Hydrogen bond of QCD

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Using the Born-Oppenheimer approximation, we show that exotic resonances, X and Z, may emerge as QCD molecular objects made of colored two-quark lumps, states with heavy-light diquarks spatially separated from antiquark. With the same method we confirm that doubly heavy tetraquarks are stable against strong decays. Tetraquarks described here provide a new picture of exotic hadrons, as formed by the QCD analog of the hydrogen bond of molecular physics.

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I. INTRODUCTION

In this paper we present a description of tetraquarks [1–3] in terms of color molecules: two lumps of two-quark (colored atoms) held together by color forces. The variety of tetraquarks described here identifies a new way of looking at multiquark hadrons, as formed by the QCD analog of the hydrogen bond of molecular physics.

We restrict to heavy-light systems, $\bar{Q}Qq\bar{q}$ or $Q\bar{Q}q\bar{q}$, and apply the Born-Oppenheimer (BO) approximation, see e.g., [4], the method used for the hydrogen molecule, see [5]. The method consists in solving the eigenvalue problem for the light particles at fixed coordinates of the heavy ones, $x_A, x_B$, and then solve the Schrödinger equation of the heavy particles in the BO potential

$$V_{\text{BO}}(x_A, x_B) = V(x_A, x_B) + \mathcal{E}(x_A, x_B).$$

$V(x_A, x_B)$ is the interaction between the heavy particles, e.g., the electrostatic repulsion, and $\mathcal{E}(x_A, x_B)$ is the lowest energy eigenvalue of the light particles at fixed heavy particles coordinates. The approximation improves with $m_q/M_Q \to 0$.

The application of the Born-Oppenheimer method to doubly heavy tetraquarks in lattice QCD has been suggested recently in [6,7], both for hidden flavor tetraquarks, $[cq][\bar{c}\bar{q}]$, i.e., the exotic resonances X, Z [3,8–10], and for double beauty open flavor tetraquarks, $bb\bar{q}q$, introduced in [11,12] and, more recently, studied in [13–16].

We fix the $Q\bar{Q}$ pair to be in color 8 and we consider both possibilities, 3 and 6, for $Q\bar{Q}$. Had we taken $Q\bar{Q}$ in color singlet, the interaction with the light quark pair would be mediated by color singlet exchanges, as in the hadroquarkonium model proposed in [17].

For hidden flavor tetraquarks, we obtain color repulsion within the heavy $Q\bar{Q}$ and the light $q\bar{q}$ quark pairs, and mutual attraction between heavy and light quarks or antiquarks. Thus, in the $[Qq] - [\bar{Q}\bar{q}]$ color singlet molecule, repulsions and attractions among constituents are distributed in the same way as for protons and electrons in the hydrogen molecule. Assuming one-gluon exchange forces, Fig. 1(a) describes a configuration of a tight $Q\bar{Q}$ similar to the “quarkonium adjoint meson” discussed in [18], see also [19]. Increasing the repulsion between light quarks beyond the naive one-gluon exchange force, we obtain a configuration of the potential which separates the diquarks from each other, Fig. 1(b), as envisaged in [20], with the phenomenological implications discussed in [10] and [21]. The most compelling one is that decays of $X, Z$ particles into quarkonia + mesons are suppressed with respect to decays into open charm mesons: the tunneling of heavy quark pairs through the barrier gets a larger suppression factor. At difference from what was done originally in [3,8,10], the two lumps of two-quark states $Qq + \bar{Q}\bar{q}$ are found in a superposition of diquark-antidiquark in the $3 \otimes 3$ and $6 \otimes 6$ color configurations.

The two light particles are not equal and there are two different heavy-light orbitals: in addition to $Qq + \bar{Q}\bar{q}$, we examine the $Q\bar{q} + \bar{Q}q$ case. In the latter, $Q\bar{q}$ and $\bar{Q}q$ orbitals have a color octet component. As we shall see, however, at large separations between heavy quarks the lowest state will correspond to a pair of color singlet charmed mesons. A minimum of the BO potential is not
The picture of diquark-antidiquark states segregated in space by a potential barrier is compatible with the existence of charged partners of the $X^{0}(3872)$ to be found in $X^{\pm} \rightarrow \rho^{\pm}J/\psi$ final states, with branching fractions considerably smaller than in the neutral channel. This requires to push way further on the available experimental bounds. It also gives an independent thrust to the idea of stable $bb\bar{q}q$ tetraquarks, still awaiting an experimental confirmation.

