Study of the structures of four-quark states in terms of the Born-Oppenheimer approximation*

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Abstract: In this work, we use the Born-Oppenheimer approximation, where the potential between atoms can be approximated as a function of distance between the two nuclei, to study the four-quark bound states. By this approximation, Heitler and London calculated the spectrum of the hydrogen molecule, which includes two protons (heavy) and two electrons (light). Generally, the observed exotic mesons $Z_b(10610)$, $Z_b(10650)$, $Z_c(3900)$ and $Z_c(4020)$ ($Z_c(4025)$) may be molecular states made of two physical mesons and/or diquark-anti-diquark structures. Analogous to the Heitler-London method for calculating the mass of the hydrogen molecule, we investigate whether there exist energy minima for these two structures. Contrary to the hydrogen molecule case where only the spin-triplet possesses an energy minimum, there exist minima for both of these states. This implies that both molecule and tetraquark states can be stable objects. Since they have the same quantum numbers, however, the two states may mix to result in the physical states. A consequence would be that partner exotic states co-existing with $Z_b(10610)$, $Z_b(10650)$, $Z_c(3900)$ and $Z_c(4020)$ ($Z_c(4025)$) are predicted and should be experimentally observed.

Key words: exotic states, Born-Oppenheimer approximation, molecule, tetraquark

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1 Introduction

The naive quark model suggests that a meson is made of a quark and an anti-quark, whereas a baryon consists of three quarks. The constituents in hadrons are bound together by the QCD interaction to constitute a color singlet. However, neither the quark model nor the QCD theory ever forbids the existence of multi-quark states as long as they are color-singlets. The fact that after several years of hard work all experimental trials to observe pentaquarks have failed, has greatly discouraged high energy physics theorists and experimentalists, even though the idea of pentaquarks is really stimulating. One may ask if nature indeed only favors the most economic structures for hadrons. The situation has changed with the discovery of the exotic states $Z_b(10610)$ and $Z_b(10650)$ [1], and especially the newly observed $Z_c(3900)$ [2], $Z_c(4020)$ [3] and $Z_c(4025)$ [4]. The characteristics of such states are that Z_b and Z_c-mesons contain hidden bottom $b\bar{b}$ or charm $c\bar{c}$ respectively and both are charged; therefore, they cannot be simple $b\bar{b}$ or $c\bar{c}$ bound states, but multi-quark states, and compared to the regular structures are called exotic states.

The inner structure of the multi-quark states is more complicated than the regular mesons, in that the exotic states can be molecular states or tetraquarks or their mixtures. The molecular state is constructed by two color singlet mesons. A strong point in support of such a structure is that the mass of the newly discovered meson $Z_b(10610)$ is close to the sum of the masses of B and $\bar{B}^*$, while the mass of $Z_c(3900)$ is also close to a sum of D and D^* masses. The study of the decay modes of such mesons, however, seems to support the tetraquark structure [5, 6]. To clarify the structures of those exotic states, one may need to investigate their overall characteristics based on fundamental dynamics, instead of simply considering the closeness of their masses to the sum of the constituents.

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One observation may draw our attention. The resonances $Z_b(10610)$, $Z_b(10650)$, $Z_c(3900)$, $Z_c(4020)$ and $Z_c(4025)$ have been experimentally observed and confirmed as exotic four-quark states. Many authors [7–11] have assumed them to be molecular states of B, B^*, D and D^* (and the corresponding anti-mesons) which are well-measured experimentally. A common point is that the masses of the observed exotic mesons are larger than the sum of the supposed constituent mesons. Specifically, 10608.4±2.0 MeV [1] (the mass of $Z_b(10610)$) is larger than the sum of the masses of B and B^* (10604.45 MeV); 10653.2±1.5 MeV [1] (the mass of $Z_b(10650)$) is larger than the sum of the masses of B^* and B^* (10650.4 MeV); 3899±3.6±4.9 MeV [2] (the mass of $Z_c(3900)$) is larger than the sum of D and D^* (3876.6 MeV); 4022.9±0.8±2.7 MeV [3] (the mass of $Z_c(4020)$) is larger than the sum of D^* and D^* (4013.96 MeV). Generally, unless there exists a linearly increasing potential (such as the confinement potential for quarks) or a barrier, the binding energy of two constituent mesons which is caused by exchanging color-singlet hadrons must be negative. Thus, the mass of a composite meson should be smaller than the sum of the two (or more) constituent masses. Moreover, as estimated by some authors [12, 13], the masses of those exotic states are also larger than the sums of the masses of the diquark and anti-diquark concerned. In our calculation, even though the sum of the two diquark masses is larger than the mass of the corresponding exotic meson, the negative binding energy still makes the resultant total energy smaller than the exotic meson. This may imply that neither molecular nor tetraquark states alone correspond to the observed exotic mesons. Our study indicates that only their mixture provides a reasonable picture for the four-quark states. Thus, both molecular and tetraquark states should exist, even though they may not be the physical states which we observe in experiments.

By the Born-Oppenheimer [14] approximation, the potential between atoms can be approximated as a function of the distance between the two nuclei; by this scheme, Heitler and London [15] calculated the spectrum of the hydrogen molecule. In that case, the two protons are supposed to be at rest and the two electrons are moving. Since the two electrons are identical fermions, the wavefunction of the two-electron system must be totally anti-symmetric. It was found that there is only one energy minimum corresponding to the triplet. Namely, in the hydrogen molecule the two electrons must be in the spin-triplet.

Compared with the hydrogen molecule, Z_b (or Z_c) is made of four quarks: Q, $\bar{Q}$, u($\bar{u}$), $\bar{d}$(d), where Q stands for b or c quark. Since Q, $\bar{Q}$ are much heavier than the light flavors, we can approximate them to be at rest. Thus it is natural that we separate the four quarks into two groups. One possibility is that each group is in a color singlet, which corresponds to a molecular state, whereas another possibility is that one group containing Qu is in a color-anti-triplet (or a sextet) and the other group containing $\bar{Q}\bar{d}$ is in a color-triplet (or an anti-sextet), i.e. the dipole-anti-dipole structure. Since u and $\bar{d}$ are not identical particles, the wavefunction does not need to be anti-symmetrized. By the Born-Oppenheimer approximation, the potential between two groups can be a function of distance between Q and $\bar{Q}$ and interactions between the two groups are taken as a perturbation. Since the interactions between quarks are complicated, calculation of the energy spectrum of the exotic states is much more difficult than for the hydrogen molecule. It is noted that Braaten et al. [16] also consider the Born-Oppenheimer potential to deal with the four-quark states.

