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TWO THEOREMS ON THE LEVEL ORDER IN POTENTIAL MODELS

H. Grosse^{*)} and A. Martin
CERN - Geneva

A B S T R A C T

We study the potentials of the form

$$U(r) = -\frac{1}{r} + \lambda V(r), \quad \left| \frac{d}{dr} \left(r^2 \frac{dV}{dr} \right) \right| \geq 0$$

and show that the energy levels satisfy the inequalities

$$E(N_c, \ell) \geq E(N_c, \ell+1)$$

to first order in λ , where N_c denotes the Coulombic principal quantum number and ℓ the angular momentum. Similarly for potentials

$$U(r) = r^2 + \lambda V(r), \quad \left(\frac{d}{dr^2} \right)^2 V(r) \geq 0$$

We prove to first order in λ that

$$\tilde{E}(N_H, \ell) \geq \tilde{E}(N_H, \ell+2)$$

where N_H denotes the harmonic oscillator quantum number. In the latter case, we give also quantitative restrictions on the relative positions at the ℓ -th and $(\ell+1)$ -th states.

^{*)} Permanent address: Institut für Theoretische Physik, Universität Wien, Austria.

Since the discovery of the J/ψ , and its interpretation as $c\bar{c}$ bound state, attempts to explain the spectrum and the decay widths, with the help of potential models^{1),2)}, have been very successful. This is even more true now with the observation of four $\ell = 0$ levels and two triplets of $\ell = 1$ levels of the γ system³⁾. From the semi-classical formula predicting the number of narrow $\ell = 0$ states of a $Q\bar{Q}$ system:

$$n = \frac{1}{4} + \frac{7}{4} \sqrt{\frac{m_Q}{m_c}} \quad (1)$$

We expect, for the $t\bar{t}$ system, at least six narrow $\ell = 0$ states if the t quark mass is 20 GeV which is the present lower limit from Petra and seven or eight $\ell = 0$ states if it is 35 GeV.

The form of the $q\bar{q}$ potential is not exactly known, though some impressive progress has been made recently in lattice QCD calculations^{4),5)}; and though numerical solutions of the Schrödinger equation are now accurately and quickly obtained by computers, it remains of some interest to obtain some general results on the spectrum from general properties of the potentials used.

Crudely speaking, the potentials used are between the Coulomb and the harmonic oscillator potential. In these two extreme cases, accidental degeneracy of the levels occurs and it is interesting to be able to make statements on the order of levels in intermediate situations.

Several years ago the authors have separately proposed two theorems, related to the comparison of the order of levels of the two extreme cases mentioned above, but limited to the order of the lowest lying levels:

1) if the following conditions are fulfilled⁶⁾:

$$\frac{d^3}{dr^3} (r^2 V(r)) > 0, \quad \lim_{r \rightarrow 0} \frac{d}{dr} (r^2 V(r)) \leq 0, \quad \lim_{r \rightarrow 0} r^2 V(r) = 0 \quad *) \quad (2)$$

the first excited $\ell = 0$ level has an energy above the lowest $\ell = 1$ level. This means that if we call $E(N_c, \ell)$ the energy of the eigenvalue with angular momentum ℓ , where $N_c = n + \ell$ is the Coulomb principal quantum number (n is the number of nodes plus one unit), we have $E(2,0) > E(2,1)$. This result was also proved for a superposition of powers

$$V(r) = \int_{-2}^{\infty} d\alpha \, \rho(\alpha) r^{\alpha} \in (\alpha(\alpha+1)), \quad \rho(x) = \frac{x}{|x|}, \quad \rho \geq 0 \quad (3)$$

*) This last condition was not explicitly stated in Ref. 6).

In fact all potentials of class (3) with $\rho = 0$ for $-2 < \alpha < -1$ satisfy condition (2).

ii) Similarly, another theorem⁷⁾ gives a sufficient condition to ensure that the energy of the first radially excited $\ell = 0$ state is below the energy of the lowest $\ell = 2$ state (degenerate for a pure harmonic oscillator). Then conditions are, using $\rho = r^2$ as a variable

$$\left(\frac{d}{d\rho}\right)^3 (\rho V(\rho)) < 0, \quad \lim_{\rho \rightarrow +\infty} \frac{d}{d\rho} (\rho V(\rho)) > -\infty, \quad \lim_{\rho \rightarrow 0} \rho V(\rho) = 0 \quad *) \quad (4)$$

For instance,

$$V(r) = \int_{-1}^2 d\alpha \rho(\alpha) r^\alpha E(\alpha), \quad \rho \geq 0 \quad (5)$$

will satisfy conditions (2) and (4) and have the "canonical" order of level⁸⁾.

