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ON THE ORDER OF LEVELS IN CHARMONIUM

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ABSTRACT

We prove a theorem concerning the energies of the 2S and 3D states in a potential $V(r) = -g^2/r + V_c(r)$, where V_c is a non-singular confining potential. If $(d/dr)^3 (r^2 V_c)$ is positive, then the 3D state lies above the 2S state, provided

$$\frac{d}{dr} \frac{1}{r} \frac{d}{dr} \left(2V_c + r \frac{dV_c}{dr} \right) < 0 \quad \forall r > 0.$$

For $V_c = r^\alpha$, this corresponds to $0 < \alpha < 2$.

1. INTRODUCTION

The charmonium states are usually described by a non-relativistic potential, which is the sum of a Coulombic and a confining part $V_c^{1,2)}$. Since there is no deep understanding of the confining mechanism, one has no detailed knowledge about V_c , and model-independent assertions seem to be of great value. A result of this type has been given recently by Martin³⁾. He obtains a sufficient condition for the first three levels to be ordered 1S-2P-2S, as observed in the ψ, χ, ψ' spectroscopy^{4,5,6)}. This condition is fulfilled by $V_c = r^\alpha$ for $\alpha > 0$, for example. Here we will apply similar ideas to the next level, denoted by 3D, according to the spectroscopic notation in the pure Coulomb case.

First we give a condition on the confining potential, which implies the ordering 2S-3D; this condition is fulfilled by $V_c = r^\alpha$ for $0 < \alpha < 2$. For $\alpha > 2$, it is found that there exists exactly one coupling strength λ_0 for which the level difference becomes zero. For $\lambda < \lambda_0$ the canonical order 2S-3D is obtained, for $\lambda > \lambda_0$ the ordering is reversed.

Experimentally the 3D state has not been observed, but this can be attributed either to the small width or to the special ordering 2S-3D. A mixing of these states is sometimes assumed²⁾.

Finally we comment on the application of Martin's theorem to the next P level, denoted by 3P.

2. REVIEW OF RESULTS OF REF. 3)

Let us first present the main steps of Ref. 3), as much as they will be used here. We will study the energies E_{2S} and E_{3D} as given by the solution of the Schrödinger equations ($2m = \hbar = 1$)

$$-u'' - \frac{g^2}{r} u + \lambda^2 V_c(\lambda r) u = E_{2S} u \quad (1)$$

$$-v'' + \frac{6}{r^2} v - \frac{g^2}{r} v + \lambda^2 V_c(\lambda r) v = E_{3D} v \quad (2)$$

with $u(0) = v(0) = 0$. It is known that the 2S wave function $u(r)$ has exactly one node in $(0, \infty)$ and that of the 3D state $v(r)$ has none. In (1) and (2) a convenient behaviour of the confining potential on the coupling constant λ has

been chosen, which implies that the dimension of λ is minus one. V_c is regarded as a perturbation, such that the level shift is given by the Feynman-Hellman theorem⁷⁾

$$\frac{d}{d\lambda}(E_{2S}-E_{3D}) = \int_0^{\infty} dr (u^2 - v^2) \frac{d}{d\lambda} \lambda^2 V_c(\lambda r) \quad (3)$$

For the combination $(u-v)(u+v)$, which enters in (3), it has been proved in Ref. 3):

Lemma 1 : If u has one node at r_0 , v has none, $u-v$ vanishes once and only once in $(0, r_0)$.

Lemma 2 : If $E_{2S} \geq E_{3D}$, $u+v$ vanishes at most once in (r_0, ∞) .

The proofs are given by a study of the Wronskian determinant of u and v .

The energy difference $\varepsilon = E_{2S} - E_{3D}$, which we would like to study, is given by

$$\varepsilon = \int_0^{\infty} dr (u'^2 - v'^2) - 6 \int_0^{\infty} \frac{dr v^2}{r^2} + \int_0^{\infty} dr (u^2 - v^2) \left(-\frac{g^2}{r} + \lambda^2 V_c(\lambda r) \right) \quad (4)$$

where the normalization conditions

$$\int_0^{\infty} dr u^2(r) = \int_0^{\infty} dr v^2(r) = 1 \quad (5)$$

have been imposed. To eliminate the kinetic energy contributions, we make use of the Virial theorem, which states the equality of the expectation values of the kinetic energy and the Virial in a bound state w :

$$\int_0^{\infty} dr \left(w'^2 + \frac{\ell(\ell+1)}{r^2} w^2 \right) = \int_0^{\infty} dr \frac{r}{2} \frac{dV}{dr} w^2 \quad (6)$$

where the total potential enters on the right.

Applying (6) to u and v in (4) gives

$$2\mathcal{E} = \int_0^{\infty} dr (u^2 - v^2) \left[-\frac{g^2}{r} + \lambda^2 V_c(\lambda r) + \lambda^2 r \frac{d}{dr} V_c(\lambda r) \right] \quad (7)$$

So by the choice of the behaviour on the coupling constant, we obtain finally, using (3)

$$2\mathcal{E} = -g^2 \int_0^{\infty} dr \frac{u^2 - v^2}{r} + \lambda \frac{d\mathcal{E}}{d\lambda} \quad (8)$$

$$\frac{d\mathcal{E}}{d\lambda} = \int_0^{\infty} dr \frac{u^2 - v^2}{r} W(\lambda r) \quad W(x) = x \left(2V_c + x \frac{dV_c}{dx} \right) \quad (9)$$

Equations (8) and (9) are the starting point of our derivation. In the following we will deal only with non-singular confining potentials in the sense that V_c should be finite at the origin.