First we need to determine the wavefunctions of the color singlet of $Q\bar{d}(\bar{Q}u)$ and the color-anti-triplet (or sextet) dipole Qu (color-triplet or anti-sextet $\bar{Q}\bar{d}$). Here we use the Cornell potential [17, 18] as the interaction between the quarks and since the light flavors are relativistic, following the literature, we employ the Schrödinger-like equation with relativistic kinematics. The effective interaction between the quarks (quark-anti-quark) which belong to different groups is complicated, because not only is there the short-distance QCD interaction, but the long-distance interaction, which can be treated by exchanging color-singlet light mesons such as π, σ and ρ (for the molecule case) or the color-flux tube (for the tetraquark case), plays an important role. Here we do not involve the strange flavor. Analogous to the hydrogen molecule, we calculate the spectrum of the ground state of the four-quark system (the molecule and tetraquark separately). Our strategy is similar to the Heitler-London approximation, namely we take the products of the two meson wavefunctions (for the molecule) and diquark-anti-diquark wavefunctions (for the tetraquark) as two independent trial functions and calculate the interaction between the two groups to obtain the spectra as functions of the distance between b and $\bar{b}$ (c and $\bar{c}$). Our goal is to see whether the molecular state or tetraquark state can possess energy minima with respect to the distance between Q and $\bar{Q}$, by which one can judge if the molecule or tetraquark is physically allowed. If there exist minima for both cases, we can conclude that both structures are probable and the real physical state could be a mixture of the two structures. (In fact, our computations confirm that there are minima for both.)

This work is organized as follows. After this long introduction, we formulate the expressions for the energy spectra. We first present relevant effective potentials for the meson and diquark composed of a heavy quark and a light flavor, and then derive the Born-Oppenheimer potentials for both molecule and tetraquark. In Section 2, we discuss the explicit color and spin structures of the molecular and tetraquark states and solve the Schrödinger-like equation to obtain the spatial wavefunctions of color-singlet meson and color-anti-triplet diquark. In Section 3, along with all input parameters, we present our numerical results, which show that for both molecule and tetraquark there exist minima with repect to the distance between Q and $\bar{\mathrm{Q}}$. The last section is devoted to the discussion and conclusions.

2 Derivation of the relevant formulae

In this section, we derive the theoretical formulae for calculating the mass spectra and wavefunctions of both molecular and tetraquark states. We first solve the Schrödinger-like equations to obtain the mass spectra and wavefunctions of the mesons B, B^*, D and D^* and diquark (anti-diquark), which will be the trial functions for later calculations. Note that since the diquark is not a physical state, we determine its mass spectrum and wavefunction via theoretical computations. We go on using the Born-Oppenheimer approximation to evaluate the mass spectra of molecular and tetraquark states as functions of the distance between the two heavy constituents Q and $\bar{\mathrm{Q}}$.

2.1 Derivation of potentials

Here we first obtain the effective potentials between the relevant constituents inside a color-singlet, i.e. mesons and color-triplet (anti-triplet), i.e. anti-diquark (diquark). Then we go on to derive the potential between constituents from the different groups. For the two distinct configurations (the molecular state and tetraquark (diquark-antidiquark) state) (see Fig. 1), the effective interactions are different.

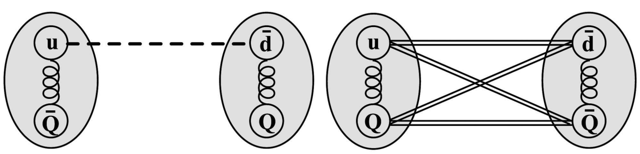

Fig. 1. Configurations of the four-quark system (left: molecular state, right: tetraquark state).

2.1.1 Meson and diquark (antidiquark) states

In this subsection, let us first discuss the interactions among the constituents inside a meson ($\mathrm{q}\bar{\mathrm{Q}}(\bar{\mathrm{q}}\mathrm{Q})$) or an (anti) diquark ($\mathrm{qQ}(\bar{\mathrm{q}}\bar{\mathrm{Q}})$). The general Hamiltonian can be written as

$$\begin{aligned} H &= \sqrt{\boldsymbol{p}_i^2+m_i^2}+\sqrt{\boldsymbol{P}_j^2+m_j^2}+V(r), \\ i &= \mathrm{q}(\bar{\mathrm{q}});j=\mathrm{Q}(\bar{\mathrm{Q}}). \end{aligned} \tag{1}$$

where the $\boldsymbol{p}_i$ and $\boldsymbol{P}_j$ are the 3-momenta of the light flavor $\mathrm{q}(\bar{\mathrm{q}})$ and heavy flavor $\mathrm{Q}(\bar{\mathrm{Q}})$ respectively. The interaction potential is

$$V(r_{ij})=V_{\mathrm{oge}}(r_{ij})+V_{\mathrm{con}}(r_{ij}), \tag{2}$$

and r_{ij} is the distance between the quarks (quark-antiquark). The one-gluon exchange (oge) term $V_{\mathrm{oge}}(r_{ij})$, which plays the main role at short distances, is [19]

$$\begin{aligned} V_{\mathrm{oge}}(r_{ij}) = \frac{1}{4}\alpha_s(\boldsymbol{\lambda}_i^{\mathrm{c}}\cdot\boldsymbol{\lambda}_j^{\mathrm{c}})\Bigg[\frac{1}{r_{ij}}-\frac{\pi}{2}\left(\frac{1}{m_i^2}+\frac{1}{m_j^2}\right. \\ \left.+\frac{4}{3m_im_j}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j\right)\delta(r_{ij})\Bigg], \end{aligned} \tag{3}$$

and the confinement part $V_{\mathrm{con}}(r_{ij})$ takes the linear form [17]

$$V_{\mathrm{con}}(r_{ij})=-\frac{1}{4}(\boldsymbol{\lambda}_i^{\mathrm{c}}\cdot\boldsymbol{\lambda}_j^{\mathrm{c}})(br_{ij}+c) \tag{4}$$

where $\boldsymbol{\lambda}_i^{\mathrm{c}}$ and $\boldsymbol{\sigma}_i$ are, respectively, the color $SU_{\mathrm{c}}(3)$ and spin operators acting on quark i, and m_{i} is the quark mass. b is the string tension, and c is a global zero-point energy. α_s is the QCD running coupling constant, which depends on the re-normalization scale μ^2 [20]

$$\alpha_s(\mu^2)=\frac{\alpha_0}{\ln\left(\dfrac{\mu^2+\mu_0^2}{\Lambda_0^2}\right)}, \tag{5}$$

where $\mu=m_im_j/(m_i+m_j)$ is the reduced mass of the $\mathrm{q_i}\bar{\mathrm{Q}}_{\mathrm{j}}$ system and Λ_0, α_0, μ_0 are fitted parameters. The framework can be generalized to the case for a diquark (anti-diquark) which involves two quarks (two anti-quarks).

The δ-function in Eq. (3) is replaced by a Gaussian smearing function [21] with a fitted parameter h

$$\delta(r_{ij})\to\frac{h^3}{\pi^{3/2}}\mathrm{e}^{-h^2r_{ij}^2}. \tag{6}$$

2.1.2 Molecular states

Now we specify the interaction between the two mesons for the molecular structures (Fig. 1, left). Since the constituent mesons are in a color singlet, the quarks (antiquarks) in one meson do not interact with the quarks in another meson via exchanging a single gluon, thus the interaction between $\mathrm{B}^{(*)}\mathrm{B}^{(*)}$ (or $\mathrm{D}^{(*)}\mathrm{D}^{(*)}$) only comes from meson-exchange between the light flavors $\mathrm{q}\bar{\mathrm{q}}$.