It is clear that these results, which were sufficient to "understand" the order of levels found for the J/ψ system where (ignoring multiplicities due to spin) only one P state and one D state were known, have to be generalized to higher excitations in view of the present $b\bar{b}$ spectroscopy and hopefully, the future $t\bar{t}$ spectroscopy. Two efforts have been made in this direction:

i) Feldman, Fulton and Devoto⁹⁾ have shown, in the framework of the WKB approximation, i.e., for $n \gg \ell$, that

$$E(N_c, \ell) > E(N_c, \ell+1) \quad \text{if} \quad I(r) = \frac{d}{dr} \left(r^2 \frac{dV(r)}{dr} \right) > 0, \quad (6)$$

and

$$\tilde{E}(N_H, \ell) < \tilde{E}(N_H, \ell+2) \quad \text{if} \quad J(\rho) = \left(\frac{d}{d\rho}\right)^2 V(\rho) < 0, \quad (7)$$

where $\rho = r^2$ and $\tilde{E}(N_H, \ell)$ is the energy of the state with harmonic principal quantum number $N_H = 2n + \ell$ and orbital angular momentum ℓ . We have the correspondence $E(n + \ell, \ell) = \tilde{E}(2n + \ell, \ell)$.

Notice that there is a hierarchy of conditions. It is not very difficult, using the fact that

*) See previous footnote.

$$\frac{d}{dr} r^2 \left(\frac{d}{dr} r^2 \frac{dV}{dr} \right) = r^2 \left(\frac{d}{dr} \right)^3 r^2 V, \quad (8)$$

to prove that condition (2) implies condition (6). Similarly, condition (4) implies condition (7).

ii) One of us (A.M.) has studied perturbations around the Coulomb potential. The motivation was that, even though the WKB approximation has some credibility, the errors made are difficult to control and close to a situation where levels are degenerate, it is difficult to be sure that the errors will be negligible in the difference of energies. The result¹⁰⁾ was that if V is like in Eq. (3)

$$\lim_{\lambda \rightarrow 0} \frac{E_\lambda(N_c, 0) - E_\lambda(N_c, 1)}{\lambda} > 0 \quad (9)$$

Here we generalize the latter result in several ways: we extend the result to arbitrary orbital angular momentum, replace the requirement of a superposition of power potentials as perturbation to the Coulomb potential by condition (6) of Feldman et al. Finally, we prove analogous results for the neighbourhood of the harmonic oscillator potential.

To prove (6) within perturbation theory we start from the Schrödinger equation for the unperturbed system

$$h_e u_{N_c, e} = -\frac{1}{4N_c^2} u_{N_c, e}, \quad h_e = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} - \frac{1}{r} \quad (10)$$

and determine the sign of the difference of the expectation values of $V(r)$ in the angular momentum ℓ and $\ell + 1$ state with the same principal quantum number N_c :

$$\begin{aligned} \Delta_{N_c, \ell} &= \lim_{\lambda \rightarrow 0} \frac{E_\lambda(N_c, \ell) - E_\lambda(N_c, \ell+1)}{\lambda} = \langle V \rangle_{N_c, \ell} - \langle V \rangle_{N_c, \ell+1} \\ \langle V \rangle_{N_c, \ell} &= \int_0^\infty dr V(r) u_{N_c, \ell}^2(r) \end{aligned} \quad (11)$$

where we have denoted by $E_\lambda(N_c, \ell)$ the eigenvalue of the full problem with potential $U(r) = (-1/r) + \lambda V(r)$.

In Ref. 10) a large number of properties of the moments $\langle r^\alpha \rangle_{N_c \ell}$ has been obtained, which are of interest in themselves. In this note we use a somewhat different approach, which allows us to cover the general case of potentials fulfilling (6). The main idea is rather simple: since there is a $O(4)$ symmetry in the Coulomb problem, there exist operators which increase (respectively decrease) the angular momentum within a multiplet of fixed N_c :

