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A THEOREM ON THE ORDER OF LEVELS IN CONFINING POTENTIALS

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ABSTRACT

We prove that in a two-body, non-relativistic system interacting via a potential $V = -g^2/r + V_c(r)$, where V_c is a confining potential non-singular at the origin, the 2S level is above the 2P level if V_c satisfies the following sufficient condition :

$$\left(\frac{d}{dr}\right)^2 \left[r(2V_c(r) + r \frac{dV_c}{dr}(r)) \right] > 0, \forall r.$$

This covers the well-known cases of linear potentials or harmonic oscillator potentials, which were considered in charmonium models, but also more generally, for instance,

$$V_c(r) = r^\alpha, \quad \alpha > 0.$$

I. INTRODUCTION

The description of the J/ψ and ψ' particles ^{1),2)} by a non-relativistic bound state model has been extremely successful ^{3),4)}. In this interpretation the J/ψ particle appears as a 1S state and the ψ' as a 2S state, if we use the hydrogen-like classification. A remarkable prediction, using as interaction potential a combination of a Coulomb-like potential $-g^2/r$ and a confining potential essentially linear in r , was that between the 1S state and the 2S state a triplet of 2P states must be present. This prediction was confirmed by experiment ^{5),6)}.

The argument generally used to explain qualitatively the order of the levels, 1S-2P-2S, is that the levels should lie in between two extreme cases, the Coulomb case when 2P and 2S are degenerate, and the pure harmonic oscillator in which the 2P state is half-way between the 1S and 2S states. Although there are some arguments in favour of a linear confining potential ⁴⁾, these cannot be considered as really compelling since confinement itself is not really understood yet. So, because the exact nature of the confining potential is not exactly known, it may be useful to obtain a general sufficient condition on the interaction which guarantees that the order of levels is what we believe it to be : 1S-2P-2S.

We have found such a condition, which covers in particular the linear and quadratic confining potentials, but also other cases like $V_c = r^{\frac{1}{2}}$. No attempt is made to include such things as relativistic effects.

II. PROPERTIES OF THE WAVE FUNCTIONS

The potential will be taken to be

$$V = -g^2/r + V_c(r) \quad (1)$$

where V_c is the confining potential. However, it will turn out to be convenient to vary continuously the confining potential as a function of a parameter λ

$$V(\lambda, r) = -g^2/r + V_c(\lambda, r), \quad 0 \leq \lambda \leq 1 \quad (2)$$

such that for $\lambda=0$, V_c vanishes and for $\lambda=1$, it is precisely the confining potential. The most convenient functional dependence on λ will appear in a moment.

The 2S wave function, u , satisfies the equation

$$-u'' - \frac{g^2}{r} u + V_c(\lambda, r) u = E_{2S}(\lambda) u \quad (3)$$

According to the standard Sturm-Liouville theory, $u(r)$ has one node, i.e., $u(r) > 0$ for $r < r_0$, $u(r) < 0$ for $r > r_0$; also, we obviously have $E_{2S} > E_{1S}$.

The 2P wave function, v , satisfies

$$-v'' + \frac{2v}{r^2} - \frac{g^2}{r} v + V_c(\lambda, r) v = E_{2P}(\lambda) v. \quad (4)$$

v being the ground state wave function in the $\ell=1$ angular momentum state has no node and can be taken to be positive. Clearly, $E_{2P} > E_{1S}$, because of the centrifugal term.

If λ is varied, the energy levels will move. We shall admit that the derivative of the energy levels with respect to λ is given by the perturbation theory expression :

$$\frac{d}{d\lambda} (E_{2S} - E_{2P}) = \int_0^\infty dr (u^2 - v^2) \frac{dV_c(\lambda, r)}{d\lambda} \quad (5)$$

The reason why we say "admit" is that we are in a situation where the perturbation series may not converge. In particular, it certainly does not converge around $\lambda=0$, since, at large distances the confining potential dominates over the Coulomb potential. However, we believe that the perturbation expansion holds as an asymptotic expansion [the situation is quite analogous to that of the anharmonic oscillator for which this is proved ⁷⁾]. Here our needs are much more modest, since all we need to establish (5) is the continuity of the normalized wave functions with respect to λ for finite r , together with their rapid decrease for $r \rightarrow \infty$.

Equation (5) shows that it is important to study the difference

$$u^2 - v^2$$

Lemma 1

$u-v$ vanishes once and only once.