Theorem³⁾: Assume the conditions

$$W(0) \leq 0 \quad \left(\frac{d}{dr} \right)^2 W(r) > 0 \quad \forall r > 0 \quad (A)$$

hold; then at a crossing point $\mathcal{E}(\lambda) = 0$, the slope $d\mathcal{E}/d\lambda$ has to be positive.

To be complete, let us reproduce the main steps of the proof: Assume on the contrary, that $d\mathcal{E}/d\lambda \leq 0$, then (8) implies

$$\int_0^{\infty} dr \frac{u^2 - v^2}{r} < 0 \quad (10)$$

but then it follows [using Lemma 1 and (5)] that $u^2 - v^2$ vanishes twice. A careful analysis shows that

$$\int_r^\infty dr' \int_{r'}^\infty dr'' \frac{u^2 - v^2}{r''} > 0 \quad (11)$$

has to be positive. So evaluating $d\varepsilon/d\lambda$ by two partial integrations and using (A) shows $d\varepsilon/d\lambda > 0$ contrary to the assumption.

The same arguments give immediately:

Corollary: Assume (A) holds, then for $\varepsilon > 0$, it follows that $d\varepsilon/d\lambda \neq 0$.

This version is of some help in our situation. We know from the hydrogen levels that $\varepsilon(0) < 0$. So if λ increases, $\varepsilon(\lambda)$ may cross and become positive, but then the energy difference has to be monotonic and can never cross again or go to zero. In other words: if we know $\varepsilon(\lambda) \leq 0$ for $\lambda \rightarrow \infty$, no crossing is allowed; if $\varepsilon(\lambda) > 0$ for some λ , there exists exactly one value λ_0 with $\varepsilon(\lambda_0) = 0$.

3. SCALING ARGUMENTS

To study the behaviour of ε for large λ we first return to Eqs. (1) and (2). Starting with Eq. (1), denoting more explicitly the eigenvalue by $E_{2S}(\lambda, g^2)$ we obtain, by a scale transformation

$$r \rightarrow r/\lambda \quad p \rightarrow \lambda p \quad \bar{u}(r) = u(r/\lambda) \quad (12)$$

the following equation:

$$-\bar{u}'' - \frac{g^2}{\lambda r} \bar{u} + V_c(r) \bar{u} = \lambda^{-2} E_{2S}(\lambda, g^2) \bar{u} \quad (13)$$

As is often seen, $\bar{u}$ is an eigenfunction of the operator on the left of the eigenvalue $\lambda^{-2} E_{2S}(\lambda, g^2)$. But since the operator depends only on g^2/λ we get

$$E_{2S}(\lambda, g^2) = \lambda^2 f_{2S}(g^2/\lambda) \quad (14)$$

where f_{2S} is a function of only one variable. Clearly this has to be so for dimensional reasons; g^2/λ is the only dimensionless combination, which one can form out of g^2 and λ . But then also the level difference is expressed similarly

$$\varepsilon(\lambda, g^2) = \lambda^2 [f_{2S}(g^2/\lambda) - f_{3D}(g^2/\lambda)] \quad (15)$$

So, the sign of ε for $\lambda \rightarrow \infty$ coincides with the sign of ε for $g \rightarrow 0$. Therefore it is enough to compute the sign of the level difference for the operator

$$-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \lambda^2 V_c(\lambda r) \quad (16)$$

To proceed we use the above scaling argument once more and start with

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \omega^2 r^2 + \lambda^2 V_c(\lambda r) \right] v(r) = E(\lambda, \omega) v(r) \quad (17)$$

The difference Δ of the energies of the second S state and the first D state for this operator has again a general form like (15) (changing $g^2 \rightarrow \omega^2$). $\lambda = 0$ corresponds now to the harmonic oscillator for which we know $\Delta = 0$. In the next chapter we give conditions (B) [or (C)] implying $\Delta < 0$ (or $\Delta > 0$) for all $\lambda > 0$. So we know $\Delta < 0$ (or $\Delta > 0$) for large λ , which corresponds to $\omega \rightarrow 0$, and therefore to the level difference of (16) and we are finished.

4. DERIVATION OF MAIN RESULTS

Let us denote the solutions of Eq. (17) again by u and v . Similar to (8) and (9) we obtain, with the help of the Virial theorem,

$$2\Delta = \omega^2 \int_0^\infty dr (u^2 - v^2) r^2 + \lambda \frac{d\Delta}{d\lambda} \quad (18)$$

$$\frac{d\Delta}{d\lambda} = \int_0^\infty dr (u^2 - v^2) U(\lambda r) \quad U(x) = 2V_c + x \frac{dV_c}{dx} \quad (19)$$

Theorem, Part A: Under the conditions

$$0 \leq \lim_{r \rightarrow \infty} \frac{1}{r} \frac{dU}{dr} < \infty \quad \frac{d}{dr} \frac{1}{r} \frac{dU}{dr} < 0 \quad \forall r > 0 \quad (B)$$

the slope $d\Delta/d\lambda$ has to be negative, if the levels cross $\Delta = 0$.

