Bound states of heavy quarks in QCD*

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Bound states of heavy $\bar{q}q$ quarks are reviewed within the context of QCD, paying attention to what can be derived from the theory with a reasonable degree of rigour. This is compared with the results of semiclassical arguments. Among new results, we report a very precise $O(\alpha_s^4)$ evaluation of $b, c$ quark masses from quarkonium spectrum with a potential to two loops.

1. INTRODUCTION

In the present note we are going to review some aspects of the QCD analysis of heavy quarkonia, $cc$ and especially $\bar{b}b$ states. This is fitting for a conference which (slightly ahead of time) celebrates the 25th anniversary of QCD. Indeed, the theory of quark interactions became a respectable theory, QCD, only with the advent of asymptotic freedom in 1973. Before that date we had the quark model, a somewhat inconsistent set of semiphenomenological calculations. Among these an important role was played by bound state calculations in the so-called constituent quark model, developed in the early sixties by, among others, Morpurgo, Dalitz and collaborators, and Oliver, Pene, Reynal and Le Yaouanc. In this model $u, d, s$ quarks were given phenomenological masses of 300−500 MeV, and were bound by potentials: the harmonic oscillator potential being a popular choice because of its simplicity. Quite surprisingly, a large number of properties of hadrons could be reproduced in this way.

After the advent of asymptotic freedom, and with it a consistent field theory of strong interactions, it was possible to show that, at least for heavy quarks and at short distances, the interaction is of Coulombic type. For colour singlet $\bar{q}q$ states of the form

$$-\frac{C_F \alpha_s}{r}.$$ (1.1)

In one of the first applications of QCD, De Rújula, Georgi and Glashow[1] showed that taking into account relativistic corrections and colour algebra one could calculate the spectrum of the then known hadrons, including in particular such features as the $N - \Delta$ splitting, and even the $\Sigma^0 - \Lambda$ splitting, something that had defied previous, non-QCD analyses. They were also able to predict some qualitative features of the charmonium spectrum.

Nowadays we expect more from QCD, at least for heavy quarks. The reason is that there it can be easily proved that, to leading order in $(\nu^2)$ (with $\nu$ the velocity of the quarks) the interaction can be described by a potential. At very short distances this potential has to be of the Coulombic type, Eq. (1.1); but even at long distances the corrections to this are expected to be of the form of a function $U(r)$. At short distances (1.1) should be modified by radiative corrections, but these should be of the form of a function of $r$.

Needless to say, relativistic corrections will in general not be representable by potentials, as is the case even in QED. In QCD one encounters QED-like corrections and idiosyncratic QCD ones associated with the complicated structure of the vacuum. In particular we have those involving the gluon condensate $\langle \alpha_s : G^2 : \rangle$, first studied in this context by Leutwyler and Voloshin[2] (the quark condensate also gives contributions, but, for heavy quarkonium, subleading ones).

2. SHORT DISTANCE QUARKONIUM: PURE QCD ANALYSIS. $b$ AND $c$ QUARK MASSES

For very heavy $\bar{q}q$ bound states the equivalent of the Bohr radius, $a = 2/(mC_F \alpha_s)$, is much smaller than the confinement radius, $R \sim A^{-1}$. So we expect that, for lowest $n$ states, with $n$ the principal
quantum number, confinement may be neglected, or at least treated as a first order perturbation. In this case the potential may be obtained from perturbative QCD. At tree level (Fig. 1) we get the Coulombic potential, Eq. (1.1). Including radiative corrections will yield improved approximations, in particular giving a meaning to the quantity \( \alpha_s \) in (1.1).  

\[
H^{(0)} = 2m + \frac{1}{m} \Delta - \frac{C_F \alpha_s(\mu^2)}{2} \frac{\Delta}{r} 
\]

Because of the non-abelian nature of the interaction, the Coulomb-like part of the interaction:

\[
h_1 = V_{\text{tree}} + V_1^{(L)} + V_2^{(LL)} + V_{s,\text{rel}} + V_{\text{hf}},
\]

where also some pieces of the two-loop corrections were given. A partial evaluation of the static two-loop interaction has been published by Peter.[7] While the completed calculation has been performed very recently by the author[8] for the \( n = 1, l = 0 \) state, and will be given here for the first time.

