Possible hadronic molecular states composed of $S$-wave heavy-light mesons

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(Dated: December 15, 2021)

We perform a systematic study of possible molecular states composed of the $S$ wave heavy-light mesons, where the $S - D$ mixing and $η - η'$ mixing are explicitly included. Our calculation indicates that the observed $X(3872)$ could be a loosely shallow molecular state composed of $DD^*$ $h.c.$, while neither $Z_c(3900)/Z_c(4020)$ nor $Z_b(10610)/Z_b(10650)$ is supported to be a molecule. Some observed possible molecular states are predicted, which could be searched for by further experimental measurements.

PACS numbers: 12.20.Ds, 11.15.Tk, 14.20.-c,11.27.+d

I. INTRODUCTION

In the past decade, a number of new hadron states, named $XYZ$ particles, have been observed experimentally [1]. Among these newly observed states, some of them are close to the thresholds of a pair of hadrons, which indicates these kind of new states could be good candidates for hadronic molecular states. A typical example of the new hadron states, $X(3872)$, was first observed by the Belle Collaboration in the $π^+π^- J/ψ$ invariant mass of the $B^+ → KX(3972) → K(π^+π^- J/ψ)$ process in 2003 [2]. Later, this state was successfully confirmed by Belle itself [3–6] and by the Babar \cite{7–13}, CDF \cite{14–17}, D0 \cite{18}, LHCb \cite{19–22} and BESIII \cite{23} Collaborations in the $π^+π^- J/ψ$, $D^0D_s^0π$, $D^*0D_s^0$, $γ J/ψ$ and $γψ(2S)$ processes. The $J^{PC}$ quantum numbers of the $X(3872)$ have been confirmed as $1^{++}$ and the PDG average of the mass and width are $3871.69 ± 0.17$ and $< 1.2$ MeV, respectively. The observed mass of the $X(3872)$ is just sandwiched by the thresholds of the $D^0D_s^0$ and $D^{*+}D_{s^-}$. The absence of the charge partner of the $X(3872)$ indicates that this state is an isospin singlet [24].

A very similar charmonium-like state to the $X(3872)$, the $Z_c(3900)$, was first reported by the BESIII and Belle Collaborations in the $π^+π^- J/ψ$ invariant mass spectrum of the $e^+e^- → π^+π^- J/ψ$ at a center-of-mass energy of $4.260$ GeV [25, 26]. Later, this state was confirmed at the same process but at $\sqrt{s} = 4.17$ GeV by the CLEO Collaboration [27]. The open charm decay channel $Z_c(3900) → D^*D$ was reported by the BESIII Collaboration in 2014 [28]. Recently, the neutral partner of the $Z_c(3900)$ has been observed in the $π^0 J/ψ$ and $(DD^*)^0$ invariant mass spectra by the CLEO \cite{27} and BESIII Collaborations \cite{29,30}. As an isospin triplet, the mass of the $Z_c(3900)$ is very close to the threshold of the $DD^*$. As a partner of the $Z_c(3900)$, $Z_c(4020)$ is very close to the threshold of the $D^*D^*$, which was first observed in the $π^0 h_c$ invariant mass spectrum by the BESIII Collaboration \cite{31,32} then confirmed in the $D^*D^*$ invariant mass spectrum \cite{33,34}.

All three states, $X(3872)$, $Z_c(3900)$ and $Z_c(4020)$, are close to the thresholds of a pair of charmed mesons and were first observed in hidden charm processes. States near the $D^{(*)+}D_{s^-}$ thresholds should be more easily discovered in the hidden charm process with a light meson containing $s\bar{s}$ quark components, due to the simple quark rearrangement. A series of charmonium-like states have recently been observed in the $J/ψ\phi$ invariant mass spectrum of the $B → KJ/ψ\phi$ process, the $Υ(4140)$, $Υ(4274), X(4320)$ and $X(4350)$ \cite{35–40}. Among these states, the $Υ(4140)$ is about 80 MeV below the threshold of the $D^{*+}D_{s^-}$. Here, one should notice that the thresholds of the $D^{*+}D_{s^-}$ and $D^{*+}D_{s^-}$ are below that of the $J/ψ\phi$, thus, one cannot observe the states near the $D^{*+}D_{s^-}$ and $D^{*+}D_{s^-}$ thresholds in the $J/ψ\phi$ invariant mass spectrum.

In the bottom sector, $Z_b(10610)$ and $Z_b(10650)$ were first reported in the $Υ(nS)π^\pm$, $\{n = 1, 2, 3\}$ and $h_b(mP)π^\pm$ $\{m = 1, 2\}$ invariant mass spectra of the $e^+e^- → Υ(nS)π^+π^−$ and $e^+e^- → h_b(mP)π^+π^-\gamma$ process at a center-of-mass energy of $10.860$ GeV by the Belle Collaboration in 2011 \cite{41,42}. The open bottom channels of the $Z_b(10610)$ and $Z_b(10650)$ were observed by Belle in 2012 \cite{43,44}. The neutral partners of the $Z_b(10610)$ and $Z_b(10650)$ were observed in the hidden bottom channel in 2013 \cite{45}. More recently, the signals of these two bottom-like states have also been discovered in the $e^+e^- → h_b(mP)π^+π^−\gamma$ at a center-of-mass energy of $11.020$ GeV \cite{46}.

The observed masses of the $Z_b(10610)$ and $Z_b(10650)$ are very close to the thresholds of the $B^*B$ and $B^*\bar{B}^*$, respectively, and could be considered as corresponding to the charmonium-like states $Z_c(3900)$ and $Z_c(4020)$ in the bottom sector. As the bottom counterpart of the $X(3872)$, it was proposed to search for the $X_b$ in the $Υπ^+π^−$ process \cite{47}, hidden bottom decay channels \cite{48} and the radiative decay of the $Υ(5S)$ and $Υ(6S)$ \cite{49}. The Belle Collaboration searched for the signal of the $X_b$ in the $ωΥ(1S)$ channel and found no evidence of the $X_b$ state \cite{50}.