II. HIDDEN CHARM

We indicate with $x_A$ and $x_B$ the coordinates of $c$ and $\bar{c}$, and $x_{1,2}$ the coordinates of $q$ and $\bar{q}$. Both $c\bar{c}$ and $q\bar{q}$ are taken in the 8 color representation.

Suppressing coordinates $T = (\bar{c}_1q^a_2)(\bar{q}^a_2q^a_1)$ with the sum over $a = 1,\ldots,8$ understood.

If we restrict to one-gluon exchange we find the interactions between the different pairs in terms of the quadratic Casimir operators

$$\lambda_{q_1q_2}(R) = \alpha_5 \frac{1}{2} (C_2(R) - C_2(q_1) - C_2(q_2))$$

$q_{1,2}$ are the 3 or $\bar{3}$ irreducible representations of the color group depending on whether $q_{1,2}$ are quarks or antiquarks, and $R$ is the color representation of the $q_1q_2$ pair.\(^1\)

If we find the pair $q_1q_2$ in the tetraquark $T(q_1q_2q_3q_4)$ in a superposition of two $SU(3)_c$ representations with amplitudes $a$ and $b$

$$T = a|(q_1q_2)_{R_1}\cdots\rangle_1 + b|(q_1q_2)_{R_2}\cdots\rangle_1$$

then we use

$$\lambda_{q_1q_2} = a^2\lambda_{q_1q_2}(R_1) + b^2\lambda_{q_1q_2}(R_2).$$

Since both $c\bar{c}$ and $q\bar{q}$ are in color octet we have $\lambda_{c\bar{c}} = \lambda_{q\bar{q}} = +1/6\alpha_5$. The couplings of the other pairs are found using the Fierz rearrangement formulas for $SU(3)_c$ to bring the desired pair in the same quark bilinear. We get

$$\lambda_{c\bar{c}} = \lambda_{q\bar{q}} = -\frac{1}{3}\alpha_5 \quad \lambda_{c\bar{q}} = \lambda_{\bar{c}q} = -\frac{7}{6}\alpha_5.$$  

The pattern of repulsions and attractions in (5) is the same as in the hydrogen molecule, substituting electrons with light and protons with heavy quarks. We take a perturbative approach similar to the one in the $H_2$ case [5]. For fixed coordinates of the heavy particles, $x_A$ and $x_B$, we describe the unperturbed state as the product of two orbitals, i.e., the wave functions of the bound states of one heavy and one light particle around $x_A$ and $x_B$, and

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\(^1\)We recall the results: $C_2(1) = 0$, $C_2(R) = C_2(R)$, $C_2(3) = 4/3$, $C_2(6) = 10/3$, $C_2(8) = 3$. 

We use a constituent light quark mass
constituent masses plus the energy of each orbital
of a confining linear potential

$$V_{cq} = \frac{1}{2} \alpha_S \frac{1}{r} + kr + V_0$$

We assume a radial wave-function $R(r)$ of the form

$$R(r) = \frac{A^{3/2}}{\sqrt{4\pi}} e^{-Ar}$$

and determine $A$ by minimizing the Schroedinger functional

$$\langle H(A) \rangle = \frac{(R(r), (-\frac{1}{2} \nabla^2 + V_{cq} - V_0)R(r))}{(R(r), R(r))}$$

We use a constituent light quark mass\(^2\) $M_q = 0.31$ GeV estimated from the meson spectrum [1,3], $\alpha_S = 0.30$ at the charm mass scale and $k = 0.15$ GeV\(^2\) from [23]. Another option is that $k$ follows the coefficient of the Coulombic force [24], which leads to $k = 1/4 \times 0.15$ GeV\(^2\). We comment later on this alternative.