\[
\begin{align*}
V_{\text{tree}} &= -\frac{1}{4m^3} \Delta^2 + \frac{C_F \alpha_s}{m^2} \Delta, \\
V_1^{(L)} &= -\frac{C_F \alpha_s(\mu^2)^2}{\pi} \frac{\beta_0 \log r \mu}{r}, \\
V_2^{(LL)} &= \frac{C_F \beta_0^2 \alpha_s^2}{4\pi^2} \frac{\log^2 r \mu}{r}, \\
V_{s,\text{rel}} &= \frac{C_F \beta_0^2 \alpha_s^2}{2m^2}, \\
V_{\text{hf}} &= 4\pi C_F \alpha_s s (s + 1) \delta(r).
\end{align*}
\]

In above equations,

\[
\begin{align*}
\alpha_1 &= \frac{31 C_A - 20 T_F n_f}{36} \simeq 1.47; \\
\alpha_2 &= \frac{C_F - 2 C_A}{2} \simeq -2.33; \\
b_1 &= \frac{1}{16} \left[ \frac{17388}{81} + \frac{55}{3} \xi(3) \right] C_A^2 \\
&\quad - \left[ \frac{1798}{81} + \frac{56}{3} \xi(3) \right] C_A T_F n_f \\
&\quad - \left[ \frac{55}{3} - 16 \xi(3) \right] C_F T_F n_f + \frac{400}{81} T_F^2 n_f^2,
\end{align*}
\]

with \( \alpha_1 \) calculated in ref. 3, \( b_1 \) in ref. 7 and \( a_2 \) and many of the rest of the terms in ref. 6. All terms in \( H_1 \) are to be treated as first order perturbations of \( H^{(0)} \), except for the term \( V_1^{(L)} \), which has to be treated to second order. Thus it produces, in addition to the first order contribution,

\[
\delta_{V_1^{(L)}}^{(1)} E_{10} = -m \frac{\beta_0 C_F \alpha_s^2(\mu^2)}{4\pi} \frac{\log \left( \frac{a}{2} + 1 - \gamma_E \right)}{2}.
\]
the second-order energy shift. For the ground state it is very small, of about 4 MeV.

The first order contributions of the other V’s are easily evaluated using the formulas of ref. 6.

\[ V_{\text{Gluon cond.}}(r) \sim A \Gamma^3. \]  

Let us summarize the results[6,8,9,10]. The calculation is fully justified, in the sense that higher order corrections (both perturbative and NP) are smaller than lower order ones for \( \bar{b}b \) with \( n = 1 \). The same is partially true for the energy levels of the same states with \( n = 2 \) and, for \( \bar{c}c \), for \( n = 1 \). For the wave functions of \( \bar{b}b, n \geq 2 \) and all \( \bar{c}c \) states, and for the energy levels with higher values of \( n \) than the ones reported above, the calculation is meaningless as nominally subleading corrections overwhelm nominally leading ones.

The leading nonperturbative (NP) corrections can be shown to be those associated with the contribution of the gluon condensate. They may be understood as follows. We consider that the quarks move in a medium, the QCD vacuum, represented by their field strength operators, \( G_{\mu \nu}(x) \). When \( a \ll R \), we may consider that the confinement size is infinite and, moreover, one can neglect the fluctuations of the \( G_{\mu \nu}(x) \) in the region of size \( a \) in which the quarks move. So we may approximate the effect by introducing an interaction, which in the static limit will be of dipole type, of the quarks with a constant gluonic field, \( H_{NP} = t^\alpha r_i G_{\alpha i}(0) \). We consider that \( \langle G_{\mu \nu}(x) \rangle = 0 \), but \( \langle \alpha_s : G^2 \rangle \neq 0 \). For dimensional reasons, this will give the leading NP contribution to the spin-independent energy shifts, which are of the form[2],

\[ \delta_{NP} E_{nl} = m \frac{\pi n^6 \epsilon_{nl} \langle \alpha_s : G^2 \rangle}{(m C_F \alpha_s)^4}, \]  

where the numbers \( \epsilon_{nl} \) are of order unity, \( \epsilon_{10} \approx 1.5 \). The evaluations for the spin-dependent shifts may be found in the second paper of ref. 8 (with a correction in ref. 9) and the contributions of higher order operators has been considered in ref. 10. Note that, as already remarked by Leutwyler[2], one cannot derive (2.1) from a local potential; but the effect may be approximated by a cubic one,

\[ V_{\text{Gluon cond.}}(r) \sim A \Gamma^3. \]  

