Spectra of the lightest baryons containing two heavy quarks in a potential model

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The spectra of baryons which include two heavy quarks can be treated as a two-body system, where the two heavy quarks constitute a bosonic diquark. We derive the effective potential between the light quark and the heavy diquark in terms of the Bethe-Salpeter equation. To obtain the spectra, several serious problems need to be solved: (1) the operator ordering, (2) the errors caused by the nonrelativistic expansion, (3) spin-spin coupling, and (4) the mixing between the scalar-diquark-baryon and vector-diquark-baryon. In this work we take reasonable approaches to deal with them.

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I. INTRODUCTION

Since the heavy flavor can serve as a static color source as $M_Q \gg \Lambda_{QCD}$, extra symmetries $SU_f(2)\otimes SU_s(2)$ exist [1]. On the other hand, the diquark structure in baryons draws the interest of many theorists of high energy physics [2]. The diquark structure indeed is a bit dubious for baryons which only contain light quarks because of the spatial dispersion of light quarks [3,4].

On the contrary, one can be convinced that if there are two heavy quarks (bb,bc,cc) in a baryon, they would tend to constitute a substantial diquark with small spatial size and serve as a static $\bar{3}$ color source for the light quark [5,6]. Savage and Wise estimated the spectra of baryons with two heavy quarks in heavy quark effective theory [7]. Recently, Ebert *et al.* evaluated the spectra of such baryons in terms of the local Schrödinger-like quasipotential equation [8]. In the framework of the potential model, the interaction between the light quark and the heavy diquark can be derived by calculating their elastic-scattering amplitudes [9], and the key point is the form of the effective vertices for the diquark-gluon interaction. Similarly, Gershtein *et al.* also considered the spectroscopy of doubly charmed baryons where they include angular and radial excited states [10].

In this work, we rederive the effective potential by using the Bethe-Salpeter (BS) equation and obtain the effective vertices. In the derivations, the k^2 dependence is retained explicitly. We find that this dependence leads to an extra Yukawa-type term.

There are several serious problems which have not been carefully discussed in earlier literature [8]. They are (1) to find a systematic way of deriving the form factors at the diquark-gluon vertices; (2) the operator ordering: when one transforms the scattering amplitudes derived in the momentum space into the configuration space, the ordering problem emerges; (3) the parameters obtained by fitting the data of $J/\psi,\Upsilon$, etc. cannot be applied here because a light quark exists and its relativistic effect causes intolerable errors [11]. Therefore, we re-fit the data of $D^{(*)}$ and $B^{(*)}$ mesons to obtain the effective parameters α_s and that for the confinement part; (4) how to properly evaluate the spin-spin coupling term whose coefficient is proportional to $\delta^3(|\mathbf{r}|)$. In this case, only small-distance behavior of the wave function dominates, and the diquark picture may break down, namely, the light quark does not ''see'' the diquark as a whole, but two heavy constituent quarks separately. We need to deal with such a term in a different way; (5) how to investigate possible mixing between the baryon states with the bc diquark being a scalar and an axial vector objects, respectively. We will show that in the framework of the static quantum mechanics, this mixing cannot have a nonzero value, even though it is possible in quantum field theory.

In this work, we not only evaluate the spectra of the baryons which contain two heavy quarks, but also concentrate on several interesting issues about the application of the potential model as well as the diquark structure.

The paper is organized as the following. After this introduction, we present the formulation and concerned theoretical aspects, then discuss the aforementioned problems. In Sec. III, we give the numerical results and the adopted parameters. The last section is devoted to our conclusion and discussion.

II. FORMULATION

A. The effective vertices for diquark-gluon coupling

Since the diquark is not rigorously a pointlike subject, we cannot simply use the vertices in the fundamental QCD theory. Instead, we derive such effective vertices in terms of the BS equation. The diquark contains two heavy quarks which constitute a color $\bar{3}$ triplet, for this bound state the Cornell potential would be a good approximation and we use it as the BS kernel.

We derive the effective vertices for SSg,AAg, and ASg as the following:

$$\langle S'(v')|J_\mu|S(v)\rangle=\sqrt{MM'}[f_1 v'_\mu+f_2 v_\mu] \quad \text{for } SSg \text{ coupling}, \tag{1}$$

$$\begin{aligned}\langle A'(v',\eta')|J_\mu|A(v,\eta)\rangle=\sqrt{MM'}[&f_3(\eta\cdot\eta'^*)v'_\mu+f_4(\eta'^*\cdot\eta)v_\mu+f_5(\eta\cdot v')(\eta'^*\cdot v)v'_\mu+f_6(\eta\cdot v')(\eta'^*\cdot v)v_\mu\\&+f_7\eta'^*_\mu(\eta\cdot v')+f_8(\eta'^*\cdot v)\eta_\mu+f_9 i\epsilon_{\mu\nu\rho\sigma}\eta'^{*\nu}\eta^\rho v'^\sigma\\&+f_{10}i\epsilon_{\mu\nu\rho\sigma}\eta'^{*\nu}\eta^\rho v^\sigma] \quad \text{for } AAg \text{ coupling},\end{aligned} \tag{2}$$

$$\begin{aligned}\langle A'(v',\eta')|J_\mu|S(v)\rangle=\sqrt{MM'}[&f_{11}\eta'^*_\mu+f_{12}(\eta'^*\cdot v)v'_\mu+f_{13}(\eta'^*\cdot v)v_\mu\\&+f_{14}i\epsilon_{\mu\nu\rho\sigma}\eta'^{*\nu}v'^\rho v^\sigma] \quad \text{for } ASg \text{ coupling},\end{aligned} \tag{3}$$

where S and A stand for scalar and axial vector diquarks, v',v,η',η,M',M are the velocities, polarization vectors (for axial vector diquarks only), and masses of the diquarks in the ''final'' and ''initial'' states of the scattering, respectively. The corresponding form factors are derived by solving the BS equation and the details were given in our previous work [6]. In our case, we find relations

$$f_1=f_2=f_7=f_8=-f_3=-f_4=f_{14}=f, \tag{4}$$

and

$$f_9=f_{10}=f_{11}=f_{12}=f_{13}=0. \tag{5}$$

The relations (5) can be realized by simple parity analysis. Obviously, the terms related to f_5 and f_6 are proportional to $|\mathbf{v}|^3$ $(|\mathbf{p}|^3/m^3)$ and hence can be neglected as we only keep the nonrelativistic expansion up to order $\mathbf{p}^2$.

