Study on the structure of the four-quark states in terms of the Born-Oppenheimer approximation

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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 the approximation, Heitler and London calculated the spectrum of hydrogen molecule which includes two protons (heavy) and two electrons (light). Generally, the observed exotic mesons \( Z_0(10610), Z_0(10650) , Z_c(3900) \) and \( Z_c(4025) (Z_c(4020)) \) may be molecular states of two physical mesons and/or in diquark-anti-diquark structures. In analog to the Heitler-London method for calculating the mass of hydrogen molecule, we investigate whether there exist energy minima for these two structures. By contrary to the hydrogen molecule case where only the spin-triplet possesses an energy minimum, there exist minima for both of them. It implies that both molecule and tetraquark states can be stable objects. But since they have the same quantum numbers, the two states may mix to result in physical states. A consequence would be that one may expect to experimentally observe partner exotic states co-existing with \( Z_0(10610), Z_0(10650), Z_c(3900) \) and \( Z_c(4025) (Z_c(4020)) \).

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I. INTRODUCTION

The naive quark model suggests that a meson is made of a quark and anti-quark whereas a baryon consists of three quarks. The constituents in the hadrons are bound together by the QCD interaction to constitute a color singlet. But neither the quark model nor the QCD theory ever forbids existence of multi-quark states as long as they are color-singlets. The fact that by several years of hard work all experimental trials to observe pentaquarks failed, greatly discouraged theorists and experimentalists of high energy physics even though the idea about pentaquarks is really stimulating. One may ask if the nature indeed only favors economic textures of hadrons. The situation changes by the discovery of the exotic state \( Z_0(10610) \) and \( Z_0(10650) \)[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 \( Z_0 \) and \( Z_c \)-mesons contain hidden \( b\bar{b} \) and \( c\bar{c} \) respectively and both are charged, therefore they cannot be simply \( b\bar{b} \) or \( c\bar{c} \) bound states, but multi-quark states and are called as exotic states compared to the regular structures.

The inner structure of the multi-quark states may be more complicated than the regular mesons 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 to support such a structure is that the mass of the newly discovered meson \( Z_0(10610) \) is close to the sum of the masses of \( B \) and \( B^* \), while the mass of \( Z_c(3900) \) is also close to a sum of \( D \) and \( D^* \) masses. Instead, the study on the decay modes of such mesons seem to support the tetraquark structure [5][6]. To clarify the structures of those exotic states, one may need to investigate their all characteristics based on fundamental dynamics, instead of merely account their masses. Another observation may call our attention. The resonances \( Z_0(10610), Z_0(10650), Z_c(3900), Z_c(4020) \) and \( Z_c(4025) \) have been experimentally observed and confirmed as exotic four-quark states. Many authors [7][11] assumed them to be molecular states of \( B, B^*, D \) and \( D^* \) (and the corresponding anti-mesons) which are well experimentally measured. However there is a common point that the masses of the resultant exotic mesons are larger than the sum of their constituent mesons, Concretely, \( 10608.4 \pm 2.0 \) MeV (the mass of \( Z_0(10610) \)) is larger than sum of masses of \( B \) and \( B^* \) (10604.45 MeV); \( 10653.2 \pm 1.5 \) MeV (the mass of \( Z_0(10650) \)) is larger than sum of masses of \( B^* \) and \( B^* \) (10650.4 MeV); \( 3899 \pm 3.6 \pm 4.9 \) MeV (the mass of \( Z_c(3900) \) is larger than sum of \( D \) and \( D^* \) (3876.6 MeV); \( 4026.3 \pm 2.6 \pm 3.7 \) MeV (the mass of \( Z_c(4025) \) is larger than sum of \( D^* \) and \( D^* \) (4013.96 MeV).

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Generally, unless there exists a linearly increasing potential (such as the confinement potential for quarks) or a P-wave barrier (that is not our case), the binding energy of two constituent mesons which are caused by exchanging color-singlet hadrons must be negative. Therefore, one can conclude that either the observed exotic states are not molecular states or they are mixtures of molecular states and tetraquarks. That observation requires that both molecular state and tetraquark state should exist.

By the Born-Oppenheimer [12] approximation, the potential between atoms can be approximated as a function of the distance between two nuclei, by the scheme, Heitler and London [13] calculated the spectrum of 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. Their spin-component can be either symmetric or anti-symmetric, i.e. the two electrons are in spin triplet or singlet. Accordingly by the exchange symmetry the spatial wavefunction must also be anti-symmetric or symmetric. Taking those two anti-symmetrized wavefunctions as trial functions the expectation value of the total Hamiltonian as a function of the distance between the two protons is calculated. In this approximation, the interaction between two hydrogen atoms is treated as a perturbation. 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.

Comparing with the hydrogen molecule, $Z_0$ (or $Z_e$) is made of four quarks: $Q, \bar{Q}, u(\bar{u}), d(\bar{d})$, where $Q$ stands for $b$ or $c$ quark, since $Q, \bar{Q}$ are much heavier than the light flavors, so we can approximate them to be at rest. Thus it is natural that we can separate the four quarks into two groups. One possibility is that each group is in a color singlet, and it is the 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 $Q\bar{d}$ is in a color-triplet (or an anti-sexet), i.e. the di-pole-anti-di-pole structure. Since $u$ and $d$ are not identical particles, they do not need to be anti-symmetrized. The two trial wave functions in this case are the molecular state and the dipole-anti-dipole state. By the Born-Oppenheimer approximations, 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 state is much more difficult than for hydrogen molecule.