We find $A = 0.43$ GeV, $\langle H \rangle_{\text{min}} = 0.73$ GeV.

We write the wave function of the $qq$ state

$$\Psi(1,2) = \psi(1)\phi(2) = R(\mathbf{x}_1 - \mathbf{x}_A)R(\mathbf{x}_2 - \mathbf{x}_B).$$

The unperturbed energy of $\Psi(1,2)$ is given by the quark constituent masses plus the energy of each orbital $E_0 = 2(M_c + M_q + \langle H \rangle_{\text{min}} + V_0)$.

The perturbation Hamiltonian using the values for $\lambda_{cq} = \lambda_{q\bar{q}}$ and $\lambda_{c\bar{q}} = \lambda_{\bar{q}q}$ found above, is

$$H_{\text{pert}} = -\frac{7}{6} \alpha_S \left( \frac{1}{|\mathbf{x}_1 - \mathbf{x}_B|} + \frac{1}{|\mathbf{x}_2 - \mathbf{x}_A|} \right) + \frac{1}{6} \alpha_S \left( \frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} \right)$$

To first order in $H_{\text{pert}}$ and with $r_{AB} = |\mathbf{x}_A - \mathbf{x}_B|$, the BO potential is

$$V_{BO}(r_{AB}) = \frac{1}{6} \alpha_S \frac{1}{r_{AB}} + \delta E$$

where $\delta E = \langle \Psi(1,2), H_{\text{pert}}\Psi(1,2) \rangle$ evaluates to

$$\delta E = -\frac{7}{6} \alpha_S 2 I_1(r_{AB}) + \frac{1}{6} \alpha_S I_4(r_{AB}).$$

The functions $I_{1,4}$ are given in [5] for hydrogen wave functions, and may be computed numerically for any given orbital (7)

$$I_1(r_{AB}) = \int d^3\xi \phi(\xi) \psi(\xi) \psi(\xi) \frac{1}{|\xi - \eta|}$$

where the vector $\xi$ originates from $A$ and $|\mathbf{x}_B| = r_{AB}$.

Similarly

$$I_4(r_{AB}) = \int d^3\xi d^3\eta \psi(\xi) \psi(\xi) \psi(\xi) \frac{1}{|\xi - \eta|}.$$  

In addition, we take into account the confinement of the colored diquarks by adding a linearly rising potential determined by a string tension $k_T$ and the onset point, $R_0$

$$V_{\text{conf}}(r) = k_T (r - R_0) \times \theta(r - R_0)$$

$$V(r) = V_{BO}(r) + V_{\text{conf}}(r).$$

For orientation, we choose $R_0 = 10$ GeV\(^{-1}\), greater than $2A^{-1} \sim 5$ GeV\(^{-1}\), where the two orbitals start to separate.\(^3\) As for $k_T$, we note that the tetraquark $T = |(c\bar{c})_8(\bar{q}q)_8\rangle_1$ can be written as

$$T = \sqrt{\frac{2}{3}}(cq)_3|\bar{q}q\rangle_3 - \sqrt{\frac{1}{3}}(cq)_8|\bar{q}q\rangle_8.$$  

At large distances the diquark-antidiquark system is a superposition of $3 \otimes 3 \rightarrow 1$ and $6 \otimes 6 \rightarrow 1$. The hypothesis of Casimir scaling of $k_T$ [24] and (16) would give

$$k_T = \left( \frac{2}{3} + \frac{1}{3} C_2(6) \right) = 1.5k.$$  

However, as discussed in [24], gluon screening gives the 6 diquark a component over the 3, which appears in the product $6 \otimes 8$, bringing $k_T$ closer to $k$. For simplicity, we adopt $k_T = k$.

The potential $V(r)$ computed on the basis of Eqs. (15) is given in Fig. 1(a). Also reported are the wave function and

\(^2\)For heavy quarks we take $M_c = 1.67$ GeV, $M_b = 5.0$ GeV [1,3].