For \( \bar{b}b \) one gets a precise determination of \( m_b \) and \( \bar{m}_b (\bar{m}_b^2) \) (pole and \( \overline{\text{MS}} \) masses), a reliable prediction for the hyperfine splitting, and reasonable agreement with the experimental value of \( \Upsilon \rightarrow e^+ e^- \):

\[ m_b = 4906^{+70}_{-65} \text{ MeV} \]  

\[ \bar{m}_b (\bar{m}_b^2) = 4397^{+18}_{-32} \text{ MeV}, \]  

\[ \Gamma (\Upsilon \rightarrow e^+ e^-) = 1.12 \text{ keV (exp : 1.32 \pm 0.05}). \]  

For \( \bar{c}c \) a reasonably accurate value for is also obtained for \( m_c \): not including the estimated systematic error,

\[ m_c = 1570 \pm 20 \text{ MeV} \]  

\[ \bar{m}_c (\bar{m}_c^2) = 1306^{+22}_{-36} \text{ MeV}. \]  

These results are obtained with the one-loop potential with relativistic corrections[6]. We may extend the calculation to two loops, using the Hamiltonian of Eqs. (2.1,2) above, plus leading NP corrections, Eq. (2.3). Taking \( A = 200 \) MeV, the renormalization point \( \mu = 2/a \simeq 2.5 \) GeV, and varying \( \mu^2 \) by a factor two to get the systematic errors of the calculation one finds from the \( \Upsilon \) and \( J/\psi \) masses the (pole) quark masses[8] correct up to, and including, \( O(\alpha_s^4) \) terms:

\[ m_b = 4984 \pm 62 \text{ MeV}, \]  

\[ m_c = 1797 \pm 70 \text{ MeV}. \]  

The corresponding \( \overline{\text{MS}} \) bar masses are \( \bar{m}_b (\bar{m}_b^2) = 4.446 \text{ GeV} \) and \( \bar{m}_c (\bar{m}_c^2) = 1.501 \text{ GeV} \). The values of the masses are slightly larger than those one finds with the sum rule method (see for example, refs. 12). This may be easily understood
if one realizes that the last are obtained in calculations accurate to $O(\alpha_s^2)$ while the ones reported here include terms in $\alpha_s^3$ (Eq. (2.5)) and $\alpha_s^4$, for Eq. (2.6). If we had only included the terms in $\alpha_s^4$ in a potential calculation we would have obtained $m_b = 4746$ MeV, for example. This is comparable to the sum rule value, so the discrepancy is seen to lie in the contribution of terms of order $\alpha_s^4$, not taken into account in the sum rule evaluations.

3. Quarkonia at Long Distances. Connection Between the Long and Short Distance Regimes

Here we consider bound states of heavy quarks at long distances. This certainly includes $cc$ with $n > 1$ and $\bar{b}b$ with $n > 2$; $n = 1$ for the first and $n = 2$ (and, a fortiori, $n = 1$) for the second are somewhat marginal. As stated in the previous section, perturbative QCD supplemented with leading NP effects fails now; but, fortunately, since the average velocity of bound states decreases with increasing $n$, we expect the dynamics to be governed by a potential: our task is to determine it. This has been considered by a number of people$^{13-17}$. Here we will follow the derivation of ref. 16 in the version of ref. 18, which will allow us to establish connection with the short distance analysis of the previous section.

The potential, that we denote by $V(r)$, is expected to exhibit a number of features. First of all, it should behave as $s/r$ at long distances. Secondly, it should contain a Coulombic piece, so we write

$$V(r) = -\frac{\kappa}{r} + U(r), \quad (3.1)$$

and, at short distances, one should be able to identify $\kappa = C_F \alpha_s$ + radiative corrections.

