Where are the 1^1P_1 states in heavy Quarkonia?

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Abstract

It is shown that for heavy quark-antiquark systems described by the generalized Fermi-Breit Hamiltonian with a static non-relativistic potential satisfying only a concavity condition derived from lattice QCD, a fit of the triplet 1^3P_j states implies tight bounds for the singlet P state. In particular, the candidate for $\Upsilon(1^1P_1)$ proposed by the CLEO collaboration some years ago can be excluded on the basis of these inequalities. If, in addition, the vector exchange potential satisfies the condition of asymptotic freedom, then the singlet state must be very close to the centre of gravity of the triplet state.

One of the few states of quarkonium systems as yet unobserved is the singlet 1P state. Indications for a possible candidate in the charmonium system were given by R704 [1], but the lack of statistics, due to the closing of the ISR, did not allow any definite conclusion. In the case of upsilon, a candidate was found in the inclusive spectrum of $\Upsilon'' \rightarrow \pi\pi + X$ by CLEO [2] but the signal disappeared later with increasing statistics.

It is clear that the observation of these states is of great importance as it allows us to test the structure of the spin-dependent forces. Most calculations [3] predict that the 1P_1 state, both for charmonium and for upsilon, will be very close to the centre of gravity of the triplet P states, which have been observed and are known with good accuracy. However there is not, so far, a quantitative measure of how close it should be to the centre of mass of the triplet states, and this is precisely what we want to do in this paper, with as little theoretical input as possible, and as much experimental input as possible.

Our experimental input will be:

- the masses of the triplet P states
- the masses of the 1S and 1D states (here we use the ‘Particle Data Group’ notation, not the one of atomic spectroscopy) or, in the case of upsilon, the mass of the 2S state since the 1D state has not yet been seen (this is also a state whose observation is much needed [4]).

The theoretical input is the following:

- the masses of the quarks, which are taken from potential models, and have some uncertainty which will be discussed later.
- the postulate that the spin-dependent structure of the forces between quark and antiquark is given by the Fermi–Breit Hamiltonian, with an arbitrary mixture of scalar, V_s , and vector V_v potential (which is what everybody does!)
- the requirement that the central potential $V = V_s + V_v$ be concave, i.e. $V'' < 0$, in agreement with lattice QCD [5]
- finally two admittedly questionable beliefs: that the quark–antiquark system, as far as the central part of the interaction is concerned, satisfies strictly the Schrödinger equation, and that the spin-dependent effects can be treated perturbatively.

While we have not tried to do anything to take into account non-perturbative effects in the spin-dependent interaction, which might be questionable especially for charmonium, where the $1^3P_2 - 1^3P_0$ separation is 130 MeV, to be compared to a 1P – 1S separation of 400 MeV, we have tried to estimate the effect of relativistic corrections and shown that it introduces a certain uncertainty in our bounds.

In addition, we have considered the possibility of introducing an extra requirement, which is to impose that the vector part of the potential, generally supposed to be the short range part containing for instance a gluon exchange, should have a positive Laplacian. This requirement is a kind of strong version of asymptotic freedom and is satisfied by some existing models.

As we shall see the bounds we get are very tight, and, if they had been known in 1986, would have allowed us to exclude the CLEO candidate. If, in the future, a singlet P state is seen violating our bounds, it will mean that one of our assumptions is violated. If a violation is observed in a theoretical calculation, in the pure Schrödinger picture, it means that the calculation is just wrong.

If one uses the Fermi–Breit Hamiltonian perturbatively to calculate the spin separation of the 1P states one gets [4]

$$\begin{aligned}
M(1^3P_2) &= \overline{M}_{1P} + h_{LS} + \frac{1}{5}h_T \\
M(1^3P_1) &= \overline{M}_{1P} - h_{LS} - h_T \\
M(1^3P_0) &= \overline{M}_{1P} - 2h_{LS} + 2h_T.
\end{aligned} \tag{1}$$