First we need to determine the wavefunctions of the color singlet of $Q\bar{d}(Qu)$ and the color-anti-triplet dipole $Qu(\bar{Q}d)$. Here we use the Cornell potential [14] 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 two groups is complicated, because not only the short-distance QCD interaction exists, but also the long-distance interaction which can be treated by exchanging color-singlet light mesons: $\pi, \sigma$ and $\rho$ etc. plays important roles. Here we do not involve the strange flavor. In analog to the hydrogen molecule, we calculate the spectrum of the ground state of the four quarks. Our strategy is similar to the Heitler-London approximation, namely we take the wavefunctions of the molecule and tetraquark states as two independent trial function and consider the interaction between two groups to calculate the spectra as functions of the distance between $b$ and $\bar{b}$ ($c$ and $\bar{c}$). Our goal is to see whether the molecule state or tetraquark state can possess an energy minimum with respect to the distance between $Q$ and $\bar{Q}$, by which one can judge if molecule or tetraquark can be physically allowed. If there exist minima for both cases, we would 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 would formulate the expressions for the energy spectrum along with some supplementary treatments, such as derivations of the effective potentials for the meson and diquark which are composed of a heavy quark and a light flavor in terms in the relativistic constituent models. We discuss the explicit color, spin structures of the molecule and tetraquark states and solving the Schrödinger-like equation to obtain the spatial wavefunctions in Sec. [11] In Sec. [111] we present our numerical results along with all input parameters. The last section is devoted to our discussion and conclusion.

II. DERIVATION OF THE CONCERNED FORMULAE

In this section, we derive the theoretical formulae for calculating the mass spectra and wavefunctions of molecular and tetraquark states. We first obtain the mass spectra and wavefunctions of the mesons $B, B^*$, $D$ and $D^*$ by solving the Schrödinger-like equations where the Cornell potential is adopted. We deduce the wavefunctions for scalar diquark in the same scheme. But it is noted, since diquark is not a physical state, we can only determine its wavefunction and mass up to a constant (the zero-point energy). We go on using the
Born-Oppenheimer approximation to evaluate the mass spectra of molecule and tetraquark which are functions of the distance between two heavy quarks \( Q \) and \( \bar{Q} \).

### A. Brief review of the potential model

Here for readers' convenience we briefly review some concerned contents of the theoretical framework and models which we are going to use in this work.

The basic brick for our study is the effective interactions between constituents inside the hadrons (for both regular mesons and four-quark states). Namely, in regular mesons or diquarks, the constituents are quarks and anti-quarks, instead, in the four quark states, the constituents are color-singlet-mesons (molecules) or colored diquarks (tetraquark).

Constituent quark models are based on the spontaneous breaking of the \( SU(3)_L \otimes SU(3)_R \) chiral symmetry of the QCD Lagrangian. The effective Lagrangian responsible for the constituent quarks is \(^{[15]}\)

\[
L_{\text{eff}} = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - g_s \bar{\psi}\psi \sigma \cdot \vec{F} \psi \cdot \vec{F} \psi + \frac{g_t^2}{2m} \bar{\psi}\sigma^{\mu\nu} \vec{F} \psi \cdot \partial_\nu \psi + \lambda^a \Delta L^a, \tag{1}
\]

where, \( D_\mu = \partial_\mu + ig A_\mu^a \) (\( \lambda^a \) is the Gell-Mann matrix for color \( SU_c(3) \), \( A_\mu^a \) is the gluon field); \( \vec{F} \) denotes the flavor \( SU_f(3) \) Gell-Mann matrix; \( \sigma \) denotes the scalar fields (\( \kappa_0, \kappa_0 \)); \( \vec{F} \) denotes the octet pseudoscalar fields (\( \pi, K, \eta_8 \)) and \( \vec{v}_\mu \) denotes the vector meson fields (\( \rho, K^*, \omega_8, \omega_0 \)); the term \( \lambda^a \Delta L^a \) stands for the confinement interaction (Fig. 1). \( g_s, g_p, g_v \) are the coupling constants of scalar, pseudoscalar and vector fields to fermions, respectively, and the constant \( g_t^2 \) is a tensor coupling responsible for the tensor interaction.

\begin{center}
\textbf{FIG. 1:} A Feynman diagram for QCD interaction which confines quarks inside hadrons.
\end{center}

To get the effective interactions between two constituents, one needs to include contributions of all the Feynman diagrams shown in Fig. 2 but of course it is impossible to include all the contributions, so that approximations must be taken. The constituent quark model was thoroughly studied by Glozman et al \(^{[16]}\) and Glantschnig et al \(^{[17]}\), and successful applications to phenomenology have been obtained, thus here we will employ it.

\begin{center}
\textbf{FIG. 2:} The Feynman diagrams of quark-antiquark interaction. (a) exchange of a pseudoscalar(p), scalar(s), vector(v) and gluon(g) between quark and antiquark (or quark-quark). (b) annihilation of quark-antiquark pair into pseudoscalar, scalar, vector and gluon in s-channel.
\end{center}
The general Hamiltonian of a four quark-system in the semi-relativistic framework takes the following form

$$H = \sum_{i=1}^{4} \sqrt{\mathbf{p}_i^2 + m_i^2} + \sum_{i<j=1}^{4} V(r_{ij})$$  \hspace{1cm} (2)$$

where the potential between quarks $i$ and $j$ has four pieces as

$$V(r_{ij}) = V^{oge}(r_{ij}) + V^{con}(r_{ij}) + V^{me}(r_{ij}) + V^{ann}(r_{ij}),$$  \hspace{1cm} (3)$$

and $r_{ij}$ is the distance between quarks (quark-antiquark). The one-gluon exchange(oge) term $V^{oge}(r_{ij})$, which plays the main role at short distance, is

$$V^{oge}(r_{ij}) = \frac{1}{4} \alpha_s \vec{X}_i \cdot \vec{X}_j \left( \frac{1}{r_{ij}} - \frac{1}{6m_im_jd^2} \vec{s}_i \cdot \vec{s}_j \frac{e^{-r_{ij}/d}}{r_{ij}} \right),$$  \hspace{1cm} (4)$$