To date, four charmonium-like states, $X(3872)$, $Z_c(3900)$, $Z_c(4020)$ and $Υ(4140)$, have been observed experimentally, and are near the thresholds of a pair of $S$ wave charmed or charmed-strange mesons. In the bottom sector, two bottomonium-like states, $Z_b(10610)$ and $Z_b(10650)$, have been discovered which could be the bottom counterparts of the $Z_c(3900)$ and $Z_c(4020)$. In Table I, we summarize the thresholds of pairs of $S$-wave charmed/charmed-strange and bottom/bottom-strange mesons, and the corresponding near-
threshold states are also presented.

The experimental observations have stimulated theorists to great interest in the intrinsic nature of these near-threshold states. Different interpretations of these observed states have been proposed, such as conventional charmonium to the X(3872) and Y(4140) [51–58], tetraquark states [59–69] and special production mechanisms [70–76]. Since all the above-mentioned states are near-threshold states, the hadronic molecular interpretations of these states are particularly attractive. In the following, we present a short review of the molecular interpretations of the observed near-threshold states listed in Table I.

**Molecular interpretation of X(3872):** The first observed charmonium-like state, X(3872), is very close to the threshold of the D* D̅, so it is natural to consider the X(3872) as a shallow bound state of the D* D̅ + h.c. In Ref. [77], the author proposed a microscopic model, where both the quark exchange and pion exchange induced effective potential were included and the X(3872) was interpreted as a D°D̄ + h.c molecular state. The calculation at the quark level suggested that molecular states D°D̄, D°D̄ and D°D̄ could be mixed to form components of I = 0 and I = 1 states, and the I = 0 state could correspond to the observed X(3872). The one-boson-exchange potential model calculations indicated that the X(3872) could be a D°D̄ + h.c molecular state [78–80]. The estimation by the effective Lagrangian [81], coupled channel [82] and QCD sum rule [83] also supported the X(3872) as a shallow D* D̅ bound state.

In the molecular framework the decay behaviors of the X(3872) have been extensively discussed. In Refs. [84–86], the strong and radiative decays of the X(3872) were discussed in the D°D̄ + h.c molecular scenario with the compositeness condition of the composite particle. The estimate in an effective Lagrangian approach in the molecular scenario were consistent with the corresponding experimental measurement [87], which indicated that the X(3872) could be a loosely bound state of the D°D̄ + h.c.

**Molecular interpretation of Z_b(3900) and Z_b(4020):** The observed masses of the Z_b(3900) and Z_b(4020) are very close to the thresholds of D* D̄ and D* D̄, respectively, which indicates that they could be a D* D̄ and D* D̄ hadronic molecular state with I = 1. The authors of Refs. [88–90] used the potential model to find bound state solutions for the D* D̄ + h.c and D* D̄ systems, which corresponded well to the observed Z_b(3900) and Z_b(4020). The QCD sum rule calculations in Refs. [65, 91] also supported that the Z_b(3900) and Z_b(4020) could be deuteron-like hadronic molecular states.

The decays of the Z_b(3900) and Z_b(4020) were estimated via the meson loops [92, 93]. The product and decay behaviors of Z_b(3900) and Z_b(4020) have been studied in D* D̄ + h.c and D* D̄ hadronic molecular scenarios with the Weinberg compositeness condition in Refs. [94, 95], and the theoretical estimations were consistent with the corresponding experimental measurements. Besides the observed channels, some other decay modes of Z_b(3900) and Z_b(4020) have been studied in the molecular scenario, such as the ρη, J/ψπγ, γη and γγ[96–100]. All these theoretical studies supported that the Z_b(3900) and Z_b(4020) could be assigned as D* D̄ + h.c and D* D̄ hadronic molecular states, respectively.

**Molecular interpretation of Y(4140):** The observed mass of the Y(4140) is about 80 MeV below the thresholds of the D* D̄ and the charmed-strange meson pair could easily couple to the J/ψφ final states, so it is natural to interpret the Y(4140) as a S– wave D* D̄ molecule. The potential calculations in Refs. [101–106] indicated that the Y(4140) could be a D* D̄ molecular state with JPC = 0+ +. The QCD sum rule calculations also supported the Y(4140) to be a D* D̄ molecule state [107–109]. In Ref. [110], Y(4140) was assigned as a mixing D* D̄ molecular state with D* D̄ component.

The lineshape of the radiative open-charm decay of the Y(4140) is estimated in Ref. [104], where the Y(4140) was considered as the strange counterpart of the Y(3930). The hidden charm decays of the Y(4140) were studied in the hadronic molecular state [111] with JPC = 0+ + and 2+ +.

**Molecular interpretation of Z_b(10610) and Z_b(10650):** The experimentally measured masses of the Z_b(10610) and Z_b(10650) are very close to the thresholds of the B±B̄ and B±B̄. In Refs. [78, 89], the OBE potential model indicated that the Z_b(10610) and Z_b(10650) could be molecular states composed of B±B̄ and B±B̄, respectively. The observed Z_b(10610) and Z_b(10650) were explained as molecular states in the chiral quark model [112, 113]. Using QCD sum rules, the masses of the Z_b(10610) and Z_b(10650) could be reproduced in a molecular picture [91, 109, 114].

In Ref [115], the transitions to Y(nS)π (n = 1, 2, 3) and h_0(mP)π (m = 1, 2) were analysed in the molecular picture with compositeness condition. The observed processes of the Z_b(10610) and Z_b(10650) investigated in the effective Lagrangian approach also supported the molecular scenarios [116–119]. The decays of the Z_b(10610) and Z_b(10650)

### Table I: The thresholds of pairs of S-wave heavy-light mesons and the corresponding near-threshold charmonium-like states.

| Threshold (MeV) | Possible State | Isospin Singlet | Isospin Triplet |
|----------------|----------------|-----------------|----------------|
| DD             | 3734           | ...             | ...            |
| D* D̄          | 3876           | X(3872)         | Z_b(3900)      |
| D* D̄          | 4017           | ...             | Z_b(4020)      |
| D* D̄          | 3936           | ...             | ...            |
| D* D̄          | 4080           | ...             | ...            |
| D* D̄          | 4224           | ...             | Y(4140)        |
| DD*           | 3835           | ...             | ...            |
| DD*           | 3979           | ...             | ...            |
| DD*           | 3977           | ...             | ...            |
| DD*           | 4121           | ...             | ...            |

| Bottom Sector | BB             | 10539           | ...             | 
|               | B±B̄           | 10605           | Z_b(10610)      |
|               | B±B̄           | 10651           | Z_b(10650)      |
|               | B±B̄           | 10734           | ...             | 
|               | B±B̄           | 10782           | ...             | 
|               | B±B̄           | 10830           | ...             | 
|               | B±B̄           | 10646           | ...             | 
|               | B±B̄           | 10694           | ...             | 
|               | B±B̄           | 10694           | ...             | 
|               | B±B̄           | 10740           | ...             | 



have been evaluated via the intermediate meson loops model, where more decay channels were predicted [96].