The constituent quark model has been thoroughly studied by many authors, for example, Vijande et al. [20, 22], and its successful applications to phenomenology are noted, thus here we employ it to derive the effective interaction between mesons. The interactions $V_{\mathrm{me}}(r_{ij})$ induced by meson-exchange(me) between q and $\bar{\mathrm{q}}$ include the contributions of pseudoscalar (p) and scalar (s),

$$\begin{aligned} V_{\mathrm{me}}(r_{ij}) = \sum_{a=1}^{3}V_{\pi}(r_{ij})\boldsymbol{F}_i^a\cdot\boldsymbol{F}_j^a+\sum_{a=4}^{7}V_{\mathrm{K}}(r_{ij})\boldsymbol{F}_i^a\cdot\boldsymbol{F}_j^a \\ +V_{\eta}(r_{ij})[\cos\theta_{\mathrm{p}}(\boldsymbol{F}_i^8\cdot\boldsymbol{F}_j^8)-\sin\theta_{\mathrm{p}}]+V_{\sigma}(r_{ij}), \end{aligned} \tag{7}$$

and the explicit forms of the interactions are

$$V_{\chi}(r_{ij}) = \frac{g_{ch}^2}{4\pi}\frac{m_{\chi}^2}{12m_im_j}\frac{\Lambda_{\chi}^2}{\Lambda_{\chi}^2-m_{\chi}^2}m_{\chi}\Big[\mathrm{Y}(m_{\chi}r_{ij}) -\frac{\Lambda_{\chi}^3}{m_{\chi}^3}Y(\Lambda_{\chi}r_{ij})\Big](\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j), \tag{8}$$

$$V_{\sigma}(r_{ij}) = -\frac{g_{ch}^2}{4\pi}\frac{\Lambda_{\sigma}^2}{\Lambda_{\sigma}^2-m_{\sigma}^2}m_{\sigma}\Big[\mathrm{Y}(m_{\sigma}r_{ij}) -\frac{\Lambda_{\sigma}}{m_{\sigma}}Y(\Lambda_{\sigma}r_{ij})\Big], \tag{9}$$

with χ=π, K, η and $\boldsymbol{F}_i^a(a{=}1,\ 2,\ \cdots,\ 8)$ being the SU(3) flavor matrices. $Y(x)=\mathrm{e}^{-x}/x$ is the Yukawa function, g_{ch} is the chiral coupling constant, θ_{p} is the mixing angle for the physical η and η′, and the Λs are the chiral symmetry breaking scales. Once the potential between qq is determined, the corresponding potential for $\mathrm{q\bar{q}}$ can also be obtained from a G-parity transformation [23]. It is noted that the employed framework is the SU(3) chiral quark model where the heavy quark (c or b) does not couple to the SU(3) mesons.

Furthermore, in the effective potential there also exists a part $V_{\mathrm{ann}}(r_{ij})$ induced by quark-antiquark $(\mathrm{q},\bar{\mathrm{q}})$ pair annihilation into light mesons which mediate interactions in the s-channel. To the lowest order the quark-antiquark pair resides in an S-wave state and the contribution of the σ-meson($J^{pc}{=}0^{++}$) can be neglected [23]. So here we only keep the contributions of π and ρ to the potential [24, 25]

$$V_{\mathrm{ann},\pi}(r_{ij}) = \frac{g_{\mathrm{ch}}^2\delta(r_{ij})}{4m_{\mathrm{q}}^2-m_{\pi}^2}\left(\frac{1}{3}+\frac{1}{2}\boldsymbol{\lambda}_{\mathrm{q}}^{\mathrm{c}}\cdot\boldsymbol{\lambda}_{\bar{\mathrm{q}}}^{\mathrm{c}}\right) \times\left(\frac{1}{2}-\frac{1}{2}\boldsymbol{\sigma}_{\mathrm{q}}\cdot\boldsymbol{\sigma}_{\bar{\mathrm{q}}}\right)\left(\frac{3}{2}+\frac{1}{2}\boldsymbol{\tau}_{\mathrm{q}}\cdot\boldsymbol{\tau}_{\bar{\mathrm{q}}}\right), \tag{10}$$

and

$$V_{\mathrm{ann},\rho}(r_{ij}) = -\frac{g_v^2\delta(r_{ij})}{4m_{\mathrm{q}}^2-m_{\rho}^2}\left(\frac{1}{3}+\frac{1}{2}\boldsymbol{\lambda}_{\mathrm{q}}^{\mathrm{c}}\cdot\boldsymbol{\lambda}_{\bar{\mathrm{q}}}^{\mathrm{c}}\right) \times\left(\frac{3}{2}+\frac{1}{2}\boldsymbol{\sigma}_{\mathrm{q}}\cdot\boldsymbol{\sigma}_{\bar{\mathrm{q}}}\right)\left(\frac{3}{2}+\frac{1}{2}\boldsymbol{\tau}_{\mathrm{q}}\cdot\boldsymbol{\tau}_{\bar{\mathrm{q}}}\right). \tag{11}$$

$\boldsymbol{\tau}$ is the isospin operator, and the δ-function is also rewritten in the same form as Eq. (6).

Summing all the individual parts, the interaction between the two mesons of the molecule is

$$H_{\mathrm{int}}^{(\mathrm{mol})}=V_{\mathrm{me}}(r_{ij})+V_{\mathrm{ann}}(r_{ij}). \tag{12}$$

2.1.3 Tetraquark states

For the case of the tetraquark, we are dealing with the interaction between the two groups qQ and $\bar{\mathrm{q}}\bar{\mathrm{Q}}$. The key point is to derive an effective potential. The total Hamiltonian is written as

$$H_{\mathrm{int}}^{(\mathrm{tetra})}=\sum_{\substack{i=\mathrm{u,b;}\\ j=\bar{\mathrm{d}},\bar{\mathrm{b}}}}\Big[V_{\mathrm{oge}}(r_{ij})+V'_{\mathrm{con}}(r_{ij})\Big]. \tag{13}$$