and the confinement potential(con) $V^{con}(r_{ij})$ takes the form

$$V^{con}(r_{ij}) = \begin{cases} 
    br_{ij} + c & \text{if } i, j \text{ occur in the same cluster orbit,} \\
    -\frac{1}{4} \left( \vec{X}_i \cdot \vec{X}_j \right) \left\{ \frac{3b}{4m_im_jd^2} (1 - e^{-\mu_e r_{ij}}) + \frac{3}{4} c \right\} & \text{if } i, j \text{ occur in the different cluster orbit,}
\end{cases} \hspace{1cm} (5)$$

where $\vec{X}_i$ is the color operator, $\vec{s}_i$ is the spin operator acting on quark $i$, $\alpha_s$ is the QCD running coupling constant, $m_i$ is the constituent quark mass, $\mu_e$ is a parameter in the screened potential which is obtained by the lattice QCD calculations [19], and $b$, $c$, $d$ are the parameters obtained by fitting the heavy mesons spectra and are listed in Table. [19] In order to obtain a unified description of light and heavy mesons, the running QCD coupling constant which depends on $\mu^2$ is used [20]

$$\alpha_s(\mu^2) = \frac{\alpha_0}{\ln(\frac{\mu^2 + \mu_0^2}{\Lambda^2})},$$  \hspace{1cm} (6)$$

where $\mu = m_im_j/(m_i + m_j)$ is the reduced mass of the $q\bar{q}$ system and the free parameters $\Lambda_0 = 0.133 \text{ fm}^{-1}$, $\alpha_0 = 2.118$, $\mu_0 = 36.976 \text{ MeV}$.

In Eq. (3), $V^{me}(r_{ij})$ is the interaction induced by meson-exchange(me)(the hyperfine interaction) between constituent quarks which includes contributions of pseudoscalar($p$), vector($v$) and scalar($s$), so reads as

$$V^{me}(r_{ij}) = V^p(r_{ij}) + V^v(r_{ij}) + V^s(r_{ij})$$

$$= \sum_{a=1}^{3} [V_p(r_{ij}) + V_v(r_{ij})] \lambda^a_q \lambda^a_{\bar{q}} + \sum_{a=4}^{7} [V_K(r_{ij}) + V_{K^*}(r_{ij})] \lambda^a_q \lambda^a_{\bar{q}}$$

$$+ [V_\sigma(r_{ij}) + V_{\omega}(r_{ij})] \lambda^8_q \lambda^8_{\bar{q}} + \frac{2}{3} [V_{\rho'}(r_{ij}) + V_{\omega_8}(r_{ij})] + \frac{2}{3} V_\rho(r_{ij}),$$  \hspace{1cm} (7)$$

where $\lambda^a_q (a = 1, 2, \cdots, 8)$ are $SU(3)$ flavor matrices, and the explicit form of the interactions can be found in the attached Appendix.

In Eq. (3), $V^{ann}$ is the potential induced by annihilating quark-antiquark ($u, \bar{d}$) pair into a meson(see Fig. 2) which mediates interactions in s-channel. To the lowest order the quark-antiquark pair resides in an S-wave state, the contribution of $\sigma$-meson($J^{PC} = 0^{++}$) can be neglected [21]. The potential is written as

$$V^{ann,p}_{q\bar{q}}(r_{ij}) = \frac{g_p^2}{4m_q^2 - m_p^2} \left( \frac{3}{2} + \frac{1}{2} \vec{\lambda}_q \cdot \vec{\lambda}_{\bar{q}} \right) \left( \frac{1}{2} - \frac{1}{2} \vec{s}_q \cdot \vec{s}_{\bar{q}} \right) \left( \frac{3}{2} + \frac{1}{2} \vec{r}_q \cdot \vec{r}_{\bar{q}} \right),$$  \hspace{1cm} (8)$$

and

$$V^{ann,v}_{q\bar{q}}(r_{ij}) = -\frac{g_v^2}{4m_q^2 - m_v^2} \left( \frac{3}{2} + \frac{1}{2} \vec{\lambda}_q \cdot \vec{\lambda}_{\bar{q}} \right) \left( \frac{3}{2} + \frac{1}{2} \vec{s}_q \cdot \vec{s}_{\bar{q}} \right) \left( \frac{3}{2} + \frac{1}{2} \vec{r}_q \cdot \vec{r}_{\bar{q}} \right).$$  \hspace{1cm} (9)$$
In this work, we modify the terms in Eq. (9) by introducing a free parameter. The equations shown above contain a \( \delta \)-function, it is strictly valid only for point-like particles. The constituent quarks are not point-like, but a quasi-particle, surrounded by a cloud of sea quarks and have finite size, thus its position should be smeared out, to manifest the non-local effect, we introduce a non-local Gaussian smearing function \([24]\) with an additional parameter \(r_0\)

\[
\delta (\vec{r}) \rightarrow \frac{h^3}{\pi^{3/2}} e^{-h^2 (\vec{r} - r_0)^2}.
\]

(10)

\(h\) is suggested to be 1GeV which is just the chiral symmetry breaking scale.

Once the potential between \(qq\) is determined, the corresponding potential for \(q\bar{q}\) can be obtained from a \(G\)-parity transformation \([21]\). In an effective theory inspired by QCD, one may distinguish the interactions between light-light quark pair, light-heavy quark pair and heavy-heavy quark pair \([20]\):

\[
V_{q_i q_j} = \begin{cases} 
q_i q_j : u\bar{d} \Rightarrow V_{oge} + V_{con} + V_{me} + V_{ann,p} \\
q_i q_j : q\bar{Q}(\bar{Q}) \Rightarrow V_{oge} + V_{con}, (q : u, \bar{d}) \\
q_i q_j : Q\bar{Q} \Rightarrow V_{oge} + V_{con}.
\end{cases}
\]

(11)

It is noted that the employed framework is the SU(3) chiral model where the coupling between heavy quarks (\(c\) and \(b\)) and the SU(3) mesons does not exist.