In Table I, there exist 10 thresholds of pairs of charmed or bottom mesons. As we discussed above, some near-threshold charmonium-like or bottomonium-like states have been observed experimentally, and have been intensively considered as $S$–wave hadronic molecular states. Theoretically, it is very interesting and urgent to systematically consider the possibility of hadronic molecular states composed of other combinations of charmed or bottom meson pairs [80]. Moreover, investigations of the deuteron indicated that the $D$-wave component of the wave function is crucial in understanding its static properties [120, 121]. Thus, in the present work, we further include the $S-D$ mixing in the wave functions of the hadronic molecule composed of a heavy-light meson pair. By this systematic study, we can identify whether the observed near-threshold states, i.e., $X(3872), Z_c(3900), Z_b(4020), Y(4140), Z_b(10610)$, and $Z_b(10650)$, could be hadronic molecular states and in addition, we can predict more near-threshold molecular states, which could be accessed by further experimental measurements.

This work is organized as follows. After this Introduction, we present the wave functions of the possible molecular state and the effective potentials of the heavy-light meson pair in Section II. The numerical results and discussion are given in Section III and Section IV is devoted to a summary.

## II. WAVE FUNCTIONS AND EFFECTIVE POTENTIALS

In the heavy quark effective theory, the two $S$-wave heavy-light mesons degenerate into a $H = \{P, P^*\}$ doublet, in which the $P$ and $P^*$ indicate $D_{(s)}$ and $D_{(s)}^*$ in the charm sector and $B_{(s)}$ and $B_{(s)}^*$ in the bottom sector. The molecular state composed of $HH$ can be decomposed into three types, which are $P - P^*$, $P^-P^-$ and $P^*-P^*$, respectively. In the following, we construct the wave functions and calculate the potentials of these three types.

### A. Wave function of the molecular states

For a molecular state composed of two mesons, the total wave function is

$$|\Psi\rangle = \frac{\phi(r)}{r} \otimes |\underline{L}\rangle \otimes |I, I_3\rangle$$

where the $|\phi(r)\rangle$, $|\underline{L}\rangle$ and $|I, I_3\rangle$ denote the radial, spin-orbital and flavor functions, respectively. As for the radial and the spin-orbital wave function, there exists $S - D$ mixing in the $P - P^*$ and $P^*-P^*$ types of hadronic molecular states, which will be considered explicitly in the present work. For the $S$-wave dominant $P - P^*$ type molecule, both the spin and total angular momentum are one, while the orbital momentum could be zero and two when considering the $S - D$ mixing. The corresponding spin-orbital wave functions are

$$J = 1 : |3S_1\rangle, |3D_1\rangle.$$  

### B. Potential of the $P^-(*) - P^{*-}(*)$ system

The potential of the $P^-(*) - P^{*-}(*)$ system can be estimated from the amplitude of the $P^-(*)P^{*-}(*) \rightarrow P^{(*)}P^{(*)}$ process.
TABLE III: The flavor wave functions of the $P^r - P$ systems for the charm sector. The corresponding wave functions for the bottom sector can be constructed by replacing the charmed mesons with the corresponding bottom mesons.

| state       | Charm sector |
|-------------|--------------|
| $\phi_+^s/\phi_s$ | $\frac{1}{\sqrt{3}}(D_{s}^0D_{s}^0 + cD_{s}^{-}D_{s}^{-})$ |
| $\phi_{-}^s/\phi_{s}$ | $\frac{1}{\sqrt{3}}(D_{s}^{-}D_{s}^{+} + cD_{s}^{-}D_{s}^{+})$ |
| $\phi_0^s/\phi_0$ | $\frac{1}{\sqrt{3}}(D_{s}^{-}D_{s}^{-} + cD_{s}^{-}D_{s}^{-})$ |
| $\phi_{-}^s/\phi_0$ | $\frac{1}{\sqrt{3}}[(D_{s}^0D_{s}^0 + cD_{s}^{-}D_{s}^{-})]$ |
| $\phi_0^s/\phi_0$ | $\frac{1}{\sqrt{3}}[(D_{s}^{-}D_{s}^{+} + cD_{s}^{-}D_{s}^{+})]$ |
| $\phi_{-}^s/\phi_0$ | $\frac{1}{\sqrt{3}}[D_{s}^{-}D_{s}^{-} + cD_{s}^{-}D_{s}^{-}]$ |

FIG. 1: Feynman diagrams describing $P^r = P^l$ scattering in the one-boson-exchange model. Here $\mathcal{V}$ and $\bar{\mathcal{V}}$ indicate the light vector and pseudoscalar mesons, respectively.

we adopt the one-boson-exchange model, where the interaction can be realized by exchanging a light boson as shown in Fig. 1. The interactions of the heavy-light mesons and light mesons are described by the effective Lagrangian, which are constructed in heavy quark limit and chiral symmetry. The concrete Lagrangians are [122–127],

$$L_{P^rP^l,\mathcal{V}} = \frac{1}{2} [\mathcal{V}_{a} \mathcal{P}_{a}^{\dagger} \mathcal{P}_{a}^{\dagger} - \mathcal{V}_{a} \mathcal{P}_{a}^{\dagger} \mathcal{P}_{a}^{\dagger}] \sigma (6)$$

where $g_{\sigma} = g_{\sigma}/(2\sqrt{6})$, $g_{\sigma} = 3.73$, $f_{\sigma} = 132$ MeV, $\beta = 0.59$, $g_{\mathcal{V}} = 5.8$ and $\lambda = 0.56$ GeV$^{-1}$, respectively [122, 128, 129]. The gauge coupling $g = 0.59$ is estimated from the experimental width of $D^{*+}$ with the assumption that the $D^{*+}$ dominantly decays into $D\pi$ [128]. The light pseudoscalar and vector meson matrices in the above effective Lagrangians are defined as

$$\mathcal{P} = \begin{pmatrix} V_{\pi}^0 + \alpha \eta + \beta \eta' & \pi^+ & K^+ \\ \pi^- & -V_{\pi}^0 + \alpha \eta + \beta \eta' & K^0 \\ K^- & K^0 & \gamma \eta + \delta \eta' \end{pmatrix}$$

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and in the present calculations, we use $\theta = -19.1^\circ$ [130, 131].