To find this potential consider the Green’s function in terms of the Wilson loop, working directly in the nonrelativistic approximation, and for large time $T$: for a $q\bar{q}$ pair:

$$G(x, \bar{x}; y, \bar{y}) = \int Dz D\bar{z} e^{-(K_0 + \bar{K}_0)} \langle W(C) \rangle,$$

with $K_0, \bar{K}_0$ the kinetic energies,

$$K_0 = \frac{m}{2} \int_0^T dz^2(t)^2, \quad \text{etc.}$$

and the Wilson loop operator corresponds to the contour $C$ enclosing the $q, \bar{q}$ paths from time 0 to time $T$. It should include path-ordered parallel transporters for the initial and final states, $\Phi(x, \bar{x}), \Phi(y, \bar{y})$ with e.g.

$$\Phi(x, \bar{x}) = P \int_{\bar{x}}^x dz_\mu B_\mu(z).$$

The calculation is simplified if choosing $x = \bar{x}, y = \bar{y}$ which will be enough for our purposes here. To take into account the nonperturbative character of the interaction it is convenient to work in the background gauge formalism and write $B_{\mu} = b_{\mu} + a_{\mu}$ where the $a_{\mu}$ represent the quantum fluctuations and $b_{\mu}$ is a background field which is chosen such that the vacuum expectation value of the Wick ordered products of the $a_{\mu}$ vanish. Therefore, we may express the gluon correlator in terms of $b_{\mu}$ only:

$$\langle \Phi(x) G(y) \Phi \rangle \rightarrow \langle \Phi_0(x) G_0(y) \Phi \rangle,$$

Expanding in powers of the background field $b_{\mu}$ we may write the Wilson loop average as

$$\langle W(C) \rangle = \int D\alpha \langle C \rangle^{d_{\alpha}} \alpha_{\mu}$$

$$+ \left( \frac{i q^2}{2!} \right)^2 \int D\alpha \int_C dz_\mu \int dz_\nu P \Phi_0(z, z') \cdot \times b_\mu(z) P \Phi_0(z', z) b_\mu(z') + \ldots$$

$$\equiv W_0 + W_2 + \ldots$$

and the transporter $\Phi_0$ is constructed with only the quantum field $a$. For the first term, $W_0$, the cluster expansion gives

$$W_0 = Z \exp (\phi_2 + \text{higher orders}),$$

$$\phi_2 = C_F g^2 \int_0^T dt \int_0^T dt' \frac{1 + \bar{z}z'}{r^2 + (t - t')^2}$$

$$= C_F \alpha_s \int_0^T dt + O(v^2),$$

i.e., the Coulombic piece of the potential. ($Z$ is a constant that, in particular, includes regularization).

The evaluation of the first nontrivial piece, $W_2$ is more complicated. It produces a correction to the Green’s function, $\delta G$, which in the static
We then find the basic equation
\[ f | m \text{ation would be 1} \]
rotation period (which in the Coulombic approxi-
We may write, using Lorentz invariance,
the ensuing energy shifts from the relation

Here the \( G^{(S,8)}_C \) are the singlet, octet Coulombic Green’s functions. We may then take matrix el-
ements between Coulombic states, \( |nl\rangle \), and identify the ensuing energy shifts from the relation