Lemma 1: Let

$$A_\ell^\pm = \pm \frac{d}{dr} - \frac{\ell+1}{r} + \frac{1}{2(\ell+1)} \quad (12)$$

and let $u_{N_c, \ell}$ be the solution of the Schrödinger equation (10); then we have

$$A_\ell^- u_{N_c, \ell+1} = \alpha_\ell u_{N_c, \ell}, \quad A_\ell^+ u_{N_c, \ell} = \alpha_\ell u_{N_c, \ell+1} \quad (13)$$

where the constants α_ℓ follow from normalization of the wave functions:

$$4\alpha_\ell^2 = (\ell+1)^2 - N_c^{-2} \quad (14)$$

Proof:

In order to prove (13), we notice that h_ℓ is easily expressed in terms of $A_\ell^\pm$:

$$h_\ell = A_\ell^- A_\ell^+ - \frac{1}{4(\ell+1)^2} = h_{\ell+1} - \frac{2(\ell+1)}{r^2} \quad (15)$$

in addition we notice the commutation relations

$$[h_\ell, A_\ell^+] = -\frac{2(\ell+1)}{r^2} A_\ell^+ \quad (16)$$

Now operate with $h_{\ell+1}$ on $A_\ell^+ u_{N_c, \ell}$. Use of the commutation rules (16) proves (13). Normalization determines the constants α_ℓ .

Equations (13) have rather powerful consequences for our problem. If we multiply the first of them by $V(r)u_{N_c, \ell}(r)$ and the second by $V(r)u_{N_c, \ell+1}(r)$, integrate and subtract, we get

$$\alpha_\ell \cdot \Delta_{N_c, \ell} = \int_0^\infty dr \left(\frac{d}{dr} V(r) \right) u_{N_c, \ell}(r) u_{N_c, \ell+1}(r) \quad (17)$$

On the other hand, multiplication of the first of Eqs. (13) by $V'(r)u_{N_C, \ell+1}(r)$, integration and comparison with Eq. (17) gives

$$\alpha_\ell^2 \cdot \Delta_{N_C, \ell} = \left\langle \frac{1}{2} \frac{d^2 V}{dr^2} - \frac{\ell+1}{r} \frac{dV}{dr} + \frac{1}{2(\ell+1)} \frac{dV}{dr} \right\rangle_{N_C, \ell+1} \quad (18)$$

In order to proceed, we need

Lemma 2:

Within the above definitions, we have

$$\left\langle \frac{1}{r^3} (r-r_0) \right\rangle_{N_C, \ell+1} = 0, \quad r_0 = 2(\ell+1)(\ell+2) \quad (19)$$

Proof:

Putting $V(r) = -1/r$, we see from the definition of $\Delta_{N_C, \ell}$ and the virial theorem that $\Delta_{N_C, \ell}$ vanishes; from Eq. (18) we then get the relation (19) between the moments.

In order to determine finally the sign of $\Delta_{N_C, \ell}$ we rewrite Eq. (18) by adding a multiple of (19):

$$\alpha_\ell^2 \cdot \Delta_{N_C, \ell} = \left\langle \frac{1}{2} \frac{d^2 V}{dr^2} + \frac{1}{r} \frac{dV}{dr} \right\rangle_{N_C, \ell+1} + \left\langle \frac{1}{r^3} \left(r^2 \frac{dV}{dr} - r_0^2 \frac{dV}{dr}(r_0) \right) \frac{(r-r_0)}{2(\ell+1)} \right\rangle_{N_C, \ell+1} \quad (20)$$

Assume inequality (6) at this point; the first expectation value in (20) is therefore positive. The second one is also positive, since it is the expectation of a product of two monotonically increasing functions which vanish both at the same point r_0 (by construction). Moreover, we note that the sign $\Delta_{N_C, \ell}$ is the same as the sign of $I(r)$. This allows us to state

THEOREM 1: Assume that the potential $\lambda V(r)$ is such that $I(r)$ of Eq. (6) is positive, then in first order perturbation theory in λ we have

$$E(N_C, \ell) > E(N_C, \ell+1)$$

If one has the case $I(r) < 0$ the above inequality is reversed.

Remarks:

For the class of potentials of the form of Eq. (3) we immediately get the "canonical level ordering" for any l and N_C .

Since the main reason why the above derivation works is the symmetry behind the problem, one expects a similar result for perturbations around the harmonic oscillator. This is indeed the case, as we shall show now.