With the above preparations, we can get the elastic scattering amplitudes corresponding to the diagrams in Fig. 1. In general, the scattering amplitude $iM(J, J_c)$ can be related to the interaction potential in momentum space in terms of the Breit approximation by [78, 89, 90]

$$V(q) = -\frac{M}{\sqrt{\Pi_1 \Pi_2 \Pi_3 \Pi_4}} (12)$$

Here, all the involved particles are mesons, so to depict the inner structure effect of the mesons, a monopole type form factor is introduced, which is [132–135]

$$F(q) = \frac{\Lambda^2 - m^2}{\Lambda^2 - q^2} (13)$$

where $q$ is the four-momentum of the exchanged meson. $\Lambda$ is a model parameter, which should be of order 1 GeV. The effective potential in coordinate space is the Fourier transformation of that in momentum space, and is

$$V(r) = \int \frac{d^3 p}{(2\pi)^3} e^{iq \cdot r} V(q) F(q)^2. (14)$$

In the following, we take the charm sector as an example to show the potentials of the $P - P$, $P^r - P$ and $P^r - P^r$ systems one by one.

1. $P - P$ type

As shown in Fig. 1(a), the interactions between $P - P$ can be realized by exchanging a $\sigma$ meson or a vector meson. The corresponding potentials are

$$V_{\sigma}^\mu(r) = -g_{\sigma}^2 Y(\Lambda, m_{\sigma}, r),$$

$$V_{\mathcal{V}}^\mu(r) = -\frac{1}{2} g_{\mathcal{V}}^2 Y(\Lambda, m_{\mathcal{V}}, r),$$

where $g_{\mathcal{V}} = g_{\mathcal{V}}/(2\sqrt{6})$, $g_{\mathcal{V}} = 3.73$, $f_{\mathcal{V}} = 132$ MeV, $\beta = 0.59$, $g_{\mathcal{V}} = 5.8$ and $\lambda = 0.56$ GeV$^{-1}$, respectively [122, 128, 129]. The gauge coupling $g = 0.59$ is estimated from the experimental width of $D^{*+}$ with the assumption that the $D^{*+}$ dominantly decays into $D\pi$ [128]. The light pseudoscalar and vector meson matrices in the above effective Lagrangians are defined as

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$$V_{\sigma}^\mu(r) = -g_{\sigma}^2 Y(\Lambda, m_{\sigma}, r),$$

$$V_{\mathcal{V}}^\mu(r) = -\frac{1}{2} g_{\mathcal{V}}^2 Y(\Lambda, m_{\mathcal{V}}, r),$$

(15)
respectively, and the concrete form of the \( Y(\Lambda, m, r) \) is

\[
Y(\Lambda, m, r) = \frac{1}{4\pi r} e^{-\Lambda r} - \frac{\Lambda^2 - m^2}{2\Lambda} e^{-\Lambda r}.
\]  

For the \( \Phi \) and \( \Omega \) system, their components are \( D^+_1 - D^+_2 - D^-_1 \) and \( B^0 - \bar{B}/B^0 \), respectively. No proper vector meson can be exchanged in these systems due to the ideal mixing of the \( \omega - \phi \). Thus, in the present model, the potential of the \( \Phi \) and \( \Omega \) system is zero. The concrete potentials of the \( \Phi^8 \) and \( \Phi_{s1}^0 \) system are

\[
\begin{align*}
V_{\Phi^8} &= -\frac{1}{2} V_{\Phi^8}^0(r) + \frac{1}{2} V_{\Phi^8}^r(r) + V_{\Phi^8}^2(r) \\
V_{\Phi_{s1}^0} &= \frac{3}{2} V_{\Phi_{s1}^0}^0(r) + \frac{1}{2} V_{\Phi_{s1}^0}^r(r) + V_{\Phi_{s1}^0}^2(r)
\end{align*}
\]  

respectively.

2. \( P^* - P \) type

For the \( P^* - P \) system, there exist two kinds of diagrams, the direct diagram and cross diagram, which are presented in Figs. 1(b) and 1(c), respectively. For the direct diagrams, the exchanged mesons are \( \sigma \) and vector mesons, and the corresponding potentials are

\[
\begin{align*}
V_{\sigma}^b &= -\frac{g^2_s}{2} (e_1 \cdot e_3) Y(\Lambda, m_\sigma, r) \\
V_{\sigma}^b &= -\frac{1}{2} \frac{g^2_s}{2} g^2_\gamma (e_1 \cdot e_3) Y(\Lambda, m_v, r)
\end{align*}
\]  

respectively.

For the cross diagram, the exchanged light mesons are pseudoscalar and vector mesons. The potentials are

\[
\begin{align*}
V_{\gamma}^b(r) &= -\frac{g^2_s}{f}\frac{1}{3} (e_1 e_3^4) \nabla^2 Y(\Lambda_0, m_0, r) \\
&+ \frac{1}{3} S(\vec{r}, e_1, e_3 r) \frac{1}{\partial r} \frac{1}{\partial r} Y(\Lambda_0, m_0, r), \\
V_{\gamma}^b(r) &= -2\frac{g^2_s}{2} e_1 (e_1 e_3) \nabla^2 Y(\Lambda_0, m_0, r) \\
&-\frac{1}{3} S(\vec{r}, e_1, e_3 r) \frac{1}{\partial r} \frac{1}{\partial r} Y(\Lambda_0, m_0, r),
\end{align*}
\]  

respectively, where \( \Lambda_0 = \sqrt{\Lambda^2 - \Lambda^2} \), \( m_0 = \sqrt{\Lambda^2 - m^2} \) with \( \Delta \) and \( m \) being the mass difference of the \( P^* - P \) and the mass of the exchanged meson, respectively.