### B. Wave functions of four-quark states

There are two distinct configurations for a four quarks system: the molecular state and the tetraquark (diquark-antidiquark) state (see Fig. 3). Considering all the degrees of freedom of constituent quarks, the total wave function is a direct product of radial, flavor, color, and spin parts

\[|\psi_\alpha\rangle = |\phi_\alpha\rangle \otimes |F_\alpha\rangle \otimes |C_\alpha\rangle \otimes |S_\alpha\rangle, \quad \alpha = 1, 2\]

(12)

where \(\alpha = 1\) stands for molecular state, and \(\alpha = 2\) is for tetraquark state. Unlike the hydrogen molecules, the involved quarks (antiquarks) are not identical, so the Pauli principle does not impose any restrictions on the compositions.

#### 1. Radial wave function

As only the ground state \((L = 0)\) is concerned, at the lowest order the total radial wave function should be a product of the two clusters’s wavefunctions as shown in Fig. 3

\[
\phi_1 = \phi_{u\bar{Q}} \otimes \phi_{\bar{d}Q}, \quad \phi_2 = \phi_{uQ} \otimes \phi_{\bar{d}\bar{Q}}.
\]

(13)

FIG. 3: The configurations of four-quark system(the left panel is the molecular state and the right one is the tetraquark state)

The radial wavefunction for each cluster is derived by solving the Schrödinger-like equation

\[
\left[ \sqrt{\vec{p}_Q^2 + m_Q^2} + \sqrt{\vec{p}_q^2 + m_q^2} + V(r) \right] \phi_\kappa = E\phi_\kappa, \quad \kappa = u\bar{Q}, \bar{d}Q, uQ, \bar{d}\bar{Q}.
\]

(14)
where the potential \( V(r) \) takes one-gluon exchange potential plus the confinement potential (see Eq.\(^{(4)}\) and Eq.\(^{(5)}\)), \( m_q \) and \( m_Q \) are the masses of light \((u,d)\) and heavy \(c,b\) quarks (or the antiquarks). The color matrix elements (the expectation values of the Casimir operator) for meson and diquark (or antidiquark) in \( V(r) \) are different, since the former is in color-singlet and the latter is in either triplet or sextet which will be discussed in details later. We solve the Schrödinger-like equation numerically in terms of the program offered by the authors of Ref.\(^{25}\), then we deduce the radial wavefunction \( u(r) \), defined as in

\[
\phi\left(\vec{r}\right) = u\left(l\right) r Y_{lm}\left(\hat{r}\right), \quad l = 0.
\]

In Fig. 4 the wavefunctions of \( B^{(*)} \) and \( D^{(*)} \) are shown. The eigenvalues are given in the Table. I as well as the constituent quarks masses as inputs.

### TABLE I: Masses of heavy mesons calculated by solving the Schrödinger-like equation with the one-gluon exchange and confinement potentials(Eq.(4)), and a comparison with experimental data \(^{26}\), as quarks masses being \( m_u(d) = 0.33\text{GeV}, m_b = 5.1\text{GeV}, m_c = 1.7\text{GeV} \).

| mesons | \( B \) | \( B^* \) | \( D \) | \( D^* \) |
|--------|--------|--------|--------|--------|
| Exp.(MeV) | 5279.25 ± 0.17 | 5325.2 ± 0.4 | 1869.62 ± 0.15 | 2006.98 ± 0.15 |
| This work(GeV) | 5.271 | 5.3255 | 1.869 | 2.007 |

![FIG. 4: The reduced wavefunction \( u(r) \) in the coordinate space. (a) the solid curve is for \( B \) and the dashed one is for \( B^* \). (b) the solid curve is for \( D \) and the dashed one is for \( D^* \).](attachment:figure4.png)

2. **Color 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 following:

\[
\begin{align*}
\vert \bar{3}_uQ \otimes \bar{3}_d\bar{Q} \rangle, & \quad \vert \bar{6}_uQ \otimes \bar{6}_d\bar{Q} \rangle, \\
\vert \bar{1}_u\bar{d} \otimes \bar{1}_Q\bar{\bar{Q}} \rangle, & \quad \vert \bar{8}_u\bar{d} \otimes \bar{8}_Q\bar{\bar{Q}} \rangle, \\
\vert \bar{1}_u\bar{Q} \otimes \bar{1}_d\bar{\bar{Q}} \rangle, & \quad \vert \bar{8}_u\bar{Q} \otimes \bar{8}_d\bar{\bar{Q}} \rangle,
\end{align*}
\] (15) (16) (17)

as the three orthonormal basis vectors. Here, the expression in Eq.\(^{(15)}\) is the so-called tetraquark state with a diquark-anti-diquark structure, whereas Eq.\(^{(16)}\) and Eq.\(^{(17)}\) are the molecular states with a meson-meson
structure, specially, the state \( |1_{uQ} \otimes 1_{Qd} \rangle \) (denoted as \( |C_1 \rangle \)) corresponding to the \( B^{(*)}B^{(*)} \) (or \( D^{(*)}D^{(*)} \)) which is the concern of this work.

The three basis vectors are related to each others through rearrangements \[27\]

\[
|1_{uQ} \otimes 1_{Qd} \rangle = \sqrt{\frac{1}{3}} |3_{uQ} \otimes 3_{dQ} \rangle + \sqrt{\frac{2}{3}} |6_{uQ} \otimes 6_{dQ} \rangle , \tag{18}
\]

\[
|8_{uQ} \otimes 8_{Qd} \rangle = -\sqrt{\frac{2}{3}} |3_{uQ} \otimes 3_{dQ} \rangle + \sqrt{\frac{1}{3}} |6_{uQ} \otimes 6_{dQ} \rangle , \tag{19}
\]

and

\[
|1_{ud} \otimes 1_{QQ} \rangle = -\sqrt{\frac{1}{3}} |3_{uQ} \otimes 3_{dQ} \rangle + \sqrt{\frac{2}{3}} |6_{uQ} \otimes 6_{dQ} \rangle , \tag{20}
\]

\[
|8_{ud} \otimes 8_{QQ} \rangle = \sqrt{\frac{2}{3}} |3_{uQ} \otimes 3_{dQ} \rangle + \sqrt{\frac{1}{3}} |6_{uQ} \otimes 6_{dQ} \rangle . \tag{21}
\]