Where $\overline{M}_{1P}$ is the centre of gravity of the triplet P states and

$$\begin{aligned}
h_{LS} &= \frac{1}{6m^2} \left[9 \left\langle \frac{1}{r} V'_v \right\rangle - 3 \left\langle \frac{1}{r} V'_s \right\rangle \right] \\
h_T &= \frac{1}{6m^2} \left\langle V''_v - \frac{1}{r} V'_v \right\rangle,
\end{aligned} \tag{2}$$

m being the quark mass, where the expectation values are taken in the state $n = 0$ (zero node) and $\ell = 1$. For the singlet state

$$M(1^1P_1) = \overline{M}_{1P} - \frac{4}{6m^2} \langle \Delta V_v \rangle. \tag{3}$$

The basic trick of this paper is that one can find a combination of the four masses which can be expressed entirely in terms of the expectation value of $\frac{1}{r} \left[\frac{dV_v}{dr} + \frac{dV_s}{dr} \right]$. One gets

$$M(1^1P_1) = \tilde{M}_{1P} - \frac{1}{2m^2} \left\langle \frac{1}{r} \frac{dV}{dr} \right\rangle \tag{4}$$

with

$$\tilde{M}_{1P} = \frac{1}{12} \left[-5M(1^3P_2) + 27M(1^3P_1) - 10M(1^3P_0) \right].$$

We now generalize inequalities that have been previously obtained [6] on purely angular excitations, i.e. states with zero-node radial wave functions. We have obtained the following theorem on the expectation values of V'/r , on the state $n = 0$, $\ell = 1$ of the Schrödinger equation with two equal masses m : if V is concave,

$$\left\langle \frac{V'}{r} \right\rangle_{n=0, \ell=1} \geq \frac{5}{8} m (E(0, 2) - E(0, 1))^2 \tag{5}$$

$$\left\langle \frac{V'}{r} \right\rangle_{n=0, \ell=1} \leq \frac{1}{2} m (E(0, 1) - E(0, 0))^2, \tag{6}$$

where the energies are labelled by n , number of nodes and ℓ orbital angular momentum.

A corollary of (5) is

$$\left\langle \frac{V'}{r} \right\rangle_{n=0, \ell=1} \geq \frac{5}{8} m (E(1, 0) - E(0, 1))^2, \tag{7}$$

if the parenthesis is positive.

Indeed, if $V'' < 0$, $V' > 0$ is implied, and hence $\frac{d}{dr} \frac{1}{r} \frac{dV}{dr} < 0$. By a known theorem on the order of energy levels [7], $E(1, 0) < E(0, 2)$.

Another obvious but interesting corollary, obtained by eliminating $\langle \frac{1}{r} V' \rangle$ between (5) and (6) is

$$(E(0,2) - E(0,1)) < \sqrt{\frac{4}{5}}(E(0,1) - E(0,0)) \quad (8)$$

for concave potentials. $\sqrt{\frac{4}{5}} \simeq 0.894$ is not very far from the best possible constant which is known to be 0.867.

We shall only sketch the proof of inequalities (5) and (6) (the uninterested reader can skip it!). A detailed derivation of the bounds and the generalization to arbitrary angular momentum ℓ will be published elsewhere. As in previous work one basic tool is Chebychev's inequality

$$\langle fh \rangle_1 \langle gh \rangle_1 \leq \langle fgh \rangle_1 \langle h \rangle_1, \quad (9)$$

where f and g are decreasing and h is non-negative. Again the expectation values are taken with respect to the first angular excitation, i.e. $u^2 dr$. Since V is supposed to be concave one may take $f = V'$, $g = 1/r^2$ and $h = r$. We obtain

$$\langle \frac{V'}{r} \rangle_1 \geq \langle rV' \rangle_1 \frac{\langle r^{-1} \rangle_1}{\langle r \rangle_1}. \quad (10)$$

The second fact we use is that since $V'' - 1/rV'$ is negative we have the following inequality for the moments (which is sharper than the usual Schwarz inequality) [8]:

$$\frac{\langle r^{-1} \rangle_1}{\langle r \rangle_1} \geq \frac{5}{4} \frac{1}{\langle r^2 \rangle_1}. \quad (11)$$

By the virial theorem $\langle rV' \rangle_1$ equals twice the kinetic energy. The kinetic energy can be bounded below by the uncertainty principle. Hence

$$\langle rV' \rangle_1 = 2 \langle T \rangle_1 \geq \frac{25}{2} \frac{1}{\langle r^2 \rangle_1}. \quad (12)$$

Therefore we have the lower bound

$$\langle \frac{V'}{r} \rangle_1 \geq \frac{125}{8} \langle r^2 \rangle_1^{-2}. \quad (13)$$

Taking ru_{01} as a trial function for E_2 and applying the Rayleigh-Ritz variational principle one obtains after some algebraic manipulations

$$\frac{5}{\langle r^2 \rangle_1} \geq E_2 - E_1, \quad (14)$$

which implies the lower bound given in the theorem.