Here one should notice that the mass splitting of the \( D \) and \( D^* \) meson could be larger than the mass of the \( \pi \), thus the exchanged pion meson could be on shell, thus the \( Y \) function for the pion exchange is different from other pseudoscalar or vector meson exchange processes, and the \( Y \) function for the \( \pi \) exchange process is,

\[
Y(\Lambda, m_0, r) = \frac{1}{4\pi r^3} e^{-\Lambda r} - \frac{r(\Lambda^2 + m_0^2)}{2\Lambda} e^{-\Lambda r} + \cos(m_0 r).
\]  

The concrete potentials for the \( \Phi^+, \Phi^* \), \( \Phi_{s1}^0 \), and \( \Phi_{s1}^0 \) are

\[
\begin{align*}
V_{\Phi^+} &= -c \cdot \gamma V_{\Phi^+}^\gamma(r) - c \cdot \beta V_{\Phi^+}^\beta(r), \quad V_{\Phi^+}^\gamma(r) = V_{\Phi^+}^\beta(r) = \frac{3}{2} V_{\Phi^+}^\gamma(r) + \frac{1}{2} V_{\Phi^+}^\beta(r) \\
V_{\Phi^0} &= -c \cdot \gamma V_{\Phi^0}^\gamma(r) - c \cdot \beta V_{\Phi^0}^\beta(r), \quad V_{\Phi^0}^\gamma(r) = V_{\Phi^0}^\beta(r) = \frac{3}{2} V_{\Phi^0}^\gamma(r) + \frac{1}{2} V_{\Phi^0}^\beta(r) \\
V_{\Phi_{s1}^0} &= -c \cdot \gamma V_{\Phi_{s1}^0}^\gamma(r) - c \cdot \beta V_{\Phi_{s1}^0}^\beta(r), \quad V_{\Phi_{s1}^0}^\gamma(r) = V_{\Phi_{s1}^0}^\beta(r) = \frac{3}{2} V_{\Phi_{s1}^0}^\gamma(r) + \frac{1}{2} V_{\Phi_{s1}^0}^\beta(r) \\
V_{\Phi_{s1}^0} &= -c \cdot \gamma V_{\Phi_{s1}^0}^\gamma(r) - c \cdot \beta V_{\Phi_{s1}^0}^\beta(r), \quad V_{\Phi_{s1}^0}^\gamma(r) = V_{\Phi_{s1}^0}^\beta(r) = \frac{3}{2} V_{\Phi_{s1}^0}^\gamma(r) + \frac{1}{2} V_{\Phi_{s1}^0}^\beta(r)
\end{align*}
\]  

respectively. In the above potential, notice that there exist two factors related to \( \epsilon_i \), which is the polarization vector of the involved vector mesons. In the subspace formed by \( |3S_1\rangle \) and \( |1D_1\rangle \), the factor \( \epsilon_i e_i^\dagger \) and \( S(\vec{r}, e_i, e_i^\dagger) \) can be expressed in matrix form as

\[
\begin{align*}
\epsilon_i e_i^\dagger &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad S(\vec{r}, e_i, e_i^\dagger) &= \begin{pmatrix} 0 & -\sqrt{2} \\ \sqrt{2} & 1 \end{pmatrix}
\end{align*}
\]  

respectively.

3. \( P^* - P^* \) type

For the \( P^* - P^* \) system, the exchanged mesons can be \( \sigma \), pseudoscalar and vector mesons as shown in Fig. 1(d). The corresponding potentials are

\[
\begin{align*}
V_{\sigma}^d &= -\frac{2}{f} (e_1 \times e_3) \cdot (e_1 \times e_3) Y(\Lambda, m_\sigma, r) \\
V_{\sigma}^d(r) &= -\frac{2}{f} (e_1 \times e_3) \cdot (e_1 \times e_3) Y(\Lambda, m_v, r) \\
V_{\sigma}^d(r) &= -\frac{2}{f} (e_1 \times e_3) \cdot (e_1 \times e_3) Y(\Lambda, m_v, r) \\
V_{\sigma}^d(r) &= -\frac{2}{f} (e_1 \times e_3) \cdot (e_1 \times e_3) Y(\Lambda, m_v, r)
\end{align*}
\]  

respectively.

The total potentials of the \( \Phi^+ \), \( \Phi^* \), \( \Phi^* \) and \( \Phi_{s1}^0 \) systems are

\[
\begin{align*}
V_{\Phi^+} &= -c \cdot \gamma V_{\Phi^+}^\gamma(r) - c \cdot \beta V_{\Phi^+}^\beta(r), \quad V_{\Phi^+}^\gamma(r) = V_{\Phi^+}^\beta(r) = \frac{3}{2} V_{\Phi^+}^\gamma(r) + \frac{1}{2} V_{\Phi^+}^\beta(r) \\
V_{\Phi^0} &= -c \cdot \gamma V_{\Phi^0}^\gamma(r) - c \cdot \beta V_{\Phi^0}^\beta(r), \quad V_{\Phi^0}^\gamma(r) = V_{\Phi^0}^\beta(r) = \frac{3}{2} V_{\Phi^0}^\gamma(r) + \frac{1}{2} V_{\Phi^0}^\beta(r) \\
V_{\Phi_{s1}^0} &= -c \cdot \gamma V_{\Phi_{s1}^0}^\gamma(r) - c \cdot \beta V_{\Phi_{s1}^0}^\beta(r), \quad V_{\Phi_{s1}^0}^\gamma(r) = V_{\Phi_{s1}^0}^\beta(r) = \frac{3}{2} V_{\Phi_{s1}^0}^\gamma(r) + \frac{1}{2} V_{\Phi_{s1}^0}^\beta(r)
\end{align*}
\]
respectively. The factor related to the polarization vectors of the involved vector mesons can be expressed in matrix form as

\[
(e_1 e_3^†)(e_2 e_4^†) = \begin{pmatrix}
1 & 0 \\
0 & 1 \\
1 & 0 \\
0 & 0 \\
0 & 1 \\
1 & 0 \\
0 & 0 \\
1 & 0 \\
0 & 0
\end{pmatrix}
\]

\[
(e_1 \times e_3^†)(e_2 \times e_4^†) = \begin{pmatrix}
2 & 0 \\
0 & -1 \\
1 & 0 \\
0 & 1 \\
0 & 0 \\
1 & 0 \\
0 & 1 \\
0 & 0 \\
0 & 1
\end{pmatrix}
\]

\[
S(\vec{r}, e_1 \times e_3^†, e_2 \times e_4^†) = \begin{pmatrix}
0 & \sqrt{2} \\
-\sqrt{2} & 0 \\
\sqrt{2} & 0 \\
0 & -\sqrt{2}
\end{pmatrix}
\]

respectively.