The interaction among the constituents in the diquark and anti-diquark is not simply determined by perturbative QCD, becuse the short-distance and long-distance contributions exist simultaneously. Following Brodsky et al. [26], the flux tube model may properly describe the interaction for the tetraquark case. Meanwhile in this case the contribution of meson exchange can be safely ignored compared with that of gluon exchange [27]. The general form of Hamiltonian in the flux-tube model can also be decomposed into the Coulomb-type part, which is responsible for short distance interaction, and the confinement part, for long-distance interaction. As Brodsky et al. [26] suggested, in a "substantial separation", diquark and antidiquark are connected by the flux-tube. It is noted that in our pictures according to the Heitler-London approximation, we need to consider all the interactions among the constituents of different groups, thus we account for the interactions as shown on the right-hand side of Fig. 1. Obviously, summing over all the contributions a resultant Born-Oppenheimer potential would be obtained, which is also an effective flux tube between the diquark and anti-diquark and is the picture from Ref. [26]. Moreover, as is well known, when the tension on the string goes beyond a certain bound, the string will break into two strings and at the new ends a quark-anti-quark pair is created [28, 29]. One can use a step function to describe the breaking effect as

$$(br_{ij}+c)\theta(r-r_0), \tag{14}$$

where r_0 is a parameter corresponding to the strength limit of the string. A typical scale for non-perturbative QCD is Λ_{QCD}, therefore it is natural to consider $r_0=1/\Lambda_{\mathrm{QCD}}$. Just as for smearing the delta function, we need also to smear the step function. In fact

$$\theta(r-r_0)=\lim_{\varepsilon\to 0}\frac{1}{\mathrm{e}^{\frac{1}{\varepsilon}(r_{ij}-r_0)}+1},$$

so smearing the step function implies that we keep ε as a non-zero free parameter to be determined.

Here the interaction between q from the diquark and $\bar{\mathrm{q}}$ from the antidiquark at a relatively large distance is described by a modified form as

$$V'_{\mathrm{con}}(r_{ij})=-\frac{1}{4}(\boldsymbol{\lambda}_i^{\mathrm{c}}\cdot\boldsymbol{\lambda}_j^{\mathrm{c}})(br_{ij}+c)\frac{1}{\mathrm{e}^{\frac{1}{\varepsilon}(r_{ij}-r_0)}+1}, \tag{15}$$

where ε is a parameter in fm, and we set $\Lambda_{\mathrm{QCD}}=280$ MeV in this work.

2.2 Wave functions of four-quark states

Combining all the degrees of freedom of the constituent quarks, the total wave function is a direct product of the radial, spin, color, and isospin (flavor) parts:

$$|\psi_{\alpha}\rangle = |C_{\alpha}\rangle\otimes|I_{\alpha}\rangle\otimes[|\phi_{\alpha}\rangle\otimes|S_{\alpha}\rangle]^{JM}, \quad \alpha = (\mathrm{mol}),(\mathrm{tetra}). \tag{16}$$

For molecular state and tetraquark state separately, unlike the hydrogen molecules, the quarks (antiquarks) involved are not identical, so the Pauli principle does not impose any restrictions on the compositions.

2.2.1 Radial wave function

In the essence of the Born-Oppenheimer approximation, we can choose the product of the two clusters' wave-functions as the basis shown in Fig. 1

$$\phi_{(\rm mol)}=\phi_{\rm u\bar{Q}}\otimes\phi_{\rm \bar{d}Q},\ \phi_{(\rm tetra)}=\phi_{\rm uQ}\otimes\phi_{\rm \bar{d}\bar{Q}}. \tag{17}$$

The radial wave function for each cluster is obtained by solving the Schrödinger-like equation

$$\left[\sqrt{\boldsymbol{p}_{\rm q}^2+m_{\rm q}^2}+\sqrt{\boldsymbol{P}_{\rm Q}^2+m_{\rm Q}^2}+V(r)\right]\phi_\kappa=E\phi_\kappa,$$
$$\kappa={\rm u\bar{Q},\bar{d}Q,uQ,\bar{d}\bar{Q}}, \tag{18}$$

where the potential $V(r)$ takes the Cornell type potential (see Eq. (3) and Eq. (4)), $m_{\rm q}$ and $m_{\rm Q}$ are the masses of light (u, d) and heavy (c, b) quarks. It applies to both meson and diquark cases with different color factors.

We solve the Schrödinger-like equation numerically using the program offered by the authors of Ref. [30, 31] to deduce the radial wavefunction $u(r)$, defined as $\phi_\kappa(\boldsymbol{r})=\dfrac{u_l(r)}{r}{\rm Y}_{lm}(\hat{\boldsymbol{r}})$, with $l=0$. In Fig. 2 the wave-functions of $\rm B^{(*)}$ and $\rm D^{(*)}$ are shown. The eigenvalues are given in Table 1 where the constituent quark masses are input parameters.

2.2.2 Color factors in the wave function

We now turn to discuss the color part of the four-quark states. The color singlet state of a four-quark system is constructed as follows:

$$|\bar{3}_{\rm uQ}\otimes 3_{\rm \bar{Q}\bar{d}}\rangle,\quad |6_{\rm uQ}\otimes\bar{6}_{\rm \bar{Q}\bar{d}}\rangle, \tag{19}$$

$$|1_{\rm u\bar{d}}\otimes 1_{\rm Q\bar{Q}}\rangle,\quad |8_{\rm u\bar{d}}\otimes 8_{\rm Q\bar{Q}}\rangle, \tag{20}$$

$$|1_{\rm u\bar{Q}}\otimes 1_{\rm Q\bar{d}}\rangle,\quad |8_{\rm u\bar{Q}}\otimes 8_{\rm Q\bar{d}}\rangle, \tag{21}$$

which stand as three orthonormal basis-vectors. The expression in Eq. (19) is the so-called tetraquark state with a diquark-anti-diquark structure; we only consider the state $|\bar{3}_{\rm uQ}\otimes 3_{\rm \bar{Q}\bar{d}}\rangle$ (denoted as $|C_{(\rm tetra)}\rangle$) here [26]. Eq. (20) and Eq. (21) are for the molecular states with a meson-meson structure; in particular, the state $|1_{\rm u\bar{Q}}\otimes 1_{\rm Q\bar{d}}\rangle$ (denoted as $|C_{(\rm mol)}\rangle$) corresponds to the $\rm B^{(*)}B^{(*)}$ (or $\rm D^{(*)}D^{(*)}$), which is the concern of this work.

The three basis vectors are related to each other through rearrangements [33]

$$|1_{\rm u\bar{Q}}\otimes 1_{\rm Q\bar{d}}\rangle = \sqrt{\frac{1}{3}}|\bar{3}_{\rm uQ}\otimes 3_{\rm \bar{Q}\bar{d}}\rangle+\sqrt{\frac{2}{3}}|6_{\rm uQ}\otimes\bar{6}_{\rm \bar{Q}\bar{d}}\rangle, \tag{22}$$

$$|8_{\rm u\bar{Q}}\otimes 8_{\rm Q\bar{d}}\rangle = -\sqrt{\frac{2}{3}}|\bar{3}_{\rm uQ}\otimes 3_{\rm \bar{Q}\bar{d}}\rangle+\sqrt{\frac{1}{3}}|6_{\rm uQ}\otimes\bar{6}_{\rm \bar{Q}\bar{d}}\rangle, \tag{23}$$

and

$$|1_{\rm u\bar{d}}\otimes 1_{\rm Q\bar{Q}}\rangle = -\sqrt{\frac{1}{3}}|\bar{3}_{\rm uQ}\otimes 3_{\rm \bar{Q}\bar{d}}\rangle+\sqrt{\frac{2}{3}}|6_{\rm uQ}\otimes\bar{6}_{\rm \bar{Q}\bar{d}}\rangle, \tag{24}$$

$$|8_{\rm u\bar{d}}\otimes 8_{\rm Q\bar{Q}}\rangle = \sqrt{\frac{2}{3}}|\bar{3}_{\rm uQ}\otimes 3_{\rm \bar{Q}\bar{d}}\rangle+\sqrt{\frac{1}{3}}|6_{\rm uQ}\otimes\bar{6}_{\rm \bar{Q}\bar{d}}\rangle. \tag{25}$$

The color matrix elements which we need in Sec. 3 are summarized in Table 2.