This time we start with the unperturbed oscillator Hamiltonian

$$\tilde{h}_e w_{n,e} = E_{2n+e} w_{n,e}, \quad \tilde{h}_e = -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{r^2}{4}, \quad E_{N_H} = N_H + \frac{3}{2}, \quad (21)$$

where n denotes again the number of zeros of the radial wave function $w_{n,l}$ in the domain $(0, \infty)$. Note that we have energy degeneracy between states of quantum numbers $(n+1, l)$ and $(n, l+2)$. Therefore, the first order correction which replaces Eq. (11) here is

$$\tilde{\Delta}_{n,e} = \langle V \rangle_{n+1,e} - \langle V \rangle_{n,e+2}, \quad \langle V \rangle_{n,e} = \int_0^\infty dr V(r) w_{n,e}^2(r) \quad (22)$$

The main question concerns the analogue of Eqs. (13). We found them by combining ladder operators $B_\ell^\pm$ which change from levels (n, l) to $(n+1, l-1)$

$$B_e^\pm = \pm \frac{d}{dr} - \frac{l+1}{r} + \frac{r}{2}, \quad B_e^+ w_{n+1,e} = \gamma w_{n,e+1} \quad (23)$$

$$\gamma^2 = 2n+2, \quad B_e^- w_{n,e+1} = \gamma w_{n+1,e},$$

where $w_{n,l}$ is the solution of the Schrödinger equation (21), with ladder operators $C_\ell^\pm$ which map from levels (n, l) to $(n, l+1)$

$$C_e^\pm = \pm \frac{d}{dr} - \frac{l+1}{r} - \frac{r}{2}, \quad C_e^+ w_{n,e} = \beta_e w_{n,e+1} \quad (24)$$

$$\beta_e^2 = 2l+2n+3, \quad C_e^- w_{n,e+1} = \beta_e w_{n,e},$$

It is easy to derive the algebra of $B_\ell^\pm$ and $C_\ell^\pm$ with $\tilde{h}_\ell$, from which we deduce that

$$\begin{aligned} h_{\ell+2} B_{\ell+1}^+ C_{\ell}^+ &= B_{\ell+1}^+ C_{\ell}^+ h_{\ell} \\ h_{\ell} B_{\ell}^- C_{\ell+1}^- &= B_{\ell}^- C_{\ell+1}^- h_{\ell+2} \end{aligned} \quad (25)$$

From the explicit representations for $B_{\ell}^{\pm}$ and $C_{\ell}^{\pm}$, we derive

Lemma 3:

Define operators

$$D_{\ell}^{\pm} = \pm \frac{1}{r} \frac{d}{dr} - \frac{\ell+3/2}{r^2} + \frac{E_{2n+\ell+2}}{2\ell+3} \quad (26)$$

and let $v_{n,\ell} = \sqrt{r} w_{n,\ell}$. Then we have

$$D_{\ell}^+ v_{n+1,\ell} = K_{\ell} v_{n,\ell+2}, \quad D_{\ell}^- v_{n,\ell+2} = K_{\ell} v_{n+1,\ell}, \quad (27)$$

where K_{ℓ} are again normalization constants.

Remark:

The step from $w_{n,\ell}$ to $v_{n,\ell}$ allows us to get symmetrical expressions (27). They are essential for the argument which follows.

Next, we simulate the procedure from the Coulomb problem. Multiplication of the first of Eqs. (27) by $V(r)v_{n,\ell+2}(r)/r$, the second by $V(r)v_{n+1,\ell}(r)/r$, integration and subtraction, gives

$$K_{\ell} \tilde{\Delta}_{n,\ell} = \int_0^{\infty} dr W(r) v_{n+1,\ell}(r) v_{n,\ell+2}(r), \quad W(r) = \frac{d}{dr} \left(\frac{V(r)}{r^2} \right) \quad (28)$$

Next, multiplication of the second of Eqs. (27) by $W(r)v_{n,\ell+2}(r)$ and integration, gives

$$K_{\ell}^2 \tilde{\Delta}_{n,\ell} = \left\langle \frac{1}{2} \frac{dW}{dr} - (\ell+3) \frac{W}{r} + \frac{E_{2n+\ell+2}}{2\ell+3} \right\rangle_{n,\ell+2} \quad (29)$$

Since a constant potential leaves the levels degenerate, we get from (29), replacing $V(r)$ by a constant in the definition of $W(r)$:

Lemma 4:

Within the notation of Eq. (22), we have the vanishing of

$$\left\langle \frac{1}{r^4} (r^2 - r_n^2) \right\rangle_{n, \ell+2} = 0, \quad r_n^2 = \frac{(2\ell+3)(2\ell+7)}{2E_{2n+\ell+2}}. \quad (30)$$