The matrix forms of the kinetic terms for \(P-P, P^*-P/P^*-\bar{P}^*(J = 0), P^*-\bar{P}^*(J = 1), \bar{P}^* - P^*(J = 2)\) are

\[
K = \text{diag}(\frac{\Delta}{2\mu})
\]

\[
K = \text{diag}(\frac{\Delta}{2\mu} - \frac{\Delta_1}{2\mu})
\]

\[
K = \text{diag}(\frac{\Delta}{2\mu} - \frac{\Delta_1}{2\mu} - \frac{\Delta_1}{2\mu})
\]

\[
K = \text{diag}(\frac{\Delta}{2\mu} - \frac{\Delta_1}{2\mu} - \frac{\Delta_1}{2\mu} - \frac{\Delta_1}{2\mu})
\]

respectively. Here, \(\Delta = \frac{1}{2m^2}p^2\), \(\Delta_1 = \Delta - \frac{\Delta}{2}\) and \(\mu\) is the reduced mass of the considered system. With the potentials listed in Eqs. (17)-(25) and the above kinetic terms, one can get bound energies and wave functions if there exist bound states by solving the corresponding Schrödinger equation. In the present work, we rely on complex scaling methods to perform the calculations, in which the wave function of the bound state is expanded by the harmonic oscillator wave functions [136–141].

### III. Numerical Results and Discussion

In the OBE model, one additional cutoff \(\Lambda\) is introduced in the form factor, which compensates the off-shell effect of the changed light mesons. The value of the \(\Lambda\) should be of order 1 GeV and in the present work, we search the bound state solutions of different systems with \(\Lambda\) less than 3 GeV, which is a reasonable cutoff for light meson exchange processes. In the following, we will present the numerical results of the three types of system separately.

| State | \(\Lambda\) (GeV) | \(E\) (MeV) | \(r_{\text{RMS}}\) (fm) |
|-------|------------------|---------|----------------|
| \(\Phi_0^g\) | 1.50 | -0.43 | 2.27 |
| \(\Omega_0^g\) | 1.60 | -3.65 | 1.76 |
| \(\Omega_1^g\) | 1.70 | -8.34 | 1.36 |
| Bottom | 1.10 | -1.15 | 1.85 |
| \(\Omega_0^g\) | 1.20 | -8.33 | 0.97 |
| \(\Omega_1^g\) | 1.30 | -20.81 | 0.70 |
| \(\Omega_1^g\) | 1.90 | -0.26 | 2.01 |
| \(\Omega_1^g\) | 2.10 | -3.69 | 1.10 |
| \(\Omega_1^g\) | 2.30 | -9.67 | 0.77 |

### Table IV: The binding energy and the root-means-square radius of the \(P-P\) type molecular state depending on the cutoff \(\Lambda\).

| System | Molecule state | Present work | Ref. [142] |
|--------|----------------|--------------|------------|
| \(D\bar{D}\) | \(\Phi_0^g\) | \(\Phi_{0s}\) | \(\otimes\) |
| \(D, \bar{D}\) | \(\Phi_0^g\) | \(\otimes\) | \(\otimes\) |
| \(D, D\) | \(\Phi_0^g\) | \(\otimes\) | \(\otimes\) |
| \(BB\) | \(\Omega_0^g\) | \(\Omega_{0s}\) | \(\otimes\) | \(?\) |
| \(B, \bar{B}\) | \(\Omega_0^g\) | \(\Omega_{0s}\) | \(\otimes\) | \(\otimes\) |
| \(B, \bar{B}\) | \(\Omega_0^g\) | \(\otimes\) | \(\otimes\) |

### Table V: Summary of possible bound states for \(P-P\) type. Here, we also compare our results with the estimations from the chiral and extended chiral \(SU(3)\) quark model [142]. The symbols \(\otimes\), \(\otimes\) and \(?\) indicate that this bound state must, must not or maybe exists, respectively. The symbol + means this bound state does not exist in the chiral \(SU(3)\) quark model while it is possible or not excluded in the extended chiral \(SU(3)\) quark model.

#### A. \(P-P\) type

In the \(P-P\) type system, we have not observed any near threshold states which may correspond to a \(P-P\) type molecular state. However, in the present calculations, we find one bound state solution in the charm sector, the \(\Phi_0^g\) state with \(I(J^{PC}) = 0^{++}\). As shown in Table IV, when the cutoff increases from 1.5 GeV to 1.7 GeV, the binding energy varies from less than 1 MeV to nearly 10 MeV, which corresponds to the mass of the \(\Phi_0^g\) decreasing from 3738 MeV to 3729 MeV. In addition, in this cutoff range, the root-mean-square (RMS) radius of the system decrease from 2.27 fm to 1.36 fm, which indicates the \(D\bar{D}\) could form a very loosely shallow bound state by the \(\sigma\) and vector meson exchange.
In the bottom sector, we find two bound state solutions, $\Omega_{s}^{0}$ and $\Omega_{s}^{1}$. The $\Omega_{s}^{0}$ state is the bottom correspondence of the $\Phi_{s}^{0}$ in the charm sector. When we vary the cutoff from 1.10 GeV to 1.30 GeV, the binding energy of the $\Phi_{s}^{0}$ increases from about 1 MeV to more than 20 MeV, while the RMS radius decreases from 1.85 fm to 0.70 fm. Comparing the binding energies and RMS radii of the $\Phi_{s}^{0}$ and $\Omega_{s}^{0}$, the $\Omega_{s}^{0}$ is a more compact bound state than $\Phi_{s}^{0}$ for the same binding energy. In the bottom sector, we also find the bound solution of $\Omega_{s}^{1}$, which is a $l(J^{PC}) = 0(0^{++})$ state composed of $B_{s}^{0}\bar{B}_{s}^{0}$. Here we should note that the only possible exchanged meson of the $B_{s}^{0}\bar{B}_{s}^{0}$ is the $\phi$ meson, which provides an attractive potential.