We then find the basic equation\[^{[18]}\),
\[ \delta E_{nl} = \frac{1}{16} \int \frac{d^3p}{(2\pi)^4} \int d\beta d\beta' \hat{A}(p) \]
\[ \times \sum (nl|r'e^{i(3-1/2)r'}|k(8)) \] \( (3.4) \)
\[ \times \frac{1}{E_k - E_n - p_0} \]
The states \( |k(8)\rangle \) are eigenstates of the octet Hamiltonian, with energy \( E_k^{(8)} \); the \( E_n \) are the Coulombic energies. Finally, \( \Delta(p) \) is defined in terms of the correlators, being the Fourier transform of
\[ \Delta(x) = D(x) + D_1(x) + x^2 \partial^2 D_1(x)/\partial x^2 \]
and
\[ \langle g^2 : G_{0i}(x)G_{0j}(0) : \rangle = \frac{1}{12} \left[ \delta_{ij} D(x) + x_i x_j \partial^2 D_1 / \partial x^2 \right] . \]
We may write, using Lorentz invariance, \( \Delta(x) = f(x^2/T_0^2) \), with \( T_0 \) the so-called correlation time. This will play an important role in what follows.
We have now two regimes. If \( \mu_T \equiv T_0^{-1} \gg |E_n| \) the velocity tends to zero, and the nonlocality also tends to zero as compared with the quark rotation period (which in the Coulombic approximation would be \( 1/|E_n| \)). We can now neglect, in Eq. \( (3.4) \), both \( E_n, E_k^{(8)} \) as compared to \( p_0 \) so we obtain
\[ \delta E_{nl} \approx \langle nl|U|nl\rangle \]
where
\[ U(r) = \frac{2r}{36} \left\{ \int_0^r d\lambda \int_0^\infty d\nu D(\lambda, \nu) \right. \]
\[ + \int_0^r \lambda d\lambda \int_0^\infty d\nu [-2D(\lambda, \nu) + D_1(\lambda, \nu)] \} \]
\[ (3.5) \]
At large \( r \), and as this equation shows, we find
\[ U(r) \approx \sigma r. \] Here \( \sigma \) can be related to \( T_0 \) and the
\[ \mu_T = \frac{\pi}{3\sqrt{2}} \frac{\langle \alpha_s : G^2 \rangle}{\sigma^\frac{1}{2}} \approx 0.32 \text{ GeV}. \]
For small \( r,^{[16,17]} \)
\[ U(r) \approx c_0 + c_1 r^2. \]
This is different from the behaviour expected from the Leutwyler-Voloshin analysis which gives a behaviour \( \sim r^3 \); but one should understand that the present derivation holds for \( r \to 0 \) but still \( T_0^{-1} \gg |E_n| \). It may be noted that the analysis based upon the potential \( U \) gives a very good description of heavy quarkonia states\[^{[19]}\)\).

We next get the matching between the two regimes\[^{[18]}\). For this we now turn to the opposite situation, viz., \( T_0^{-1} \ll |E_n| \). Now we may approximate \( \Delta(x) \sim \text{constant} \) so that \( \Delta(p) \sim \delta_4(p) \) and Eq. \( (3.4) \) becomes
\[ \delta E_{nl} = \frac{\pi}{18} \langle \alpha_s : G^2 \rangle \langle nl|H(8) - E_n + \mu_T|nl\rangle, \]
\[ (3.7) \]
which coincides exactly with the results of the Leutwyler-Voloshin analysis\[^{[2,6]}\) in the limit \( T_0 \to \infty (\mu_T \to 0) \). In fact, Eq. \( (3.7) \) allows us to estimate the finite size corrections to the NP effects, which improves still the agreement between theory and experiment\[^{[18]}\).

4. RENORMALONS. SEMICLASSICAL UNDERSTANDING OF THE HEAVY QUARK POTENTIALS. SHORT DISTANCE LINEAR POTENTIAL AND SATURATION

In the previous section we have shown how QCD can give a very satisfactory account of the heavy quarkonia spectra, particularly of the lowest lying states; an understanding based on perturbative calculations supplemented by NP ones, in particular those associated with the gluon condensate. Here we address two questions related to that. First, one may inquire about the connection of renormalons with nonperturbative effects. Secondly, one can try to understand intuitively the potentials one finds. Finally, we will devote a few words to a speculation on a possible linear potential at short distances, and its connection with saturation.
Renormalons. Let us return to the one-gluon exchange diagram, Fig. 1. If we dress the gluon propagator with loops (Fig. 4) then the corresponding potential, in momentum space, is

$$\tilde{V}(k) = \frac{-4\pi C_F}{k^2} \frac{4\pi}{\beta_0 \log(k^2/\Lambda^2)},$$ (4.1)

and we have substituted the one-loop expression for $\alpha_s(k^2)$. The expression (4.1) is undefined for soft gluons, with $k^2 \simeq \Lambda^2$. As follows from the general theory of singular functions, the ambiguity is of the form $c\delta(k^2 - \Lambda^2)$: upon Fourier transformation this produces an ambiguity in the $x$-space potential of $\delta V(r) = c|\sin \Lambda r|/r$. At short distances we may expand this in powers of $r$ and find

$$\delta V(r) \sim C_0 + C_1 r^2 + \ldots.$$ (4.2)

The same result may be obtained with the more traditional method of Borel transforms\cite{20,21}. This coincides with the short distance behaviour of the nonperturbative potential $U(r)$ as determined in refs. 13-17, and Eq. (3.6) here. [For applications to calculations of bound states, see ref. 22 and work quoted there].