Combining Eqs. (29) and (30) so that the previously discussed steps can be repeated is a simple task:

$$K_\ell^2 \tilde{\Delta}_{n, \ell} = \frac{1}{2} \left\langle \frac{dW}{dr} + \frac{3}{r} W \right\rangle_{n, \ell+2} + \left\langle \frac{r^3 W - r_n^2 W(r_n)}{r^4} (r^2 - r_n^2) \right\rangle_{n, \ell+2} \frac{E_{2n+\ell+2}}{2\ell+3} \quad (31)$$

Eq. (31) leads to

THEOREM 2: Assume that the potential $V(r)$ is such that the quantity

$$J(\rho) = \left(\frac{d}{d\rho} \right)^2 V(\rho), \quad \rho = r^2 \quad (32)$$

has a definite sign. It follows from first order perturbation theory in λ that

$$\tilde{E}(N_H, \ell) \geq \bar{E}(N_H, \ell+2) \quad \text{if } J(\rho) \geq 0 \quad \forall \rho. \quad (33)$$

One further application of the above method is worthwhile to be mentioned. From Eqs. (24) we deduce that

$$(2n+2\ell+5) (\langle V \rangle_{n, \ell} - \langle V \rangle_{n, \ell+1}) = \left\langle \frac{1}{2} \frac{d^2}{dr^2} V - \frac{\ell+1}{r} \frac{dV}{dr} - \frac{r}{2} \frac{dV}{dr} \right\rangle_{n, \ell+1} \quad (34)$$

by the same technique used before. Similarly, from (23)

$$(2n+2) (\langle V \rangle_{n+1, \ell} - \langle V \rangle_{n, \ell+1}) = \left\langle \frac{1}{2} \frac{d^2}{dr^2} V - \frac{\ell+1}{r} \frac{dV}{dr} + \frac{r}{2} \frac{dV}{dr} \right\rangle_{n, \ell+1} \quad (35)$$

follows. Combining both expressions (34) and (35) allows us to state a result on the relative positions of the ℓ th states to the $(\ell+1)$ th states:

Corollary:

Under the assumption of Theorem 2 we conclude that within first order perturbation theory

$$\tilde{E}(N_H, l) + \tilde{E}(N_H+2, l) \geq 2 \tilde{E}(N_H+1, l+1) \text{ if } J(\rho) \geq 0 \forall \rho. \quad (36)$$

Proof:

From (34) and (35) we get

$$\begin{aligned} (2n+2l+3)(2n+2) (\langle V \rangle_{n,l} + \langle V \rangle_{n+1,l} - 2 \langle V \rangle_{n,l+1}) = \\ = E_{2n+l+1} \left\langle \frac{d^2}{dr^2} V - \frac{1}{r^2} \frac{dV}{dr} \right\rangle_{n,l+1} + (l+\frac{1}{2}) \left\langle \left(\frac{1}{r} \frac{dV}{dr} - \frac{1}{r^2} \frac{dV}{dr} \left(\frac{1}{r} \right) \right) (r^2 - r_l^2) \right\rangle_{n,l+1} \\ r_l^2 = 2 E_{2n+l+1} \end{aligned} \quad (37)$$

and the corollary follows from the assumption that $J(\rho)$ has a definite sign.

One might also be tempted to use this technique to generalize a known result on Regge trajectories. The lowest trajectory ($n = 0$) is known to be concave⁸⁾ if the harmonic oscillator is perturbed by a potential satisfying condition (7). However, this is not true for arbitrary n . In particular, when the perturbing potential is r^α , $0 < \alpha < 1$, the trajectories are convex for $n \gg l$, as can be proved starting from the expression

$$\langle V \rangle_{n,l+2} + \langle V \rangle_{n,l} - 2 \langle V \rangle_{n,l+1} = \left\langle (2n+2l+4) \frac{d^2}{dr^2} V + \frac{2n+1}{r} \frac{dV}{dr} - r \frac{dV}{dr} \right\rangle_{n,l+1} \quad (38)$$

To conclude, we should remark that it would, of course, be desirable to obtain proofs, for arbitrary n , avoiding the use of perturbation theory. However, if we put together the exact results for small n , the WKB results for large n , the perturbation theory results in the neighbourhood of Coulomb and of the harmonic oscillator potential, we, as physicists, tend to believe that conditions (6) and (7) do guarantee the canonical order of levels.

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