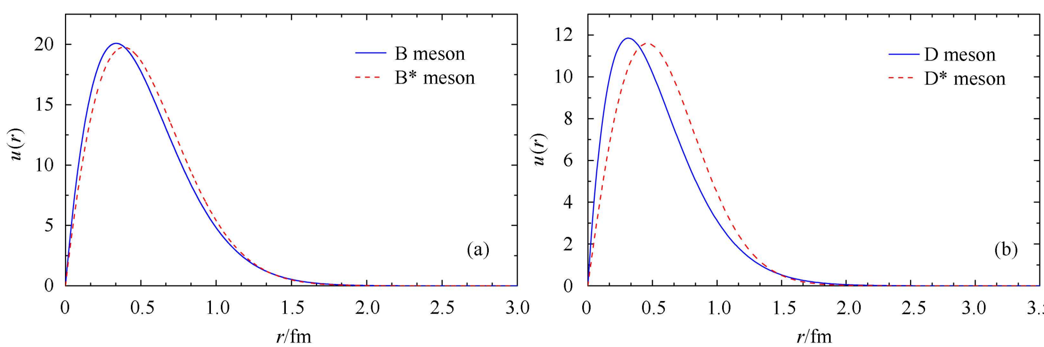

Fig. 2. (color online) The reduced wavefunction $u(r)$ in coordinate space. (a) The solid curve is for B and the dashed for $\rm B^*$. (b) The solid curve is for D and the dashed for $\rm D^*$.

Table 1. Masses of heavy mesons and diquark (with spin-0 and spin-1) calculated by solving the Schrödinger-like equation, with experimental data [32] and results from QCD sum rules presented for comparison.

mesons	B	B*	D	D*
Exp./MeV	5279.26±0.17	5325.2±0.4	1864.84±0.7	2010.26±0.07
this work/GeV	5.279	5.325	1.863	2.010
diquarks	$\rm (bq)_{S=0}$	$\rm (bq)_{S=1}$	$\rm (cq)_{S=0}$	$\rm (cq)_{S=1}$
this work/GeV	5.344	5.355	1.963	2.00
QCD sum rules [13]/GeV	5.08±0.04	5.08±0.04	1.86±0.05	1.87±0.10

Table 2. Color matrix elements [34].

$\hat{O}$	$(\vec{\lambda}_u\cdot\vec{\lambda}_Q)$	$(\vec{\lambda}_{\bar{Q}}\cdot\vec{\lambda}_{\bar{d}})$	$(\vec{\lambda}_u\cdot\vec{\lambda}_{\bar{Q}})$	$(\vec{\lambda}_Q\cdot\vec{\lambda}_{\bar{d}})$	$(\vec{\lambda}_u\cdot\vec{\lambda}_{\bar{d}})$	$(\vec{\lambda}_Q\cdot\vec{\lambda}_{\bar{Q}})$
$\langle\bar{3}_{uQ}3_{\bar{Q}\bar{d}}\|\hat{O}\|\bar{3}_{uQ}3_{\bar{Q}\bar{d}}\rangle$	$-8/3$	$-8/3$	$-4/3$	$-4/3$	$-4/3$	$-4/3$
$\langle 6_{uQ}\bar{6}_{\bar{Q}\bar{d}}\|\hat{O}\|6_{uQ}\bar{6}_{\bar{Q}\bar{d}}\rangle$	$4/3$	$4/3$	$-10/3$	$-10/3$	$-10/3$	$-10/3$
$\langle\bar{3}_{uQ}3_{\bar{Q}\bar{d}}\|\hat{O}\|6_{uQ}\bar{6}_{\bar{Q}\bar{d}}\rangle$	0	0	$-2\sqrt{2}$	$-2\sqrt{2}$	$2\sqrt{2}$	$2\sqrt{2}$

2.2.3 Spin and flavor parts of the wave function

The flavor and spin parts of the molecular states and tetraquark states associated with physical mesons $Z_b^+(10610)$, $Z_b^+(10650)$, $Z_c^+(3900)$, $Z_c^+(4020)$ are listed in Table 3, and the quantum numbers $I^G(J^P) = 1^+(1^+)$ for all states. Specifically, for the quantum number (I, I_3)=(1, +1) of light flavors u and $\bar{d}$, the isospin states are $|I_\alpha\rangle = -u\bar{d}$. A special note is that our discussion in the Introduction and numerical computation made in the next section confirm that neither molecular state nor tetraquark but their mixtures correspond to the observed physical states Z_b and Z_c. Therefore, the use here of the subscripts [10610], [10650], [3900] and [4020] only means that their quantum numbers correspond to the exotic mesons concerned.

Table 3. Flavor and spin parts of the wave functions for molecular states and tetraquark states; the subscripts [10610], [10650], [3900] and [4020] denote that those pure tetraquark states might be associated with $Z_b^+(10610)$, $Z_b^+(10650)$, $Z_c^+(3900)$ and $Z_c^+(4020)$ respectively.

state	flavor configuration	spin wave function
molecular	$\frac{1}{\sqrt{2}}(B^+\bar{B}^*-B^{*+}\bar{B})$	$\frac{1}{\sqrt{2}}(0_{b\bar{b}}\otimes 1_{u\bar{d}}+1_{b\bar{b}}\otimes 0_{u\bar{d}})$ [35]
tetraquark	$(bu)(\bar{b}\bar{d})_{[10610]}$	$\frac{1}{\sqrt{2}}(0_{bu}\otimes 1_{\bar{b}\bar{d}}-1_{bu}\otimes 0_{\bar{b}\bar{d}})$ [36]
molecular	$B^{*+}\bar{B}^*$	$\frac{1}{\sqrt{2}}(0_{b\bar{b}}\otimes 1_{u\bar{d}}-1_{b\bar{b}}\otimes 0_{u\bar{d}})$ [35]
tetraquark	$(bu)(\bar{b}\bar{d})_{[10650]}$	$1_{bu}\otimes 1_{\bar{b}\bar{d}}$ [36]
molecular	$\frac{1}{\sqrt{2}}(\bar{D}^*D^++D^{*+}\bar{D}^0)$ [6]	$1_{c\bar{c}}\otimes 1_{u\bar{d}}$ [37]
tetraquark	$(cu)(\bar{c}\bar{d})_{[3900]}$	$\frac{1}{\sqrt{2}}(0_{cu}\otimes 1_{\bar{c}\bar{d}}-1_{cu}\otimes 0_{\bar{c}\bar{d}})$ [38]
molecular	$D^{*+}\bar{D}^*$ [39]	$\frac{1}{\sqrt{2}}(0_{c\bar{c}}\otimes 1_{u\bar{d}}-1_{c\bar{c}}\otimes 0_{u\bar{d}})$
tetraquark	$(cu)(\bar{c}\bar{d})_{[4020]}$	$1_{cu}\otimes 1_{\bar{c}\bar{d}}$