\(^3\) $R_0$ should be considered a free parameter, to be fixed on the phenomenology of the tetraquark, as we discuss below.
the eigenvalue obtained by solving numerically the radial Schrödinger equation [25].

As it is customary for confined systems like charmonia, we fix \( V_0 \) to reproduce the mass of the tetraquark, so the eigenvalue is not interesting. However, the eigenfunction gives us information on the internal configuration of the tetraquark. In Eq. 1(a), with one-gluon exchange couplings, a configuration with \( c \) close to \( \bar{c} \) and the light quarks around is obtained, much like the quarkonium adjoint meson described in [18].

Figure 1(b) is obtained by increasing the repulsion in the \( q \bar{q} \) interaction: \(+1/6\alpha_s \sim 0.05 \rightarrow 2.4\). The corresponding \( c\bar{c} \) wave function clearly displays the separation of the diquark from the antidiquark. Had we used \( k = 1/4 \times 0.15 \) GeV\(^2\) in Eq. (6), the required enhancement would be \(+1/6\alpha_s \rightarrow 3.3\).

The barrier that \( c \) has to overcome to reach \( \bar{c} \), apparent in Fig. 1(b), was suggested in [10], and further considered in [21], to explain the suppression of the \( J/\psi + \rho/\phi \) decay modes of \( \chi_c(3872) \), otherwise favored by phase space with respect to the \( DD^* \) modes. Indeed, with the parameters in Fig. 1(b), we find \(|R(0)|^2 = 10^{-3}\) with respect to \(|R(0)|^2 = 10^{-1}\) with the perturbative parameters of Fig. 1(a).

The tetraquark picture of \( \chi_c(3872) \) and the related \( Z(3900) \) and \( Z(4020) \) have been originally formulated in terms of pure \( \bar{3} \otimes 3 \) diquark-antidiquark states [3,8,10]. The \( 6 \otimes 6 \) component in (16) results in the opposite sign of the \( q \bar{q} \) hyperfine interactions vs the dominant \( c\bar{c} \) and \( \bar{c}q \) one, and it could be the reason why \( \chi_c(3872) \) is lighter than \( Z(3900) \).

**B. The \( c\bar{q} \) orbital**

One obtains the new orbital by replacing \(-1/3\alpha_s \rightarrow -7/6\alpha_s \) in Eq. (6). Correspondingly \( A = 0.50 \) GeV, \( \langle H \rangle_{\min} = 0.47 \) GeV. The perturbation Hamiltonian appropriate to this case is

\[
H_{\text{pert}} = -\frac{1}{3}\alpha_s \left( \frac{1}{|x_1 - x_B|} + \frac{1}{|x_2 - x_A|} \right) \\
+ \frac{1}{6\alpha_s} \left( c - \frac{1}{|x_1 - x_2|} \right) \\
+ \frac{1}{6\alpha_s} \left( \frac{1}{|x_1 - x_B|} + \frac{1}{|x_2 - x_A|} \right) \\
+ \frac{1}{6\alpha_s} \left( \frac{1}{|x_1 - x_2|} \right).
\]

and

\[
V_{BO} = +\frac{1}{6\alpha_s} \frac{1}{r_{AB}} + \delta E.
\]

The tetraquark state is

\[
T = \sqrt{\frac{8}{9}} [(\bar{c}q)_1 (\bar{q}c)_1] - \frac{1}{\sqrt{9}} [(\bar{c}q)_8 (\bar{q}c)_8]_1.
\]

At large \(|x_A - x_B|\) the lowest energy state (two color singlet mesons) has to prevail, as concluded also in [24] on the basis of the screening of octet charges due to gluons.

There is no confining potential and \( V_{BO} \rightarrow \langle H \rangle_{\min} + V_0 \) for \( r_{AB} \rightarrow \infty \). Including constituent quark masses, the energy of the state at \( r_{AB} = \infty \) is \( E_{\infty} = 2(M_c + M_q + \langle H \rangle_{\min} + V_0) \) and it must coincide with the mass of a pair of non-interacting charmed mesons, with spin-spin interaction subtracted. Therefore we impose

\[
\langle H \rangle_{\min} + V_0 = 0.
\]

A minimum of the BO potential is not guaranteed. If there is such a minimum, as in Fig. 2(a), it would correspond to a configuration similar to the quarkonium adjoint meson in Fig. 1(a). If repulsion is increased above the perturbative value, e.g., changing \(+1/6\alpha_s \sim 0.11\) to a coupling \( \geq 1\) in analogy with Fig. 1(b), the BO potential has no minimum at all, Fig. 2(a).