In the $P-P$ system, the total spin is zero, thus there is no $S-D$ mixing in such a system. Our present results are consistent with those in Ref. [80], in which molecular states $\Phi_{s}^{0}$, $\Phi_{s}^{1}$, $\Omega_{s}^{0}$ and $\Omega_{s}^{1}$ states were established, while no bound state solution corresponding to $\Phi_{s}^{0(0)}$ and $\Omega_{s}^{0(0)}$ was found. We summarize the possible bound states of the $P-P$ system in Table V and compare with estimations in the chiral and extended chiral SU(3) quark model [142]. From the table, the present calculations in the OBE potential model are almost in line with the estimations in the chiral and extended chiral SU(3) quark model [142]. However, our calculation can exclude the possibilities of $\Phi_{s}^{0}$ and $\Omega_{s}^{0(0)}$ as molecular states, while the calculation in Ref. [142] could not fully exclude such possibilities.

| System | Molecule states | Present Work | Ref. [142] |
|--------|----------------|--------------|-------------|
| $DD^{*}$ | $\phi_{s}^{0}$ | √ | ? |
| | $\phi_{s}^{0}$ | ⊗ | ⊗ |
| | $\phi_{s}^{0}$ | ⊗ | ⊗ |

TABLE VII: The same as Table V but for the $P-P^{*}$ system.

### B. $P-P^{*}$ type

For the $P-P^{*}$ type system, both the spin and total angular momentum are 1 if only the $S$ wave dominant state is considered. In the present work, $S-D$ mixing is considered. The binding energies and RMS radii of the bound state solutions depending on the cutoff $\Lambda$ are presented in Table VI.

In the charm sector, we get four bound state solutions, $\Phi_{s}^{0(0)}$, $\Phi_{s}^{0(1)}$, $\Phi_{s}^{0(2)}$ and $\Phi_{s}^{0(3)}$, where $\Phi_{s}^{0(0)}$ corresponds to the experimentally observed $X(3872)$. When $\Lambda = 1.10$ GeV, the binding energy of the $\Phi_{s}^{0(0)}$ is very small, which agrees with the experimental observation of the $X(3872)$. In this case, the RMS radius of the $X(3872)$ could reach up to 2 fm. Thus, the estimation in the present work indicates that the observed $X(3872)$ is a very loosely shallow bound state of the $DD^{*} + h.c$, which is the same as the conclusion in Ref. [90], qualitatively. However, the binding energy of the $\Phi_{s}^{0(0)}$ is smaller than the one in Ref. [90] with the same cutoff, due to proper consideration of the $\eta - \eta'$ mixing in the present work. In addition, in the present work, the mass splittings of the charged and neutral charmed mesons are not taken into consideration. In Ref. [143], both the mass splittings of the charmed mesons and the $S-D$ mixing were considered, and the mass and decays of the $X(3872)$ were well reproduced. We find the mass splittings of the neutral and charged mesons strongly affect the decays of the $X(3872)$, while the mass could be well explained both with and without considering such mass splittings with a reasonable cutoff.

In addition, the partner of the $X(3872)$ with negative $C$ parity is also predicted in our present calculations. As the strange partner of the $X(3872)$, the state $\Phi_{s}^{0(0)}$ system has bound state solutions when we take a relative large cutoff, which is about 3 GeV. For the negative $C$ parity system, $\Phi_{s}^{0(0)}$, we can also find the bound state solution when $\Lambda$ is larger than 2.3 GeV. As listed in Table I, $Z_{c}(3900)$ is also very close to the threshold of the $DD^{*}$ with $I(J^{P}) = 1(1^-)$. In the present calculation, however, we do not find the bound state of the $DD^{*} + h.c$ with
TABLE VIII: The same as Table IV but for $P^+ - P^-$ type

| System | Molecule states | Present work | Ref. [142] |
|--------|----------------|--------------|------------|
| $D^*D'$ | $\Phi_{8}^{0s}$ | 0 | $\checkmark$ | ? |
|        | $\Phi_{8}^{0s}$ | 1 | $\checkmark$ | $\checkmark$ |
|        |                | 2 | $\checkmark$ | $\checkmark$ |
| $D^*D'$ | $\Phi_{8}^{0s}$ | 0 | $\checkmark$ | $\checkmark$ |
|        | $\Phi_{8}^{0s}$ | 1 | $\checkmark$ | $\checkmark$ |
|        |                | 2 | $\checkmark$ | $\checkmark$ |
| $D^*D'$ | $\Phi_{8}^{0s}$ | 0 | $\checkmark$ | $\checkmark$ |
|        | $\Phi_{8}^{0s}$ | 1 | $\checkmark$ | $\checkmark$ |
|        |                | 2 | $\checkmark$ | $\checkmark$ |
| $B^*\bar{B}$ | $\Omega_{8}^{0s}$ | 0 | $\checkmark$ | $\checkmark$ |
|        | $\Omega_{8}^{0s}$ | 1 | $\checkmark$ | $\checkmark$ |
|        |                | 2 | $\checkmark$ | $\checkmark$ |
| $B^*\bar{B}$ | $\Omega_{8}^{0s}$ | 0 | $\checkmark$ | $\checkmark$ |
|        | $\Omega_{8}^{0s}$ | 1 | $\checkmark$ | $\checkmark$ |
|        |                | 2 | $\checkmark$ | $\checkmark$ |
| $B^*\bar{B}$ | $\Omega_{8}^{0s}$ | 0 | $\checkmark$ | $\checkmark$ |
|        | $\Omega_{8}^{0s}$ | 1 | $\checkmark$ | $\checkmark$ |
|        |                | 2 | $\checkmark$ | $\checkmark$ |

TABLE IX: The same as Table V but for the $P^+ - P^-$ system.

$I = 1$, which indicates that the present calculation does not support the observed $Z_0(3900)$ as the $DD^*$ molecular state. In Ref. [144], the author carried out a calculation within the Bethe-Salpeter equation approach and found that $Z_0(3900)$ could be a resonance state above $DD^*$ threshold rather than a bound state below $DD^*$ threshold.