For the upper bound we need the following identity:

$$\int_0^\infty V' u_0 u_1 dr = \frac{1}{2}(E_1 - E_0)^2 \int_0^\infty ru_0 u_1 dr, \quad (15)$$

where u_0 and u_1 are the reduced Schrödinger wave functions of the 1S and 1P state respectively. In addition by analysing the Wronskian of ru_0 and u_1 one observes that ru_0/u_1 is a decreasing function. Here we use the fact that in view of the condition $\frac{d}{dr} \frac{1}{r} \frac{dV}{dr} < 0$, the functions $(1/r)u'_\ell/u_\ell - (\ell+1)/r^2$ are increasing for all $\ell > 0$ [7]. Applying Chebychev's inequality (A.1) with $f = V'/r$, $g = ru_0/u_1$ and $h = 1$ yields the upper bound.

To apply inequalities (5), (6) and (7) to our problem, we should replace the energy differences by mass differences:

$$M(1^1P_1) \leq \tilde{M}_{1P} - \frac{5}{16m}[M_{1D} - M_{1P}]^2 \quad (16)$$

$$M(1^1P_1) \leq \tilde{M}_{1P} - \frac{5}{16m}[M_{2S} - M_{1P}]^2 \quad (17)$$

$$M(1^1P_1) \geq \tilde{M}_{1P} - \frac{1}{4m}[M_{1P} - M_{1S}]^2 \quad (18)$$

Ideally M_{1S} , M_{1P} , M_{1D} , M_{2S} should be completely averaged over spins. However some states, like η_b or the D states of the $c\bar{c}$ system with $J=2$, $J=3$ and $S=0$ are not known. As far as M_{1P} is concerned one could take into account the singlet P state, but then we get a nonlinear inequality. However, as one can explicitly check for charmonium with inequality (16) the lower bounds will only differ by less than 0.5 MeV. Therefore we deal only with linear inequalities. We feel that we are not making a big error by replacing M_{1D} (in $c\bar{c}$) by the mass of 1^3D_1 which is believed to be the triplet mass anyway. We also think that the $\Upsilon - \eta_b$ separation is appreciably smaller than the $J/\psi - \eta_c$ separation and that $M_{1S} = M_\gamma$ for the $b\bar{b}$ system is not introducing a big error. In the following table we collect all the experimental data we shall use [9]:

	$M_{c\bar{c}}$ in MeV	$M_{b\bar{b}}$ in MeV
1^3S_1	3096.9 ± 0.1	9460.32 ± 0.22
1^1S_0	2979.6 ± 1.7	
1^3P_0	3415.1 ± 1.0	9859.8 ± 1.3
1^3P_1	3510.53 ± 0.2	9891.9 ± 0.7
1^3P_2	3556.15 ± 0.2	9913.2 ± 0.6
2^3S_1	3686.0 ± 0.10	10023.3 ± 0.3
1^3D_1	3769.9 ± 2.5	
$\bar{M}$	3525.3 ± 0.2	9900.17 ± 0.5
M	3571.1 ± 1.0	9909.8 ± 1.9

Now we have to insert these values in inequalities (14) and (16) for $c\bar{c}$, and (15) and (16) for $b\bar{b}$ to get upper and lower bounds. Here we have to make a choice for the quark masses, which we believe to be constituent quark masses, on which we have some flexibility according to potential models, from 1.2 to 1.9 GeV for charm and from 4.5 to 5.2 GeV for beauty. For charm we shall prefer values above 1.5 GeV which are favoured by analysis of electroweak theory [10]. At this stage we obtain, for $c\bar{c}$, for $m_c = 1.5$

$$3536.2 \pm 1.1 < M(1^1P_1) < 3558.6 \pm 1.1, \quad (19)$$

for $m_c = 1.8$

$$3541.9 \pm 1.1 < M(1^1P_1) < 3560.7 \pm 1.1, \quad (20)$$

and for $b\bar{b}$, with $m_b = 5$

$$9900.3 \pm 1.9 < M(1^1P_1) < 9908.9 \pm 1.9. \quad (21)$$

Here, the errors are only experimental errors on masses, and they are dominated by errors on the masses of the P states, since the S states, directly produced in e^+e^- collisions are extremely well determined. The bounds are seen to be extremely tight and seem to exclude the old CLEO candidate, at 9894.8 ± 1.5 as well as the R704 candidate at 3525 ± 0.4 .