**III. DOUBLE BEAUTY TETRAQUARKS: \( bb \) IN \( \bar{3} \)**

The lowest energy state corresponds to \( bb \) in spin one and light antiquarks in spin and isospin zero. The tetraquark state \( T = [(bb)_{\bar{3}}, (\bar{q}q)_{\bar{3}}]_1 \) can be Fierz transformed into

\[
T = \sqrt{\frac{1}{3}} [(\bar{q}b)_1, (\bar{q}b)_1] - \frac{\sqrt{2}}{\sqrt{3}} [(\bar{q}b)_8, (\bar{q}b)_8]
\]

with all attractive couplings

\[
\lambda_{bb} = \lambda_{\bar{q}b} = -\frac{2}{3}\alpha_s \quad \lambda_{b\bar{q}} = -\frac{1}{3}\alpha_s.
\]

As in Eq. (20), the \( 8 \) charges are screened by gluons, so at large separations the state in Eq. (22) behaves like the product of two color singlets. There is only one possible orbital, namely \( b\bar{q} \), but the unperturbed state now is the superposition of two states with \( \bar{q} \) bound to one or to the other \( b \)

\[
\Psi(1,2) = \psi(1)|\phi(2) + \phi(1)|\psi(2)|\sqrt{2(1 + S^2)}\]

The denominator is needed to normalize \( \Psi(1,2) \) and it arises because \( \psi(1) \) and \( \phi(1) \) are not orthogonal, with the overlap \( S \) defined as

\[
S = \int d^3\xi \psi(\xi)\phi(\xi).
\]

The perturbation Hamiltonian is

\[
H_{\text{pert}} = -\frac{1}{3}\alpha_s \left( \frac{1}{|x_1 - x_B|} + \frac{1}{|x_2 - x_A|} + \frac{1}{|x_1 - x_2|} \right)
\]

and

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tends to zero, for large
mesons are

couplings are reported in Fig.

\[ V_{BO}(r_{AB}) = 2(\langle H \rangle_{\text{min}} + V_0) - \frac{2}{3} \alpha_s \frac{1}{r_{AB}} + \delta E \]  

(27)

where \( \delta E = \langle \Psi(1, 2), H_{\text{pert}} \Psi(1, 2) \rangle \) evaluates to

\[ \delta E = \frac{1}{1 + S^2} \left[ \frac{2}{3} \alpha_s (I_1 + S I_2) - \frac{2}{3} \alpha_s (I_4 + I_6) \right]. \]  

(28)

\( I_{1,4} \) were defined previously whereas [5]

\[ I_2(r_{AB}) = \int d^3 \xi \psi(\xi) \phi(\xi) \frac{1}{|\xi - x_B|}. \]  

(29)

\[ I_6(r_{AB}) = \int d^3 \xi d^3 \eta \psi(\xi) \phi(\xi) \psi(\eta) \phi(\eta) \frac{1}{|\xi - \eta|}. \]  

(30)

For the orbital \( b\bar{q} \) we find \( A = 0.44 \text{ GeV}, \langle H \rangle_{\text{min}} = 0.75 \text{ GeV} \). The BO potential, wave function and eigenvalue for the \( bb \) pair in color 3 and the one-gluon exchange couplings are reported in Fig. 3. There is a bound tetraquark with a tight \( bb \) diquark, of the kind expected in the constituent quark model [13,14,16].