The color matrix elements which we need in Sec. [III][4] have been summarized in Table. [III]

| \( \hat{O} \) | \( \lambda_u \cdot \lambda_Q \) | \( \lambda_Q \cdot \lambda_d \) | \( \lambda_u \cdot \lambda_d \) | \( \lambda_Q \cdot \lambda_Q \) |
|----------------|----------------|----------------|----------------|----------------|
| \( < 3_{uQ}3_{dQ} | \hat{O} | 3_{uQ}3_{dQ} > \) | -8/3 | -8/3 | -4/3 | -4/3 | -4/3 |
| \( < 6_{uQ}6_{Qd} | \hat{O} | 6_{uQ}6_{Qd} > \) | 4/3 | 4/3 | -10/3 | -10/3 | -10/3 |
| \( < 3_{uQ}3_{dQ} | \hat{O} | 6_{uQ}6_{Qd} > \) | 0 | 0 | -2\sqrt{2} | -2\sqrt{2} | 2\sqrt{2} |

3. Spin and flavor wave function

The flavor and spin parts of \( Z_0(10610) \), \( Z_b(10650) \), \( Z_c(3900) \), \( Z_c(4025) \) are listed in Table. [III] along with their quantum numbers \( I^G(J^P) \). Note that isospin of heavy quarks \( (b, c) \) is zero, so the isospin of the hadron is contributed by only the light quarks \( u(\bar{u}) \) and \( d(\bar{d}) \).

For instance, in Table. [III] \( Z_b(10610) \) is written as \( \frac{1}{\sqrt{2}} (B^+ \bar{B}^- - B^{*-} \bar{B}) \) which is the flavor part of the molecular state (then denoted as \( |F_1 \rangle \)), while \( [bu][\bar{b}d] \) is for the tetraquark state (denoted as \( |F_2 \rangle \)). Along with the flavor wave functions, the corresponding spin wave functions \( \frac{1}{\sqrt{2}} (0_{\bar{b}d} \otimes 1_{ud} + 1_{\bar{b}d} \otimes 0_{ud}) \) \[29\] (denoted as \( |S_1 \rangle \)) and \( \frac{1}{\sqrt{2}} (0_{bu} \otimes 1_{\bar{b}d} - 1_{bu} \otimes 0_{\bar{b}d}) \) \[30\] (denoted as \( |S_2 \rangle \)) are presented. And the same information for other four-quark states \( (Z_b(10650), Z_c(3900), Z_c(4025)) \) is also listed in the table.

We close this section by presenting the spin matrix elements in the following equation

\[
\langle S_{ij} | \vec{\sigma}_i \cdot \vec{\sigma}_j | S'_{ij} \rangle = 2S_{ij}(S_{ij} + 1) - 3|\delta_{S_{ij},S'_{ij}}| \tag{22}
\]

It is particularly noted that even though with all the inputs and the given effective Hamiltonian, one still cannot obtain the eigen-energies of the constituent mesons or diquarks because there may exist a zero-point energy which emerges from the QCD vacuum and cannot be properly accounted. In the potential model, generally, one should determine the zero-point energy for mesons by fitting the well measured data. Thus in the typical computations of the spectra of a class of mesons, one can accurately calculate the gaps among different resonances, but the absolute value of the ground state must be fixed by data, for example to determine the mass of \( J/\psi \), one needs to introduce the zero-point energy, but once it is set, the masses of \( \psi' \) and other higher resonances would be obtained. Here, we can fix the zero-point energies for \( B, B^*, D \) and \( D^* \) by fitting data. By contrast, we cannot determine the zero-point energies for the diquarks because they are not physical states and no data are available. So even though we obtain their wave functions by solving the Schrödinger-like equation, we still cannot determine the spectra of diquarks. However, it does not prohibit us to investigate their qualitative behaviors. We will discuss this issue in the last section.
and \( b_d \) diquark-antidiquark) can be written as a function of distance between interacting constituents are in different groups. The explicit forms are presented in Eq.(11).

In molecular states, since the constituent mesons are in color singlet, the quarks (antiquarks) in one group (a \( c_u \) and \( \bar{c}_d \), respectively, where the superscript denotes the concerned constituent quark (antiquark) is in meson-1 or meson-2). The perturbative Hamiltonian \( H' \) is the effective interaction between a quark in meson-1 and another quark (antiquark) in meson-2 of the molecular state which is a sum of a few independent pieces

\[
H'_1 = V_{ud} + V_{Qu} + V_{Qd} + V_{QQ},
\]

the terms \( V_{ud}, V_{Qu}, V_{Qd}, \) and \( V_{QQ} \) are the interactions between \( u^1 \) and \( \bar{d}^2; Q^1 \) and \( u^2; \bar{Q}^1 \) and \( \bar{d}^2; Q^1 \) and \( \bar{Q}^2 \), respectively, where the superscript denotes the concerned constituent quark (antiquark) is in meson-1 or meson-2. In later expressions, we do not label the superscripts anymore, but it is understood that the two interacting constituents are in different groups. The explicit forms are presented in Eq.(11).

In molecular states, since the constituent mesons are in color singlet, the quarks (antiquarks) in one group (a meson) cannot interact with the quarks in another group via exchanging a single gluon, thus the perturbative interaction between \( B^{(*)} B^{(*)} \) (or \( D^{(*)} D^{(*)} \)) only comes from the meson-exchange between \( ud \). In the chiral SU(3) framework, the interactions \( V_{Qu}, V_{Qd}, \) and \( V_{QQ} \) do not exist.