3 Numerical results

As believed by theorists, the two clusters in an exotic state are bound by the QCD Van der Waals interaction. In fact, the interactions among the quarks belonging to different clusters reduce to an effective interaction between the two clusters. Following the Born-Oppenheimer approximation, we can write the binding energy between the two clusters (for molecule or tetraquark case) as a function of the distance of two heavy constituents, and the interactions among quarks(antiquarks) from the two clusters are taken as a perturbation. In this work, although we do not write up the effective interaction between the two clusters, we do assume it. We will derive an explicit form for the effective interaction in a future work. Using the wave function described above, we can calculate the binding energy with the Heitler-London method. The binding energy is

$$W_\alpha = \langle\psi_\alpha|H^\alpha_{\rm int}|\psi_\alpha\rangle, \qquad (26)$$

where $H^\alpha_{\rm int}$ (see Sec.2.1 for details) is a perturbative term for both the molecular structure and the tetraquark.

In this work, we take the meson-quark coupling constants g_{ch} and cut-off parameters Λ_χ from Ref. [20]. The masses of the light mesons are taken from the Particle Data Group (PDG) values [32], and the other parameters, such as b, c, h, α_0 etc, have been determined by fitting the heavy meson spectra (see Table 1). They are presented in Table 4.

3.1 Molecular structure

In this subsection, we discuss the case of molecular structure. In terms of the obtained wave functions and eigen-energies of the two constituent mesons, we estimate the expectation values shown in Eq. (26). The color, spin and flavor parts of Eq. (26) are shown in Table 2 and Table 3, and integration of the radial part is carried out numerically. The binding energy of molecular states $W_{\rm (mol)}$ versus the distance between Q and $\bar{Q}$ is drawn in Fig. 3. The plots indicate that there exist minima $E_{\rm (mol)}$ for all the states concerned. As we expect, in the Born-Oppenheimer approximation, a molecular state of the four-quark system possesses a minimum which corresponds to a stable structure. Then, the masses of the molecular states are $M_{\rm (mol)} = m_1+m_2+E_{\rm (mol)}$, where m_1 and m_2 are the masses of the constituent mesons, and are presented in Table 5.

Here we define R as the distance between Q and $\bar{Q}$. The minima are located at around $R\sim 1$ fm, and the $B^{(*)}$–$\bar{B}^{(*)}$, $D^{(*)}$–$\bar{D}^{(*)}$ structures can be considered as loosely bound states with binding energies of −3–−5 MeV.

3.2 Tetraquark structure

Now let us turn to discuss the tetraquark case. With the same procedure as for the molecular states, we obtain the dependence of the binding energies of tetraquark $W_{\rm (tetra)}$ on the distance between Q and $\bar{Q}$ with various values of the parameter ε. The results are shown in Fig. 4 and Fig. 5.

Interestingly, we find that there indeed exists a minimum $E_{\rm (tetra)}$ with respect to the distance between Q

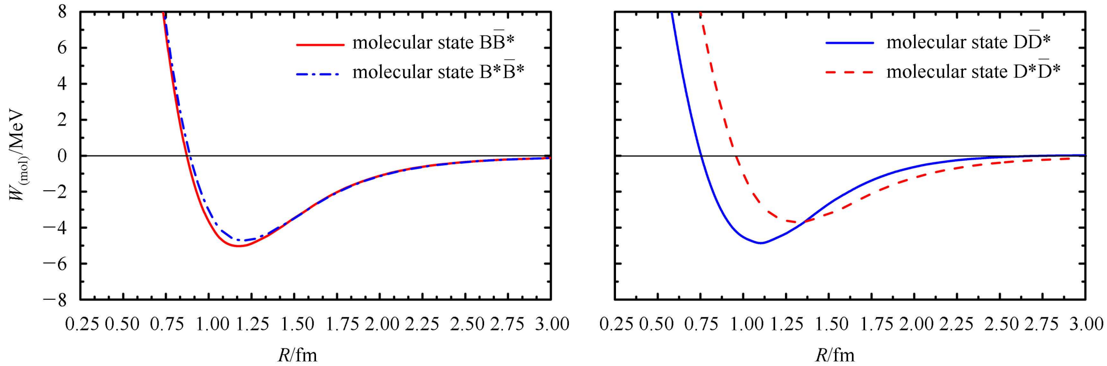

Fig. 3. (color online) The obtained binding energies for $B\bar{B}^*$, $B^*\bar{B}^*$, $D\bar{D}^*$ and $D^*\bar{D}^*$ molecular structures.

Table 4. Parameters of the model and masses of related mesons.

$m_{u(d)}$	m_b	m_c	μ_σ	μ_π	μ_η
0.313 GeV	4.80 GeV	1.40 GeV	490 MeV	139.57 MeV	547.862 MeV
μ_ρ	$g_{ch}^2/4\pi$	Λ_π	Λ_σ	Λ_η	Λ_0
775.26 MeV	0.54	4.2 fm^{-1}	4.2 fm^{-1}	5.2 fm^{-1}	0.113 fm^{-1}
μ_0	α_0	h	b	c	
36.976 MeV	2.118	0.79 GeV	0.148 GeV^2	−0.319 GeV	

Table 5. Binding energy minima ($E_{(\mathrm{mol})}$ (MeV)), distance R (fm) between $Q\bar{Q}$ and the calculated masses $M_{(\mathrm{mol})}$ (MeV) of $B\bar{B}^*$, $B^*\bar{B}^*$, $D\bar{D}^*$ and $D^*\bar{D}^*$ molecular structures.

$(\bar{b}u)(b\bar{d})_{B\bar{B}^*}$			$(\bar{b}u)(b\bar{d})_{B^*\bar{B}^*}$			$(\bar{c}u)(c\bar{d})_{D\bar{D}^*}$			$(\bar{c}u)(c\bar{d})_{D^*\bar{D}^*}$		
R	$E_{(\mathrm{mol})}$	$M_{(\mathrm{mol})}$	R	$E_{(\mathrm{mol})}$	$M_{(\mathrm{mol})}$	R	$E_{(\mathrm{mol})}$	$M_{(\mathrm{mol})}$	R	$E_{(\mathrm{mol})}$	$M_{(\mathrm{mol})}$
1.17	−5.034	10598.966	1.2	−4.717	10645.283	1.15	−4.909	3868.091	1.35	−3.705	4016.295

Table 6. Binding energy minima ($E_{(\mathrm{tetra})}$ (MeV)), distance R (fm) between $Q\bar{Q}$ and the calculated masses $M_{(\mathrm{tetra})}$ (MeV) of $(bu)(\bar{b}\bar{d})_{[10610]}$, $(bu)(\bar{b}\bar{d})_{[10650]}$, $(cu)(\bar{c}\bar{d})_{[3900]}$ and $(cu)(\bar{c}\bar{d})_{[4020]}$ tetraquark structures, with respect to the free parameter ε(fm) .