The situation just described applies for states $\bar{q}q$ at short distances; but not so short that zero frequency gluons cannot separate the pair. If this last is the case, soft gluons do not resolve the $\bar{q}q$ pair and only see a dipole. The basic diagram is no more that of Fig. 1, but that of Fig. 5. The generated renormalon may then be seen\cite{21,23} to correspond to the contribution of the gluon condensate in the Leutwyler-Voloshin mechanism.

Semicalssical picture We have seen that one can get a consistent QCD description of heavy quarkonium ground states both for large and small $T_g$. Here we will try and show how one can give an intuitive picture of what we have found\cite{21}. For this we consider a model for quarkonium to be that of a $e^+e^-$ pair inside a conducting cavity of radius $R \sim A^{-1}$. The potential energy of the pair is given as an integral over space of the corresponding electric fields,

$$V(r) = \frac{1}{4\pi} \int d^3r \mathcal{E}_1(r') \mathcal{E}_2(r + r').$$ (4.3)

In particular, the Coulomb potential is obtained when the $\mathcal{E}_i$ correspond to point charges. If these fields are modified at long distances, this will give rise to a modification of this interaction also at small distances. In our case, the modification arises because, since the charges are confined, the integral in (4.3) should only be extended to $r \leq R$. Thus,

$$\delta V(r) \sim e^2 r^2 \int_R^\infty \frac{d^3r'}{r'^6} \sim \frac{\alpha r^2}{R^3},$$

which reproduces the quadratic term in (3.6). The constant term appears because now we cannot fix the Coulomb potential by requiring it to be zero at infinity.

This calculation does not take into account retardation effects. When these become important, which is when the $e^+e^-$ pair is rotating very closely, the quadratic potential is wiped out and there remains a cubic one -again as in the QCD case. The situation is fully analogous to that of the ordinary Casimir effect\cite{24}.

A linear potential at short distances? To finish this note we are going to speculate on the possibility of a linear correction to the potential at
short distances. We have no proof of the existence of such term, but we have three different indications for its existence. First of all we have the possibility that the QCD coupling saturates at long distances\textsuperscript{[25]} so that one has,
\begin{equation}
\alpha_s(k^2) \simeq \frac{4\pi}{k^{\beta_0} \log[(k^2 + M^2)/\Lambda^2]},
\end{equation}
with $M \sim \Lambda$ (the possibility that $M = \Lambda$ is suggested by the deep inelastic scattering evaluations of the second paper of ref. 25). This yields a linear potential correction when inserted in a Coulombic potential at short distances.\textsuperscript{[25]}

The second indication comes from lattice QCD calculations, where a linear correction to the short distance Coulombic potential is apparently seen\textsuperscript{[26]}. The third indication comes from the following intuitive argument\textsuperscript{[21]}. Consider a simplified model according to which the chromo-electrostatic field of quarks is a correct zeroth-order approximation only so far as it exceeds some specific, confining properties. From this condition we get an estimate of distances $R_{cr}$ where the chromo-electrostatic field of quarks is strongly modified:
\begin{equation}
\frac{\alpha_s r^2}{R_{cr}^2} \lesssim \Lambda^4
\end{equation}
where for simplicity we have neglected the effect of the running of $\alpha_s(r^{-2})$.

The corresponding change in the potential is then of order
\begin{equation}
\delta V \sim \frac{\alpha_s r^2}{R_{cr}^2} \sim \alpha_s^{1/2} \Lambda^2,
\end{equation}
i.e., we get a leading correction linear in $r$ to the potential at short distances.

It is not easy to see how one could get a handle on this linear potential. The agreement between the orthodox QCD calculations and experiment is so good (see above and e.g. refs. 6, 8, 10) that there seems to be little room for (4.5). The saturation modification of $\alpha_s$ would also be masked by the errors in $\Lambda$. Perhaps lattice calculations may give a hint, as they seem to be doing already\textsuperscript{[26]}.

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