### C. Obtaining the binding energies for the four-quark states

By the Born-Oppenheimer approximation, the binding energy between the two groups (two molecules or diquark-antidiquark) can be written as a function of distance between \( b(c) \) and \( \bar{b}(ar{c}) \) quarks and interactions between the two groups are taken as a perturbation. Using the wave function described above, we can calculate the binding energy between the two groups with the Heitler-London method. Since the interactions between the constituents (quark, antiquark) in different groups are treated as perturbations, one just needs to calculate the binding energy of the four-quark states which include two separate groups in terms of the common perturbation method, it is the expectation

\[
W_\alpha = \langle \psi | H'_\alpha | \psi \rangle, \quad \alpha = 1, 2,
\]

where \( H'_\alpha \) is a perturbative term for the molecular or tetraquark structure.

#### 1. Molecular structure

For the case of the 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.(23). The perturbative Hamiltonian \( H'_1 \) is the effective interaction between a quark in meson-1 and another quark (antiquark) in meson-2 of the molecular state which is a sum of a few independent pieces

\[
H'_1 = V_{ud} + V_{Qu} + V_{Qd} + V_{QQ},
\]

the terms \( V_{ud}, V_{Qu}, V_{Qd}, \) and \( V_{QQ} \) are the interactions between \( u^1 \) and \( \bar{d}^2; Q^1 \) and \( u^2; \bar{Q}^1 \) and \( \bar{d}^2; Q^1 \) and \( \bar{Q}^2 \), respectively, where the superscript denotes the concerned constituent quark (antiquark) is in meson-1 or meson-2. In later expressions, we do not label the superscripts anymore, but it is understood that the two interacting constituents are in different groups. The explicit forms are presented in Eq.(11).

In molecular states, since the constituent mesons are in color singlet, the quarks (antiquarks) in one group (a meson) cannot interact with the quarks in another group via exchanging a single gluon, thus the perturbative interaction between \( B^{(*)} B^{(*)} \) (or \( D^{(*)} D^{(*)} \)) only comes from the meson-exchange between \( ud \). In the chiral SU(3) framework, the interactions \( V_{Qu}, V_{Qd}, \) and \( V_{QQ} \) do not exist.

#### 2. Tetraquark structure

Now let us turn to discuss the case of tetraquark. The perturbative Hamiltonian \( H'_2 \) between \( q \) in the diquark and \( \bar{q} \) in the anti-diquark is also a sum of a few pieces which are different however from those in Eq.(24)

\[
H'_2 = V_{ud} + V_{Qu} + V_{Qd} + V_{QQ},
\]
the terms $V_{ud}, V_{Qd}, V_{uQ}$, and $V_{QQ}$ are the interactions between constituents $u$ and $d$; $Q$ and $\bar{d}$; $u$ and $\bar{Q}$; $Q$ and $\bar{Q}$, respectively. All the four $V$’s contain contributions of one gluon-exchange and confinement interactions, while $V_{ud}$ contains also contribution from the meson-exchange interaction (i.e. the long-distance interaction). Here by a phenomenological consideration, we use the screened confinement potential between quark pairs in different clusters rather than the linear confinement for the quark pairs in the same cluster [19].

Generally, the color wave function of a tetraquark can be written as a linear combination

$$|C_0\rangle = \cos \theta |\bar{3}_{uQ} \otimes 3_{d\bar{Q}}\rangle + \sin \theta |6_{uQ} \otimes \bar{6}_{d\bar{Q}}\rangle,$$

(26)

with a proper normalization for the color wave function.

The diquark-antidiquark structure can be a composition of $6 \otimes \bar{6}$ and $3 \otimes \bar{3}$ components. The effects of the different color configurations on the tetraquark binding energy have been studied by Vijaide et al [31], they observed that for the bound-states of color-singlet, the fraction of $|6_{uQ} \otimes \bar{6}_{d\bar{Q}}\rangle$ is almost negligible, but it increases as the heavy quark mass decreases. By contrast, to guarantee the tetraquark as a stable structure, the role of $|6_{uQ} \otimes \bar{6}_{d\bar{Q}}\rangle$ is indispensible even though $|\bar{3}_{uQ} \otimes 3_{d\bar{Q}}\rangle$ is still dominant. That is because the $6 \otimes \bar{6}$ configuration causes a repulsion between the dipole and antidipole, while the $3 \otimes \bar{3}$ configuration makes an attraction, the competition of the two opposite effects results in a minimum which corresponds to the stable point. We take $\cos \theta = 0.93$ for the numerical computation of this work.

### III. NUMERICAL RESULTS

In this work, we take the meson-quark coupling constants $g_p$, $g_v$, $g_s$, $g_t$ and cut-off parameters $\Lambda_{\pi}$ (see the Appendix for details) from Ref. [35] which are presented in Table. [IV].

| $\mu_{\pi}$ | $\mu_{\rho}$ | $\mu_{\omega}$ | $\mu_{\omega'}$ |
|------------|-------------|--------------|-------------|
| 0.5 GeV    | 0.139 GeV   | 0.547 GeV    | 0.958 GeV   |
| $\mu_{\omega}$ | $g_p^2/4\pi$ | $g_v^2/4\pi$ | $(g_v^2/4\pi)\sqrt{(g_v^2+g_s^2)/4\pi}$ |
| 0.947 GeV | 0.67 | 0.67 | 0.55 | 1.107 | 1.31 |
| $(g_v^2+g_s^2)/4\pi$ | $\Lambda_{\pi}$ | $\Lambda_{\rho}$ | $\Lambda_{\omega}$ | $\Lambda_{\omega'}$ |
| 1.25 | 3.55 fm$^{-1}$ | 6.08 fm$^{-1}$ | 4.4 fm$^{-1}$ | 6.03 fm$^{-1}$ | 8.53 fm$^{-1}$ |
| $\Lambda_{\omega}$ | $\Lambda_{\omega}$ | b | c | d | $\mu_{c}$ |
| 6.68 fm$^{-1}$ | 7.16 fm$^{-1}$ | 0.101 GeV$^2$ | -0.312 GeV | 1.29 GeV$^{-1}$ | 1.1 fm$^{-1}$ |

### A. Molecular structure

In this subsection, we discuss the case of the molecular structure. With the color, spin and flavor parts of Eq.(23) are shown calculated in Table. [IV], Table. [II], and Eq.(22), and the integral of the radial part is computed numerically. The binding energy of molecular states $W_1$ versus the distance between $Q$ and $\bar{Q}$ with various values of $r_0$ is drawn in Fig. [4] and Fig. [5].