The BO potential in the origin is Coulomb-like and it tends to zero, for large \( r_{AB} \), due to (21). The (negative) eigenvalue \( E \) of the Schrödinger equation is the binding energy associated with the BO potential. The mass of the lowest tetraquark with \( (bb)_{S=1}, (\bar{q}\bar{q})_{S=0} \) and of the \( B \) mesons are

\[ M(T) = 2(M_b + M_q) + E + \frac{1}{2} \kappa_{bb} - \frac{3}{2} \kappa_{\bar{q}q}, \]  

(31)

\[ M(B) = M_b + M_q - \frac{3}{2} \kappa_{b\bar{q}}. \]  

(32)

where \( \kappa_{bb} = 15 \text{ MeV}, \kappa_{q\bar{q}} = 98 \text{ MeV} \) and \( \kappa_{b\bar{q}} = 23 \text{ MeV} \) [3] are the hyperfine interactions and \( E = -84 \text{ MeV} \) is the eigenvalue shown in Fig 3(a) with \( \alpha_s(m_b) = 0.20 \).

The \( Q \)-value for the decay \( T \to 2B + \gamma \) is then

\[ Q_{bb} = E + \frac{1}{2} \kappa_{bb} - \frac{3}{2} \kappa_{q\bar{q}} + 3 \kappa_{b\bar{q}} = -154(-137) \text{ MeV}. \]  

(33)

TABLE I. \( Q \) values in MeV for decays into meson + meson + \( \gamma \). The models in [13,14,16] are different elaborations of the constituent quark model we use throughout this paper. More details can be found in the original references. We also refer the reader to the lattice QCD literature providing alternate conclusions on these states [22]. Results in parentheses are obtained with a string tension \( k = 1/4 \times 0.15 \text{ GeV}^2 \) in Eq. (6).

| \( Q' \bar{q} \bar{d} \) | This work | K&R [13] | E&Q [14] | Luo et al. [16] |
|-----------------|-----------|---------|---------|---------------|
| \( cc \bar{b} \bar{c} \) | -10(+7)   | +140    | +102    | +39           |
| \( cb \bar{u} \bar{d} \) | -73(-58)  | ~0      | +83     | -108          |
| \( bb \bar{u} \bar{d} \) | -154(-137)| -170    | -121    | -75           |

Results for \( Q_{cc,bc} \) are reported in Tab. I using \( \alpha_s((m_b + m_c)/2) = 0.23 \). Eq. (33) underscores the result obtained by Eichten and Quigg [14] that the \( Q \)-value goes to a negative constant limit for \( M_Q \to \infty \): \( Q = -150 \text{ MeV} + O(1/M_Q) \).

IV. DOUBLE BEAUTY TETRAQUARKS: \( bb \) IN 6

We start from \( T = (bb)_6, (\bar{q}\bar{q})_6 \), also considered in [16], to find

\[ T = \sqrt{\frac{5}{3}}(\bar{q}b)_{1}, (\bar{q}b)_{1} + \sqrt{\frac{1}{3}}(\bar{q}b)_{8}, (\bar{q}b)_{8} \]  

(34)

therefore

\[ \lambda_{bb} = \lambda_{\bar{q}q} = + \frac{1}{3} \alpha_s \quad \lambda_{b\bar{q}} = - \frac{5}{6} \alpha_s. \]  

(35)

The situation is entirely analogous to the \( H_2 \) molecule, with two identical, repelling light particles. For the orbital \( b\bar{q} \), we find \( A = 0.43 \text{ GeV} \) and \( \langle H \rangle_{\text{min}} = 0.72 \text{ GeV} \). The BO potential with the one-gluon exchange parameters admits a very shallow bound state with \( E = -32 \text{ MeV} \), quantum numbers: \( (bb)_{6,S=0} \) and \( (\bar{q}\bar{q})_{6,S=0,J=1} \). \( J^{PC} = 0^{++} \), and charges \(-2,-1,0 \). The \( Q \)-value for the decay \( T \to 2B \) is then

\[ Q_{bb} = E - \frac{3}{2} \kappa_{bb} - \frac{3}{2} \kappa_{q\bar{q}} + 3 \kappa_{b\bar{q}} = -133(-131) \text{ MeV} \]  

(36)

with the same notation of Table I.

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