Proof From $u \sim r$ $v \sim r^2$ for $r \rightarrow 0$ we get $u-v > 0$ for $r \rightarrow 0$, and from $u(r_0) = 0$, $u-v < 0$ for $r = r_0$. In general, combining (3) and (4), one gets

$$v u' - u v' = - \int_0^r v r \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] dr \quad (6)$$

the integrand, in the right-hand side of (6) vanishes either once at $r = r_0$, if $E_{2S} \geq E_{2P}$, or twice if $E_{2S} < E_{2P}$, at $r = r_0$ and $r^2 = (E_{2P} - E_{2S}/2)$. In both cases we notice that applying (6) to $r = r_0$ we get

$$\begin{aligned} v(r_0) u'(r_0) &= - \int_0^{r_0} v r \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] dr \\ &= \int_{r_0}^{\infty} v r \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] dr < 0 \end{aligned} \quad (7)$$

This shows that $uv \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right]$ cannot be everywhere positive in $r_0 < r < \infty$. Therefore $uv \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right]$ is positive in $0 < r < r_0$. Therefore, if r_1 is such that $u(r_1) - v(r_1) = 0$, we get

$$v(r_1) [u'(r_1) - v'(r_1)] = - \int_0^{r_1} dr \, v r \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] < 0$$

This proves that $u-v$ can only vanish once in $0 < r < r_0$.

Lemma 2

If $E_{2S} \geq E_{2P}$ $u+v$ vanishes at most once in $r_0 < r < \infty$.

Proof We use again Eq. (6), setting $u(r_2) = -v(r_2)$. We get

$$v(r_2) [u'(r_2) + v'(r_2)] = \int_{r_2}^{\infty} v r \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] dr \quad (8)$$

since $r_2 > r_0$ and $E_{2S} \geq E_{2P}$ $(u'+v')$ is negative at r_2 . Hence $u+v$ vanishes at most once. There is no compelling reason why it should vanish so far.

Lemma 3

If $E_{2S} < E_{2P}$ $u+v$ vanishes at most twice.

Proof In that case we know that $2/r^2 + E_{2S} - E_{2P}$ vanishes once for $r_0 < r < \infty$, that

$$\int_{r_0}^{\infty} u v \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] dr < 0$$

while, clearly,

$$\int_r^{\infty} u v \left[\frac{2}{r^2} + E_{2S} - E_{2P} \right] dr' > 0$$

for r very large. If $u+v$ vanishes at least in three successive points r_1, r_2, r_3 , we get from (8) that the sign of $(u+v)'$ at two successive points, r_1 and r_2 or r_2 and r_3 will be the same, which is impossible.

We turn now to a very important relation, which we may call the virial theorem. If we start in general from a Schrödinger equation for a bound state

$$-u'' + Vu = Eu \quad (9)$$

we get, after multiplication by u and integration by parts

$$\int_0^{\infty} u'^2 dr + \int_0^{\infty} V u^2 dr = E \int_0^{\infty} u^2 dr \quad (10)$$

On the other hand, multiplying (9) by $2u'$ and integrating from r to ∞ we get

$$(u'(r))^2 - V(r)(u(r))^2 - \int_r^{\infty} \frac{dV}{dr'} (u(r'))^2 dr' = -E(u(r))^2$$

Integrating again, we get

$$\int_0^{\infty} u'^2 dr - \int_0^{\infty} V u^2 dr - \int_0^{\infty} r \frac{dV}{dr} u^2 dr = -E \int_0^{\infty} u^2 dr \quad (11)$$

and, by combination of (10) and (11), we get

$$\int_0^{\infty} \left(2 V(r) + r \frac{dV}{dr} \right) u^2(r) dr = 2 E \int_0^{\infty} u^2(r) dr \quad (12)$$

This remarkable equation shows in particular that in the pure Coulombic case ($V(r) = -e^2/r$) the ground state energy is half the potential energy. Notice also that if a centrifugal term $\frac{l(l+1)}{r^2}$ is present in V it automatically disappears from the left-hand side of (12).

Applying this equation to our problem, we get

$$\begin{aligned} & \int_0^{\infty} (u^2 - v^2) \left[-\frac{g^2}{r} + 2V_c(\lambda, r) + r \frac{dV_c(\lambda, r)}{dr} \right] dr \\ &= E_{2S} \int_0^{\infty} u^2 dr - E_{2P} \int_0^{\infty} v^2 dr = E_{2S} - E_{2P} \end{aligned} \quad (13)$$

if the wave functions are normalized

$$\int_0^{\infty} u^2 dr = \int_0^{\infty} v^2 dr = 1 \quad (14)$$

III. STUDY OF THE LEVEL CROSSING SITUATION

We want to study what happens when the 2S and 2P levels cross for some given value of the parameter λ and, in particular, we want to find the derivative of $E_{2S} - E_{2P}$ with respect to λ . We want to exploit both equation (13) and equation (5). Here we choose the functional dependence of $V_c(\lambda, r)$ in such a way that $\partial/\partial\lambda V_c(\lambda, r)$ is proportional to

$$2V_c(\lambda, r) + r \frac{\partial V_c(\lambda, r)}{\partial r}.$$

We take

$$V_c(\lambda, r) = \lambda^2 V_c(\lambda r), \quad 0 \leq \lambda \leq 1 \quad (15)$$