In the bottom sector, there also exist four bound states in our calculations, $\Omega_{8}^{0s}$, $\Omega_{8}^{0s}$, $\Omega_{8}^{0s}$, and $\Omega_{8}^{0s}$. Compared to the charm correspondence of these states, we find that cutoffs in the bottom sector are smaller than those in the charm sector and in addition, the RMS radii of these states are smaller than their correspondences in the charm sector with the same binding energy. The corresponding state of the $Z_0(10610)$ could not be found in our present calculations, which is the same case as the $Z_0(3900)$. In Ref. [90], the estimation in the OBE potential model indicated that the $Z_0(10610)$ could be a molecular state of $B\bar{B}^*$, which is different from our present calculation. The main reason for such a difference is that $\eta - \eta'$ mixing is considered in the present work, which increases repulsive interaction for the isospin triplet. In addition, the authors in Ref. [145], indicated that the $Z_0(10610)$ could be a $B\bar{B}^* + h.c$ molecular state, which is different from our present calculation. In Ref. [145], the authors considered $B\bar{B}^* - B\bar{B}^*$ mixing but only included the potentials induced by $\pi, \rho$ and $\omega$ exchange, which may be the reason for the different conclusions drawn from our present calculation.

In Table VII, we summarize our calculation for the $P^+ - P^-$ system and compare with the chiral and extended chiral $SU(3)$ quark model [142]. Our estimations in the OBE quark model are consistent with those in Ref. [142] except for the $\Phi_{0}^{0s}$. In this work, we found a bound state solution for $\Omega_{8}^{0s}$, while in Ref. [142], their calculation indicated that such a state may exist.

C. $P^- - P^-$ type

For the system composed of two red heavy $S$-wave vector mesons, the total angular momentum of the system could be 0, 1, and 2 for the $S$-wave interaction. The binding energies and RMS radii of the possible bound states depending on the cutoff are presented in Table VIII. From our calculations, we can find the bound states of $\Phi_{8}^{0s}$ and $\Phi_{8}^{0s}$ for different total angular momenta. However, $Y(4140)$ is about 80 MeV below the threshold of the $D_{s}^{+*}D_{s}^{-*}$, which is larger than the binding energy of the $\Phi_{8}^{0s}$ state. In addition, the LHCb Collaboration have measured the $J^{PC}$ quantum numbers of the $Y(4140)$ to be $1^{++}$ [39, 40], which is different from $\Phi_{8}^{0s}$. Thus, the $Y(4140)$ cannot be a $D_{s}^{+*}D_{s}^{-*}$ molecular state. When taking both the $S - D$ mixing and $\eta - \eta'$ mixing into consideration, we do not find the bound state corresponding to the observed $Z_0(4020)$. The calculation in Ref. [90] also indicated that there is no bound state for isovector states with $J = 0, 1, 2$, and only isoscalar bound states could be found. Our present calculations are consistent with those in Ref. [90], qualitatively, but the binding energies of the obtained molecular states in the present work are a little
bigger than the corresponding ones with the same cutoff due to \( \eta - \eta' \) mixing [90].

In the bottom sector, we also find two group bound states with different total angular momenta, the \( Q_{s}\) and \( \Omega_{b} \). Similar to the charm sector, our calculations also do not support the molecular interpretations of the \( Z_{b}(10650) \). Similar to the case of \( Z_{b}(10610) \), the estimation in Ref. [90] indicated that \( Z_{b}(10650) \) could be a bound state composed of \( B^{+} B^- \). While in the present work, we cannot find a bound state solution for this system due to the consideration of the \( \eta - \eta' \) mixing.

A summary for the possible \( P^* - P^* \) molecular state and the comparison with the estimation in the chiral and extended chiral quark model are presented in Table IX. The present calculations indicate there exist isoscalar bound states of the \( D^{*+} D^{*-} \) and \( B^+ B^- \) with \( J = 0 \), 1 and 2, while the estimations in Ref. [142] could only confirm the molecular state with \( J = 2 \) for \( D^{*+} D^{*-} \) system and \( J = 1 \) and 2 for the \( B^+ B^- \) system.

IV. SUMMARY

We have performed a systematic study of the possible molecular states composed of \( S \) wave heavy-light mesons, where \( S - D \) mixing and \( \eta - \eta' \) mixing are taken into consideration. From the present calculations and the comparison with the experimental observation, we can conclude:

1. Our calculation supports the \( X(3872) \) as a loosely shallow \( D^{*}D^{*-} + h.c \) molecular state with \( I(J^{PC}) = 0(1^{++}) \).
2. The counterpart of the \( X(3872) \) in the bottom sector could be a molecular state composed of \( BB^* + h.c. \).
3. The molecule assignments of the \( Z_c(3900), Z_c(4020), Z_b(10610) \) and \( Z_b(10650) \) are not supported by the present calculations.
4. We find three bound states composed of \( D^{*+} D^{*-} \) with \( J^{PC} = 0^{++}, 1^{--} \) and \( 2^{++} \), which is different from the quantum numbers of the \( Y(4140) \) reported by the LHCb Collaboration. Thus, the \( Y(4140) \) cannot be assigned as a molecular state composed of \( D^{*+} D^{*-} \) in our calculations.
5. We predict more molecular states in the present calculations. For the \( P - P \) type, three molecular states, \( \Phi_{s}^{0}, \Omega_{b}^{0} \) and \( \Omega_{b}^{*} \), are predicted. In the \( P - P \) system, besides the \( X(3872) \) and its bottom counterpart, we also predict six new molecular states.

To summarize, in the present work, we have systematically studied the molecular states composed of \( S \) wave heavy-light mesons, where the \( S - D \) mixing and \( \eta - \eta' \) mixing are explicitly considered. In the present calculation, the observed \( X(3872) \) could be interpreted as a loosely shallow \( D^{*}D^{*-} + h.c \) molecular state, while \( Z_c(3900)/Z_c(4020) \) and \( Z_b(10610) \) and \( Z_b(10650) \) cannot be molecular states. We have also predicted some new molecular states, which could be searched for in forthcoming experimental measurements.

Acknowledgements

This project is supported by the National Natural Science Foundation of China under Grant No. 11375240, No. 11565023.

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