,2.5}$).

Proof: For a monotonous potential V we can take as an upper bound a potential $\tilde{V}(r)$ being a constant $V(R)$ for $r < R$ and being infinite

for $r > R$. This gives an upper bound on $E_{1,0} < 4\pi^2/R^2 + V(R)$ for all R . On the other hand the ground state energy for angular momentum ℓ is always bounded from below by

$$E_{0,\ell} > \inf_R \left[V(R) + \frac{\ell(\ell+1)}{R^2} \right] .$$

Taking $\ell = 6$ gives a chain of inequalities and proves the assertion. The improvement mentioned (replacing 6 by 2.5) needs a more refined argument. This means that the conjecture (3.1) holds for α sufficiently large and n sufficiently small.

IV. Conclusion - Applications

There are at least three important applications of our results. Our first motivation came from quarkonium physics but they can be applied also to muonic atoms as well as to atomic physics. In the first two cases both conditions

$$\Delta V(r) > 0 \quad \text{and} \quad D_2 V(r) < 0 \quad (4.1)$$

are satisfied. In quarkonium physics all proposed potentials fulfill conditions (4.1) as can be verified by explicit calculations. Let us also note that the standard potential

$$V(r) = -\frac{\alpha(r)}{r} + k r, \quad \alpha(r)_{\text{small } r} \sim -1/\ln r \quad (4.2)$$

with a running coupling constant modifying the Coulomb-like behaviour at short distances fulfills (4.1). For small r , $\Delta V > 0$ is nothing but the antiscreening typical of QCD. In order to check (4.1) for the muonic case we consider the charge density ρ generated by V : $\rho = \Delta V$. A straightforward calculation, using the "running elastic force constant" $K(r)$ and Newton's theorem

$$K(r_0) = r_0^{-3} \int_0^{r_0} dr \, r^2 \, \rho(r) \quad (4.3)$$

yields

$$r_0^2(D_2V)(r_0) = r_0 K'(r_0) = \rho(r_0) - \langle \rho \rangle_{r \leq r_0} = \frac{3}{r_0^3} \int_0^{r_0} dr r^2 [\rho(r_0) - \rho(r)] \quad (4.4)$$

where we denote by $\langle \rho \rangle_{r \leq r_0}$ the mean value of $\rho(r)$ in the ball of radius r_0 . A decreasing charge density thus generates a potential with $D_2V \leq 0$.

So for both, quarkonium systems as well as muonic atoms the level ordering is between the level ordering of the hydrogen atom and the harmonic oscillator in the sense that (see Fig. 1)

$$E_{n+1,\ell} \geq E_{n,\ell+1} \geq E_{n+1,\ell-1} \quad (4.5)$$

The third application to atomic physics was already discussed in previous publications [6,7]. Let us note here in addition that for excited state energy levels of the neutral alkali-metal atoms Sternheimer [14] introduced a new ordering scheme. Motivated by measured values of levels he observed near degeneracy of levels if one introduces $n+2\ell$ as a new quantum number. This situation corresponds to $\alpha = 1/2$. From Theorem 2 we observe that there exists a potential giving exact degeneracy for such levels at one energy.

Table 1

ℓ	n	0	1	2	3	4	5	6	7
0		3.8	11.6	21.2	32.1	44.0	56.7	70.3	84.5
$\sqrt{6}$		12.6	22.8	34.0	46.2	59.2	72.9	87.3	102.3
1		7.1	16.0	26.4	37.8	50.1	63.3	77.2	91.7
$1 + \sqrt{6}$		16.9	27.7	39.5	52.2	65.6	79.7	94.4	109.7
2		10.8	20.6	31.6	43.6	56.4	69.9	84.2	99.0
$2 + \sqrt{6}$		21.4	32.8	45.2	58.3	72.1	86.6	101.6	117.2
3		14.9	25.5	37.0	49.5	62.7	76.7	91.2	106.4
$3 + \sqrt{6}$		26.1	38.1	51.0	64.5	78.7	93.5	108.9	124.8
4		19.3	30.5	42.6	55.5	69.2	83.5	98.4	113.9
$4 + \sqrt{6}$		31.1	43.6	56.9	70.9	85.6	100.6	116.2	
5		23.9	35.7	48.3	61.7	75.7	90.4	105.6	
$5 + \sqrt{6}$		36.3	49.3	63.0	77.3	92.2	107.7	123.7	

Table Caption

In Table 1 we give energy levels for the potential $V(r) = r^4$ for angular momentum ℓ and $\ell + \sqrt{6}$. As it is seen for $0 \leq n \leq 7$ and $0 \leq \ell \leq 5$ we find $E_{n-1, \ell+\sqrt{6}} > E_{n, \ell}$. Furthermore $(E_{n-1, \ell+\sqrt{6}} - E_{n, \ell})(E_{n, \ell} - E_{n-1, \ell})^{-1}$ does not exceed 15% for $n \leq 6$.

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Figure 1: Ordering of levels for potentials fulfilling $\Delta V > 0$ and $D_2 V < 0$