Then Eq. (5) becomes

$$\frac{d}{d\lambda}(E_{2S} - E_{2P}) = \int_0^{\infty} (u^2 - v^2) [2\lambda V_c(\lambda r) + \lambda^2 r V_c'(\lambda r)] dr \quad (16)$$

(13) becomes

$$E_{2S} - E_{2P} = \frac{1}{2} \int_0^{\infty} (u^2 - v^2) \left[-g^2 + 2\lambda^2 V_c(\lambda r) + \lambda^3 r V_c'(\lambda r) \right] dr \quad (17)$$

Hence

$$2(E_{2S} - E_{2P}) = -g^2 \int_0^{\infty} \frac{u^2 - v^2}{r} dr + \lambda \frac{d}{d\lambda}(E_{2S} - E_{2P}). \quad (18)$$

Let us now proceed to prove ab absurdo that at a crossing where $E_{2S} - E_{2P} = 0$, we necessarily have $\frac{d}{d\lambda}(E_{2S} - E_{2P}) > 0$.

Assume the contrary

$$\frac{d}{d\lambda}(E_{2S} - E_{2P}) \leq 0 \quad (19)$$

then from (18) we get

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

Condition (20) has the implication that $u^2 - v^2$ vanishes twice in $0 < r < \infty$. Indeed we know from Lemma 1 that $u^2 - v^2$ vanishes once in $0 < r < r_0$ at $r = r_1$. For $r < r_1$, $u^2 - v^2 > 0$. Suppose $u^2 - v^2$ vanishes only once. Then from (20) and from the normalization condition (14)

$$\int (u^2 - v^2) \left(\frac{1}{r} - \frac{1}{r_1} \right) dr < 0$$

which is absurd. Hence $u^2 - v^2$ must also vanish once in $r_0 < r < \infty$ at $r = r_2$:

$$u^2 - v^2 > 0 \text{ for } r < r_1; \quad u^2 - v^2 < 0 \text{ for } r_1 < r < r_2; \quad u^2 - v^2 > 0 \text{ for } r > r_2 \quad (21)$$

Now we shall evaluate $\frac{d}{d\lambda}(E_{2S}-E_{2P})$ by two successive integrations by parts. We define

$$I(r) = \int_r^{\infty} \frac{u^2 - v^2}{r'} dr' \quad (22)$$

$$J(r) = \int_r^{\infty} I(r') dr' \quad (23)$$

From (21) we see that $I(r)$ has a minimum at $r=r_1$ and a maximum at $r=r_2$. For r large, it is positive. On the other hand, $I(0) < 0$ from inequality (20). Hence $I(r)$ vanishes only once, somewhere between r_1 and r_2 . $J(r)$ has a unique maximum, and $J(r)$ is positive for r large. However, let us notice that

$$J(0) = \int_0^{\infty} dr \int_{r'}^{\infty} \frac{u^2 - v^2}{r'} dr' = \int_0^{\infty} (u^2 - v^2) dr = 0 \quad (24)$$

from the normalization condition. Therefore

$$J(r) \geq 0 \quad (25)$$

The integral we want to compute can be written as

$$\int_0^{\infty} \frac{u^2 - v^2}{r} W_c(\lambda r) dr \quad (26)$$

with

$$W_c(x) = x \left[2V_c(x) + x \frac{dV_c}{dx} \right] \quad (27)$$

The integrated terms vanish in the successive partial integrations if

$$1) \quad W_c(0) = 0$$

$$2) \quad \lim_{x \rightarrow \infty} (x(dW_c/dx)) = 0, \text{ noticing that } J(r) \sim \text{const} \times r \text{ for } r \rightarrow 0.$$

Then we get

$$\frac{d}{d\lambda} (E_{2S} - E_{2P}) = \int_0^{\infty} J(r) \left(\frac{d}{dr} \right)^2 W_c(\lambda r) dr \quad (28)$$