Since $r_0$ is a phenomenological parameter describing the spreading of the constituent quark, its value cannot be reliably fixed from our underlying theory. A reasonable estimate that its magnitude should be within a range of 0~0.2 fm which is about $1/\Lambda_{\text{chiral}}$, where $\Lambda_{\text{chiral}}$ is the chiral symmetry breaking scale of about 1 GeV, therefore, in this work, we adopt $r_0$ to be in the range of 0~0.15 fm. In the figures, we show the dependence of the resultant binding energy on the distance between $Q$ and $\bar{Q}$ with various values of $r_0$.

The figures indicate that there exist minima whose positions depend on $r_0$. 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. Here we define $R$ as the distance between $Q$ and $\bar{Q}$. In the case of $Z_b$, the $R$ is
about 1.2~1.8 fm, while for the $c$ system $Z_c$ the minima are located within a range of 1.45~2.05 fm, slightly larger than that for $Z_b$.

![Graphs showing the variation of binding energy for $Z_b(10610)$ and $Z_b(10650)$](I)

FIG. 5: The variation of the obtained binding energy for $Z_b(10610)$, $Z_b(10650)$ as molecular states with respect to various values of $r_0$. Here, the values of $r_0$ are taken as 0, 0.05, 0.10, 0.15 fm.

![Graphs showing the variation of binding energy for $Z_c(3900)$ and $Z_c(4025)$](III)

FIG. 6: The variation of the obtained binding energy for $Z_c(3900)$, $Z_c(4025)$ as molecular states. Here, the values of $r_0$ are taken as 0, 0.05, 0.10, 0.15 fm.

B. Tetraquark structure

Now let us turn to the case of tetraquark. With the same procedure as for the molecular states, we obtain dependence of the binding energies of tetraquark $W_2$ on the distance between $Q$ and $\bar{Q}$ with various values of parameter $r_0$. The results are shown in Fig. 7 and Fig. 8. It is noted that the total mass of the tetraquark is $m_{D1} + m_{D2} + W_2 + \Delta E$ where $m_{D1}$ and $m_{D2}$ are the masses of the two diquarks and $\Delta E$ is the possible undetermined zero-point energy.
It is interesting, we find that there are indeed existing minima with respect to the distance between $Q$ and $\bar{Q}$, but the stable point corresponds to the distance at $R \approx 0.7 \sim 1.2$ fm which is shorter than that for the molecular states. It seems reasonable.

**IV. CONCLUSION AND DISCUSSION**

As discussed in the introduction, many authors suggested that the newly observed four-quark states $Z_b(10610)$, $Z_b(10650)$, $Z_c(3900)$, $Z_c(4020)$ etc. are hadronic molecules, the reason is that their masses are close to the sum 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. V confirm the
allegation. Therefore, assuming them to be molecular states bring up an inconsistency. The solution is simple
that there must be corresponding tetraquark states which mix with the molecular states.

The possible energy matrix can be written as

\[
H = \begin{pmatrix}
E_1 & \Delta_Q \\
\Delta_Q & E_2
\end{pmatrix},
\]

(27)

where \(E_1\) and \(E_2\) are the masses of pure molecular state and tetraquark calculated in the theoretical framework,
\(\Delta_Q\) whose subscript \(Q\) means that it may be flavor-dependent (\(b\) or \(c\)), is a mixing parameter which so far we
do not know how to evaluate yet. Solving the secular equation:

\[
\begin{vmatrix}
E_1 - \lambda & \Delta_Q \\
\Delta_Q & E_2 - \lambda
\end{vmatrix} = 0
\]

(28)

we obtain two eigenvalues

\[
\lambda_{1,2} = \frac{E_1 + E_2 \pm \sqrt{(E_1 - E_2)^2 + 4\Delta_Q^2}}{2},
\]

(29)

and \(\lambda_{1,2}\) are the masses of physical states i.e. mixtures of molecular states and tetraquarks. Let us make a
rough estimate. Supposing that the molecular state and tetraquark are degenerate (or \(E_1 \approx E_2 = M\) are
close to each other), then \(\lambda_1 = M + \Delta_Q\), and \(\lambda_2 = M - \Delta_Q\), thus \(\lambda_1 > M\) and \(\lambda_2 < M\). We expect that \(\lambda_1\)
corresponds to the observed exotic states. Indeed it is the case of maximal mixing, i.e.

\[
|Z_{phys}| = (|Z_{mol}| + |Z_{tet}|) / \sqrt{2},
\]

where \(|Z_{phys}|\), \(|Z_{mol}|\) and \(|Z_{tet}|\) are the physical, molecular and tetraquark states respectively. In practice the
mixture may deviate from the maximal mixing.

If so, we may predict existence of some partner exotic states whose masses are smaller than the observed
states by \(2\Delta_Q\) or so (not accurately).

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

By the Born-Oppenheimer model, we calculate the masses of the molecular states which are made of
\(B, B^*, D, D^*\) respectively. The effective potential based on the chiral Lagrangian is adopted. Here the
constituent mesons are physical states, so that we can determine the relevant parameters by fitting data. To
calculate the binding energies of the molecular states we need the wavefunctions of the constituent mesons,
thus with several input parameters, by solving the Schrödinger-like equation, we derive them, then eventually
we find the binding energies \(W_1\), and \(E_1 = m_1 + m_2 + W_1\) where \(m_1\) and \(m_2\) are the masses of the constituent
mesons.