However, these bounds should be taken with a grain of salt. They hold if no relativistic effect is present, i.e. the energy differences occurring in the parenthesis should be Schrödinger energy differences. In calculations where relativistic effects are taken into account it is clear that corrections of the order of $p^4/4m^3$ are not negligible, especially for the $c\bar{c}$ system. Then we have

$$E_1 - E_0 \simeq M_{1P} - M_{1S} \pm 2\Delta M,$$

where we approximate ΔM by $\frac{1}{4m}\langle p^2/m \rangle^2$, and, again, we know [11] that $\langle p^2/m \rangle$ is of the order of $M_{1P} - M_{1S}$. A similar estimation can be made for the 1D-1P difference.

The net result of that is that the bounds are seriously weakened in the $c\bar{c}$ case. For instance with $m_c = 1.5$ we get:

$$3536.2 \pm 12.2 \leq M(1^1P_1) \leq 3558.6 \pm 12.2 \quad (22)$$

and for $m_c = 1.8$:

$$3541.9 \pm 10 \leq M(1^1P_1) < 3560.7 \pm 10 \quad (23)$$

For the $b\bar{b}$ case the error remains dominated by pure experimental errors:

$$9900.3 \pm 2.8 < M(1^1P_1) < 9908.9 \pm 2.8. \quad (24)$$

This latter result confirms that a value like 9894.8 ± 1.5 is definitely excluded. The question remains to decide whether inequalities (20) and/or (21) really exclude the R704 candidate at 3525 MeV. Superficially they do, but we must remember that the fine and hyperfine splittings have been treated perturbatively and that, as we said at the beginning, it is not clear that this does not introduce a certain error for charmonium. So we take the position that the R704 candidate is marginally compatible with the data.

So far we have used only one requirement which is that the central potential $V_s + V_v$ be concave. Many models, however, possess the property that the Laplacian of the vector part of the potential is positive. An exception is the model of Gupta et al. and of Pantaleone and Tye [3], [12]. If ΔV_v is positive, we have $M(1^1P_1) < \bar{M}(1P)$, and this imposes a compatibility condition on the triplet P states themselves:

$$\bar{M}_{1P} > \tilde{M}_{1P} - \frac{1}{4m}[M_{1P} - M_{1S}]^2. \quad (25)$$

For the upilon system this is compatible with experiment, while for the $c\bar{c}$ effect it seems not to be the case, though the blame can perhaps be put on relativistic effects and non-perturbative effects.

It should be noted that as one increases m_c , inequality (23) is more and more violated while the errors made by perturbation theory are expected to become smaller.

To summarize, our inequalities (22) to (24) seem to indicate that the singlet state is likely to be above the centre of gravity of the triplet state, but in view of the errors made, no definite conclusion in this direction is possible. The same prediction is obtained

by using the perturbative QCD expression for the hyperfine potential [12]. On the other hand, if one accepts the physical condition of strong asymptotic freedom our bounds show that then the singlet state is necessarily very close to the centre of gravity of the triplet state. In this case we expect a difference smaller than 5 MeV in $c\bar{c}$ and smaller than 3 MeV in $b\bar{b}$ as indicated by inequalities (22) to (24). For a recent discussion about the different predictions of hyperfine splittings given by perturbative QCD and models involving the condition of asymptotic freedom we refer to [13].

The upper bounds are still very crude, but they can be significantly lowered if one imposes additional constraints on the Lorentz components V_S and V_V respectively. This will be done in a future publication.

Finally, we would like to stress that our bounds suggest that in future experiments [14] not only the immediate neighbourhood of the centre of gravity of the triplet P state should be scanned, but also a somewhat broader interval especially above the centre of gravity.

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