Therefore, under the following three sufficient conditions

$$\left. \begin{aligned} W_c(0) &= 0 \\ \lim_{x \rightarrow 0} x \frac{dW_c}{dx} &= 0 \\ \left(\frac{d}{dx} \right)^2 W_c(x) &> 0, \forall x > 0 \end{aligned} \right\} \quad (29)$$

we get, in combination with positivity property (25),

$$\frac{d}{d\lambda} (E_{2S} - E_{2P}) > 0 \quad (30)$$

contrary to assumption (19). The conclusion is that, at any crossing, (30) holds under conditions (29). Since $E_{2S} - E_{2P}$ is a continuous function of λ (in this paper it is assumed, but it could be proved), we see that there is at most one crossing for $0 < \lambda \leq 1$.

IV. THE WEAK COUPLING LIMIT

The only missing step to establish from conditions (29) that the 2S level is above the 2P level is to prove that for small λ , under conditions (29), $E_{2S} - E_{2P} > 0$. It is then impossible for $E_{2S} - E_{2P}$ to vanish with a negative derivative for larger values of λ . Strangely enough, this latter question is the most easy to establish if one accepts not to be very rigorous, but a completely rigorous proof would be lengthy, to say the least. The non-rigorous proof is as follows: at $\lambda=0$, $E_{2S} - E_{2P} = 0$. For sufficiently small λ perturbation theory is applicable in the sense that

$$\lim_{\lambda \rightarrow 0} \frac{\Delta E_{\text{exact}}}{\Delta E_{\text{perturbation}}} = 1 \quad (31)$$

Now

$$\Delta E_{\text{perturbation}} = \int_0^{\infty} (u^2 - v^2) \lambda_0^2 V_c(\lambda_0 r) dr \quad (32)$$

where u and v are the unperturbed wave functions. We can define $I(r)$ and $J(r)$, with all the nice properties obtained in the previous section. Here $I(0)=J(0)=0$. $J(r)$ is positive and from the convexity properties of $rV_c(\lambda_0 r)$, which follow from (29) by integration, we prove that ΔE perturbation is positive. There is no convergence problem if V_c is polynomial bounded for $r \rightarrow \infty$. Notice that u and v , for $\lambda=0$, decrease exponentially (for $\lambda > 0$ they decrease faster than any exponential). Then by combination with Section III, we deduce that $E_{2S} - E_{2P}(\lambda)$ remains positive for $\lambda_0 \leq \lambda \leq 1$ which is what we wanted to prove.

We shall try to sketch the lines of a somewhat more rigorous proof which consists in integrating the exact equation (16) from 0 to λ_0 . Since we can always assume

$$V_c(x) + x \frac{dV_c}{dx} > 0$$

we can apply the mean value theorem to the integration over λ and get

$$E_{2S} - E_{2P}(\lambda) = \int_0^{\infty} [u^2(r, \bar{\lambda}(r)) - v^2(r, \bar{\lambda}(r))] \lambda^2 V_c(\lambda r) dr$$

with $0 < \bar{\lambda}(r) < \lambda$.

It is certainly possible to establish that for finite r , $u(r, \lambda)$ and $v(r, \lambda)$ are continuous functions of λ . Therefore, for λ small enough, they are as close as one wishes from the unperturbed wave functions for $r < R$, R arbitrarily large. The non-uniformity of the continuity in λ for $r \rightarrow \infty$ is harmless because of the rapid decrease of the wave functions. These are the lines that one should follow in a rigorous derivation.

In any case we have no doubt that under conditions (29) the difference $E_{2S}(\lambda) - E_{2P}(\lambda)$ is positive, for $0 \leq \lambda \leq 1$ and, in particular, for $\lambda = 1$.

V. DISCUSSION

If conditions (29), under which we get the "canonical" level order for a two-particle system bound by a Coulomb-like plus confining force, 1S-2P-2S, seem to be mysterious, let us give some explicit examples of potentials for which these conditions are met. First of all we have the linear potential $V_c = a+br$, the harmonic oscillator potential $V_c = a+br^2$, but also any potential like r^α or $\int \rho(\alpha) r^\alpha d\alpha$, with $\int \rho(\alpha) d\alpha$ convergent and $\rho \geq 0$. At least for the author it was a surprise to learn that a potential like $V_c = r^{\frac{1}{2}}$ would produce the right order of levels. Our theorem consolidates, in a certain way, the predictions on the level ordering. What may be criticized is that it is a local convexity property which is required. It would certainly be much more satisfactory to have conditions appearing as inequalities on moments of the confining potential. This is not impossible, but would necessitate some extra work and in particular a better knowledge of the wave functions.

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