Coming to the tetraquark case, the situation is more complicated. The constituents in different groups
exchange single gluon and are also interacting with the non-perturbative QCD part which manifests in the
confinement piece of the Cornell potential. But since the interacting quark and antiquark (light and heavy) are
separated in two groups, we adopt a screened potential form. The interaction between two groups is taken as
a perturbation and repeat what we did for the molecular states, we also obtain the dependence of the binding
energy on the distance between \(Q\) and \(\bar{Q}\). Indeed, the total mass of the tetraquark is determined up to a
zero-point energy for the diquark or antidiquark.

Our numerical results indicate that for both molecular state and tetraquark, the functions of the binding
energies possess minima. For the case of the molecular state, the minimum occurs at \(R=1.25\sim 2.05\) fm (for \(Z_b\)
and \(Z_c\), see Table. \(\checkmark\) depending on the parameter \(r_0\) whereas, for the tetraquark, \(R=0.7\sim 1.15\) fm where \(R\)
is the distance between \(Q\) and \(\bar{Q}\). The situations for \(Z_b\) and \(Z_c\) are slightly different, but roughly the tendency
is the same. It is also noted that the distance \(R\) is flavor dependent, but no matter for \(c\) or \(b\), it falls within a
reasonable range.

The important conclusion is that there are minima for both molecular states and tetraquark, so that both of
them can exist, a natural mixture would be expected. Unfortunately, so far, we do not have an appropriate way
to calculate \(\Delta_Q\) yet, but if we assume that the molecular state and tetraquark are almost degenerate, setting
\(M + \Delta_Q = M^{exp}\) where \(M^{exp}\) is the experimentally measured mass of the four-quark state, we can determine the
value of \(\Delta_Q\), for example, using the values given in Table. \(\checkmark\), roughly, \(\Delta_Q = 2.70 \sim 23.88\) MeV. Definitely,
that value is obtained based on the degeneracy assumption, which is by no means reliable but we can expect
that the order of magnitude of the mixing parameter is plausible. If the picture is right, we expect partners of $Z_b(10510)$, $Z_b(10650)$, $Z_c(3900)$ and $Z_c(4025)$ (or $Z_c(4020)$) to be at the ranges which are smaller than the observed masses of those exotic states within a range around the value of about 2$\Delta Q$.

Since there are still a few parameters such as $r_0$, the zero-point energy of the diquark etc. which cannot be fixed by the available theory and experimental measurements yet, our results are only qualitatively reliable. To require quantitatively reliable conclusion, more information (theoretical and especially experimental) is needed. However, so far, the presently available data are not accurate enough to make our theoretical effort to go further, we hope that more measurements will be carried out at BES, SuperBelle and LHCb soon.

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**APPENDIX**

The explicit expressions of the Goldstone-boson-exchange potentials from Ref. [17]. By using a monopole-type form factor for the constituent quark-meson vertex [36]

$$F(q^2) = \frac{\Lambda_\gamma^2 - \mu_\gamma^2}{\Lambda_\gamma^2 + q^2},$$

(30)

where $\mu_\gamma$ represents meson masses, and $\Lambda_\gamma$ determines the chiral symmetry-breaking scale which have to be taken differently for different mesons [37].

Then one can get the spatial dependence meson-exchange potentials as follow. The pseudoscalar meson-exchange interaction produces spin-spin force, the corresponding potential is

$$V_\gamma(r_{ij}) = \frac{g_{\rho,\gamma}^2}{4\pi} \frac{1}{12m_im_j} (\vec{\sigma}_i \cdot \vec{\sigma}_j) \left[ \mu_\gamma^2 \exp(-\mu_\gamma r_{ij}) - \left( \mu_\gamma^2 + \frac{\Lambda_\gamma^2 - \mu_\gamma^2}{2} r_{ij} \right) \exp(-\Lambda_\gamma r_{ij}) \right],$$

(31)

with $\gamma = \pi, K, \eta, \eta'$. And $g_{\rho}$ can be derived phenomenologically from the pion-nucleon coupling constant [37].

The vector meson-exchange interaction produces central and spin-spin forces, the potentials are

$$V_\gamma(r_{ij}) = V_\gamma^c(r_{ij}) + V_\gamma^{ss}(r_{ij}) \quad \gamma = \rho, K^*, \omega_8, \omega_0,$$

(32)

with

$$V_\gamma^c(r_{ij}) = \frac{(g_{\nu,\gamma})^2}{4\pi} \left[ \exp(-\mu_\gamma r_{ij}) \right] - \left( 1 + \frac{\Lambda_\gamma^2 - \mu_\gamma^2}{2\Lambda_\gamma} \right) \exp(-\Lambda_\gamma r_{ij}),$$

(33)
and
\[
V_{\sigma}^{ss}(r_{ij}) = 2 \left( g_{v,\gamma} + g_{t,\gamma} \right)^2 \frac{1}{4\pi} \frac{1}{12m_im_j} (\vec{\sigma}_i \cdot \vec{\sigma}_j) \left[ \mu_\gamma^2 \frac{\exp(-\mu_\gamma r_{ij})}{r_{ij}} - \left( \mu_\gamma^2 + \frac{\Lambda_\gamma^2}{2} r_{ij} \right) \exp\left(-\frac{\Lambda_\gamma^2}{2} r_{ij} \right) \right],
\]

(34)

The scalar meson-exchange interaction produces central force
\[
V_{\sigma}(r_{ij}) = - \frac{g_\sigma^2}{4\pi} \frac{\exp(-\mu_\sigma r_{ij})}{r_{ij}} - \left( 1 + \frac{\Lambda_\sigma^2}{2\Lambda_\sigma} r_{ij} \right) \frac{\exp(-\Lambda_\sigma r_{ij})}{r_{ij}},
\]

(35)

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