ε	$(bu)(\bar{b}\bar{d})_{[10610]}$			$(bu)(\bar{b}\bar{d})_{[10650]}$			$(cu)(\bar{c}\bar{d})_{[3900]}$			$(cu)(\bar{c}\bar{d})_{[4020]}$		
	R	$E_{(\mathrm{tetra})}$	$M_{(\mathrm{tetra})}$	R	$E_{(\mathrm{tetra})}$	$M_{(\mathrm{tetra})}$	R	$E_{(\mathrm{tetra})}$	$M_{(\mathrm{tetra})}$	R	$E_{(\mathrm{tetra})}$	$M_{(\mathrm{tetra})}$
0.02	0.79	−97.387	10601.613	0.79	−98.158	10611.842	0.79	−105.080	3857.92	0.79	−104.813	3895.187
0.03	0.82	−94.181	10604.819	0.82	−94.846	10615.154	0.82	−101.780	3861.22	0.82	101.533	3898.467
0.04	0.865	−90.99	10608.010	0.85	−91.510	10618.490	0.85	−98.495	3864.505	0.85	−98.241	3901.759
0.05				0.88	−88.136	10621.864	0.88	−95.146	3867.854	0.88	−94.916	3905.084
0.06				0.94	−84.735	10625.265	0.91	−91.753	3871.247	0.91	−91.552	3908.448
0.07				0.97	−81.380	10628.62	0.97	−88.335	3874.665	0.94	−88.157	3911.843
0.08				1.0	−78.010	10631.990	1.0	−84.925	3878.048	1.0	−84.767	3915.233
0.09				1.06	−74.661	10635.339	1.03	−81.562	3881.438	1.03	−81.408	3918.592
0.10				1.09	−71.421	10638.579	1.09	−78.180	3884.820	1.06	−78.052	3921.948
0.11				1.15	−68.289	10641.711	1.12	−74.911	3888.089	1.12	−74.760	3925.234
0.12				1.21	−65.296	10644.704	1.18	−71.717	3891.283	1.18	−71.555	3928.445
0.13				1.30	−62.463	10647.537	1.24	−68.646	3894.354	1.24	−68.468	3931.532
0.14				1.36	−59.826	10650.174	1.3	−65.720	3897.280	1.30	−65.530	3934.470
0.16										1.45	−60.138	3939.862
0.17										1.51	−57.705	3942.295

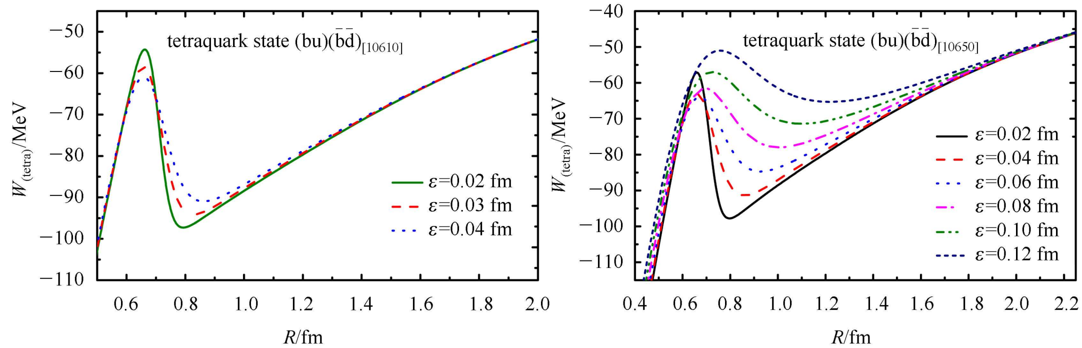

Fig. 4. (color online) Variation of the obtained binding energy for $(\mathrm{bu})(\bar{\mathrm{b}}\bar{\mathrm{d}})_{[10610]}$, $(\mathrm{bu})(\bar{\mathrm{b}}\bar{\mathrm{d}})_{[10650]}$ tetraquark structures, for values of ε from 0.02 to 0.12 fm.

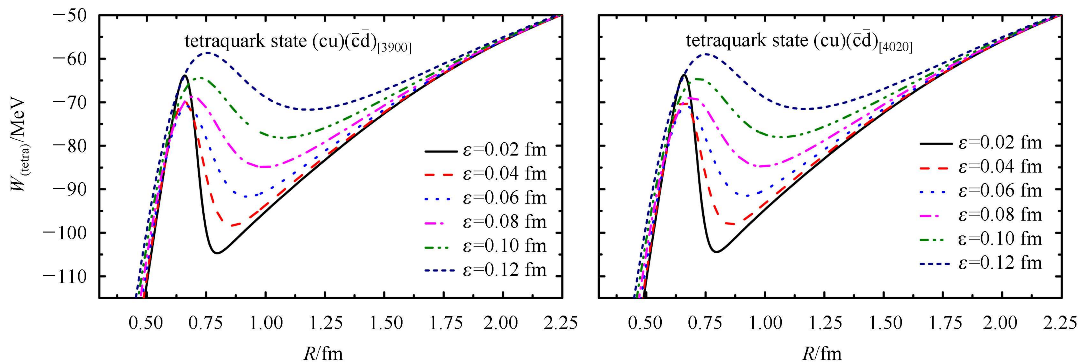

Fig. 5. (color online) Obtained binding energies for $(\mathrm{cu})(\bar{\mathrm{c}}\bar{\mathrm{d}})_{[3900]}$ and $(\mathrm{cu})(\bar{\mathrm{c}}\bar{\mathrm{d}})_{[4020]}$ tetraquark structures, for values of ε from 0.02 to 0.12 fm.

and $\bar{\mathrm{Q}}$, and the stable point corresponds to the distance at $R\approx0.79$–1.5 fm, which is comparable with that for molecular states, but is generally shorter. It seems reasonable. The masses of the tetraquark (defined as $M_{(\mathrm{tetra})}=m_{\mathrm{D1}}+m_{\mathrm{D2}}+E_{(\mathrm{tetra})}$), where m_{D1} and m_{D2} are the masses of the diquark and anti-diquark, are presented in Table 6.

4 Discussion and conclusion

As discussed in the introduction, many authors suggested that the newly observed four-quark states $\mathrm{Z_b}(10610)$, $\mathrm{Z_b}(10650)$, $\mathrm{Z_c}(3900)$, $\mathrm{Z_c}(4020)$ etc. are hadronic molecules, the reason being that their masses are close to the sums of some mesons B, B^*, D, D^*. However, for all of them the sum of the masses of the constituent mesons is smaller than the mass of the concerned exotic meson. By the potential model, the binding energy should be negative, and the calculated values of the binding energies shown in Table 5 confirm this allegation. Therefore, assuming them to be molecular states brings up an inconsistency. To solve this puzzle, there must be corresponding tetraquark states which mix with the molecular states to result in the observed physical hadrons.