Proof: Assume on the contrary $d\Delta/d\lambda \geq 0$; this implies

$$\int_0^{\infty} dr (u^2 - v^2) r^2 < 0 \quad (20)$$

Consider

$$I(r) = \int_r^{\infty} dr' (u^2 - v^2) \quad (21)$$

$$J(r) = \int_0^r dr' r' I(r') \quad (22)$$

Obviously $I(0) = J(0) = 0$; furthermore $J(\infty) < 0$ by (20). Note, by Lemmas 1 and 2, $u^2 - v^2$ has either one or two zeros; in the first case $J'(r) \leq 0$ for all r , in the second case $J(r)$ falls off first, has exactly one minimum and goes then to zero. In both cases $J(r) < 0$. Next we calculate the slope by partial integrations, using condition (B)

$$\frac{d\Delta}{d\lambda} = - \int_0^{\infty} dr J(r) \frac{d}{dr} \left[\frac{1}{r} \frac{d}{dr} U(r) \right] \quad (23)$$

Note that $I(r)$ goes like $-r^3$ for small r and u and v drop exponentially at infinity. $J(r) < 0$ implies $d\Delta/d\lambda < 0$, contrary to our assumption.

To exclude the crossing situation, we note that for small λ the level shift is given by the perturbation theoretic expression

$$\Delta_{\text{pert}} = \int_0^{\infty} dr (u_0^2 - v_0^2) \lambda^2 V_c(\lambda r) \quad (24)$$

where u_0 and v_0 denote the unperturbed wave functions. Observing that (B) implies

$$\frac{d}{dr} \frac{1}{r} \frac{d}{dr} V_c(r) < 0 \quad (25)$$

we have only to assume the following boundary condition at infinity

$$0 \leq \lim_{r \rightarrow \infty} \frac{1}{r} \frac{dV_c}{dr} < \infty \quad (B')$$

and can proceed as above with the result that $\Delta_{\text{pert}} < 0$.

Theorem, Part B: Impose the conditions

$$0 \leq \lim_{r \rightarrow 0} \left(\frac{1}{r} \frac{d}{dr} U(r) \right) < \infty \quad \frac{d}{dr} \left[\frac{1}{r} \frac{d}{dr} U(r) \right] > 0 \quad \forall r > 0 \quad (c)$$

then the slope $d\Delta/d\lambda$ has to be positive at the crossing point $\Delta = 0$.

The by now familiar ideas of the proof are as follows. The contrary to $d\Delta/d\lambda > 0$ implies

$$\int_0^{\infty} dr r^2 (u^2 - v^2) > 0 \quad (26)$$

In this case $u^2 - v^2$ has to have two zeros; otherwise we would have

$$\int_0^{\infty} dr (r^2 - r_0^2) (u^2 - v^2) > 0 \quad (27)$$

which is impossible. Consider again $I(r)$ as given in (21) and

$$K(r) = \int_r^{\infty} dr' r' I(r') \quad (28)$$

Here $K(0) > 0$, $K(r)$ rises near $r = 0$, and has to have one maximum; furthermore, $K(\infty) = 0$, so we get $K(r) > 0 \forall r > 0$. Calculating the slope by two partial integrations and using conditions (C) we get again a contradiction, implying that $d\Delta/d\lambda > 0$ for $\Delta = 0$.

From the perturbation expression (24) we can again conclude the positivity of Δ_{pert} near $\lambda = 0$ if

$$0 \leq \lim_{r \rightarrow 0} \frac{1}{\pi} \frac{dV}{dr} < \infty \quad (C')$$

5. CONCLUSION

Let us summarize: conditions (A) imply the monotonicity of the difference ϵ of the energies 2S-3D for our original Hamiltonian (for $\epsilon > 0$); (B, B') [or (C, C')] imply a negative (or positive) value for large λ . As a result (A, B, B') give a negative level difference for all λ ; (A, C, C') one and only one value for which the levels cross. Especially for a linear superposition of potentials $V = r^\alpha$ with a positive weight, we obtain the canonically level order if $0 < \alpha < 2$, while for the other case $\alpha > 2$ is required.

Immediately, we may conclude for the next state 3P: E_{3P} has to be above E_{2S} because the angular momentum operator is positive, but if condition (A) is fulfilled by an application of Martin's theorem, it has to lie also above the 3D state, whatever the stronger condition is.

Concerning mathematical rigour, we naturally should remark that we assumed that the perturbation series will give at least an asymptotic expansion, as is the case for the anharmonic oscillator⁸⁾ and that for small λ ³⁾

$$\lim_{\lambda \rightarrow 0} \frac{\Delta_{\text{pert}}}{\Delta_{\text{exact}}} = 1 \quad (29)$$

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