The possible energy matrix is written as

$$H=\begin{pmatrix} M_{(\mathrm{mol})} & \Delta_{\mathrm{Q}} \\ \Delta_{\mathrm{Q}} & M_{(\mathrm{tetra})} \end{pmatrix}, \tag{27}$$

where $M_{(\mathrm{mol})}$ and $M_{(\mathrm{tetra})}$ are the masses of a pure molecular state and a tetraquark calculated in the theoretical framework, and the off-diagonal element Δ_{Q} whose subscript Q means that it may be flavor-dependent (b or c), and is a mixing parameter. Solving the secular equation:

$$\begin{vmatrix} M_{(\mathrm{mol})}-\lambda & \Delta_{\mathrm{Q}} \\ \Delta_{\mathrm{Q}} & M_{(\mathrm{tetra})}-\lambda \end{vmatrix}=0 \tag{28}$$

we obtain two eigenvalues

$$\lambda_{\pm}=\frac{M_{(\mathrm{mol})}+M_{(\mathrm{tetra})}\pm\sqrt{(M_{(\mathrm{mol})}-M_{(\mathrm{tetra})})^2+4\Delta_{\mathrm{Q}}^2}}{2}, \tag{29}$$

and $\lambda_{\pm}$ are the masses of physical states i.e. mixtures of molecular states and tetraquarks.

It is noted that $\lambda_{+}>\mathrm{Max}(M_{(\mathrm{mol})},\ M_{(\mathrm{tetra})})$ and $\lambda_{-}<\mathrm{Min}(M_{(\mathrm{mol})},\ M_{(\mathrm{tetra})})$. In our framework, the masses of both molecular states and tetraquark states are below those of the observed exotic mesons, so we expect that the λ_{+}'s correspond to the physical exotic states which are the experimentally observed $\mathrm{Z_b}(10610)$, $\mathrm{Z_b}(10650)$,

$Z_c(3900)$ and $Z_c(4020)$. If so, it is natural to predict the existence of partner exotic states whose masses are λ_-'s smaller than the observed states, as listed in Table 7.

In this scheme, we conclude that the tetraquark states must exist.

Our numerical results indicate that for both molecule and tetraquark states, the functions of the binding energies possess minima. For the case of molecular states, the minimum occurs at $R\sim 1$ fm (for Z_b and Z_c, see Table 5), whereas, for the tetraquark, R=0.79–1.5 fm depending on the parameter ε where R is the distance between Q and $\bar{Q}$. The situations for Z_b and Z_c are slightly different, but the tendency is roughly the same. It is also noted that the resultant R is flavor dependent, but no matter whether c or b, it falls within a reasonable range i.e. roughly $1/\Lambda_{QCD}$.

The following are a few observations on the results. First, from Fig. 4 and Fig. 5, one notices that the local minimum is a metastable one and for $R<0.6$ fm, the binding energy drops drastically. This may imply that there could be an anarchy state for a four-quark system. This is only a qualitative inference, though, and in that case the computed value for the binding energy would not be reliable because here the adopted picture is only valid for the diqark-anti-diquark structure rather than the anarchy state.

The main conclusion is that there are minima for both molecule and tetraquark structures, so both of them can exist, and a mixture would naturally be expected. The mixing between molecular structure and tetraquark is induced by exchanging quarks and anti-quarks which reside in different groups (Fig. 6). Such a mechanism has been discussed in the literature [40], and a more specific study can be found in Ref. [41, 42]. Because it is a non-perturbative QCD effect, however, in this work we do not directly calculate Δ_Q from an underlying principle or a concrete model. Instead, we fix it phenomenologically; for example, using the values given in Table 5, Table 6 and λ_+ of Eq. (29), we obtain Δ_Q=2–35 MeV.

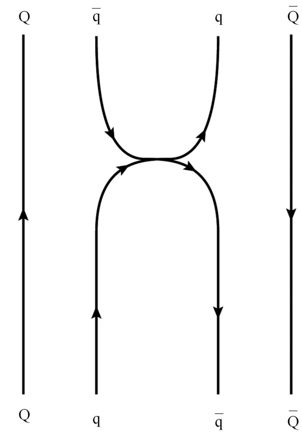

Fig. 6. Mixing mechanism.

With the provided model, we predict the positions of the partners of $Z_b(10510)$, $Z_b(10650)$, $Z_c(3900)$ and $Z_c(4020)(Z_c(4025))$ which weakly depend on the value of ε. Therefore, the key point to validate or negate our model is to look for the counter-partners of the observed exotic mesons. However, since the masses of the expected mesons are below the production thresholds of $B^{(*)}$-$\bar{B}^{(*)}$ or $D^{(*)}$-$\bar{D}^{(*)}$ (which can be realized in Z_b decays but not in Z_c's), one should look for them in the decay modes such as KKπ etc.

Table 7. The mixing parameter Δ_Q and the masses M' of the predicted counterparts of $Z_b(10610)$, $Z_b(10650)$, $Z_c(3900)$ and $Z_c(4020)$, with respect to the free parameter ε.

	$Z_b(10610)$		$Z_b(10650)$		$Z_c(3900)$		$Z_c(4020)$	
ε/fm	Δ_b/MeV	M'/MeV	Δ_b/MeV	M'/MeV	Δ_c/MeV	M'/MeV	Δ_c/MeV	M'/MeV
0.02	8.0	10592.2	18.10	10603.9	35.63	3827.01	29.04	3888.58
0.03	5.81	10595.4	17.36	10607.2	34.17	3830.31	28.67	3891.86
0.04	1.92	10598.6	16.58	10610.6	32.65	3833.60	28.29	3895.15
0.05			15.75	10613.9	31.03	3836.94	27.90	3898.48
0.06			14.87	10617.3	29.29	3840.34	27.49	3901.84
0.07			13.95	10620.7	27.43	3843.76	27.08	3905.24
0.08			12.96	10624.1	25.45	3847.14	26.67	3908.63
0.09			11.89	10627.4	23.30	3850.53	26.25	3911.99
0.10			10.76	10630.7	20.94	3853.91	25.82	3915.34
0.11			9.54	10633.8	18.36	3857.18	25.40	3918.63
0.12			8.20	10636.8	15.44	3860.37	24.98	3921.84
0.13			6.70	10639.6	11.98	3863.44	24.57	3924.93
0.14			4.89	10642.3	7.29	3866.37	24.17	3927.87
0.16							23.42	3933.26
0.17							23.07	3935.69

For a quantitatively reliable conclusion, more information (theoretical and especially experimental) is needed. Indeed, more accurate data are being accumulated, and we hope that further measurements will be carried out at BES, SuperBelle and LHCb, as well as the other proposed colliders.

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