Here we would like to emphasize that in expressions (2) and (3), the order of η and η'^* is not trivial. When we derive these formulas in quantum field theory (QFT), they are commutative, so we can put them in any order. However, as we turn η and η'^* into spin operators of quantum mechanics (QM), the order problem exists. Because the $\mathbf{S}$ operator is not self-commutative, in the operator form, $\eta\cdot\eta'^*\neq\eta'^*\cdot\eta$. Therefore, when we write the expressions, we must be very careful about the order.

The form factors f_i's involve the BS integrals and cannot be analytically expressed. One can only obtain numerical results instead. However, in order to serve our final goal to derive an effective potential, we need an analytical expression for the Fourier transformation. Thus we have simulated the numerical results with various function forms, finally we decide that the following expression:

$$\begin{aligned}\frac{f}{\mathbf{k}^2}&=\left(\frac{A}{\mathbf{k}^2}+\frac{B}{\mathbf{k}^2+C^2}\right)\frac{1}{1+\dfrac{\mathbf{k}^2}{\Lambda^2}}\\&=\frac{A}{\mathbf{k}^2}+\left(\frac{B}{1-\dfrac{C^2}{\Lambda^2}}\right)\frac{1}{\mathbf{k}^2+C^2}-\left(A+\frac{B}{1-\dfrac{C^2}{\Lambda^2}}\right)\frac{1}{\mathbf{k}^2+\Lambda^2},\end{aligned} \tag{6}$$

where $\mathbf{k}$ is the exchanged three-momentum, gives the best fit. The parameters A, B, C and Λ are given from our numerical fit. In this expression, we keep the explicit k dependence of the form factor. In fact, expression (6) can be rewritten as

$$f=\frac{(A+B)\mathbf{k}^2+AC^2}{(\mathbf{k}^2+C^2)}\cdot\frac{1}{1+\dfrac{\mathbf{k}^2}{\Lambda^2}}, \tag{7}$$

and $\mathbf{k}^2+C^2=-(k^2-C^2)$ where k is the four-momentum in the $k_0=0$ case. It is the familiar polelike form factor which is widely used in phenomenology [4].

It is noted that the form factor has the following limits:

$$f\to A=1 \quad \text{as} \quad |\mathbf{k}|\to 0 \quad \text{and} \quad f\to 0 \quad \text{as} \quad |\mathbf{k}|\to\infty,$$

which guarantee the required asymptotic behavior.

B. Effective potential

We derive the effective potential by calculating the elastic-scattering amplitude, then we need to turn the corresponding quantities into the quantum mechanics operators. The polarization vectors η or η' of the axial vector diquarks must be normalized as $\eta^2=\eta'^2=-1$ according to the quantum field theory. Turning $\eta(\eta')$ into a QM spin operator, we have

$$\eta=\frac{1}{\sqrt{2}}\left((\vec{\beta}\cdot\mathbf{S})\gamma,\mathbf{S}+\frac{\gamma-1}{\vec{\beta}^2}(\vec{\beta}\cdot\mathbf{S})\vec{\beta}\right), \tag{8}$$

where $\mathbf{S}$ is the spin operator, $\vec{\beta}=\mathbf{p}/M$, $\gamma=E/M$ are the boost factors, and $\mathbf{p},E,M$ are the momentum, energy and mass, respectively, the factor $1/\sqrt{2}$ guarantees the right normalization for the axial vector diquark $s(s+1)=2$.

The concrete forms of the scattering amplitudes induced by one-gluon exchange, are derived in the standard way:

$$\begin{aligned}M^{gluon}(\mathbf{p},\mathbf{k})=&\langle\lambda^a\lambda^a\rangle g_s^2\frac{1}{16\sqrt{E_1E_1'E_2E_2'}}\\&\times\overline{u}(\mathbf{p}_1')\gamma^\nu u(\mathbf{p}_1)D_{\mu\nu}(\mathbf{k})\langle p_2'|J^\mu|p_2\rangle,\end{aligned} \tag{9}$$

where the Coulomb gauge for the gluon propagator is chosen,

$$D^{00}(k)=-\frac{1}{\mathbf{k}^2},\quad D^{ij}(k)=-\frac{1}{k^2}\left(\delta^{ij}-\frac{k^ik^j}{\mathbf{k}^2}\right),\quad D^{0i}=D^{i0}=0. \tag{10}$$

Thus we have the expressions for the transition amplitudes as the following:

$$\begin{aligned}V^{SS}_{gluon}(\mathbf{p},\mathbf{k})=&-\frac{16\pi\alpha_s}{3}\frac{f}{\mathbf{k}^2}\Bigg[1+\frac{\mathbf{p}^2}{m_1m_2}-\frac{\mathbf{k}^2}{4m_1}\\&\times\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)+\frac{i\mathbf{S}_1\cdot(\mathbf{k}\times\mathbf{p})}{2m_1}\\&\times\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\Bigg]\quad(\text{for } Sq\to Sq);\end{aligned} \tag{11}$$

$$\begin{aligned}V^{AA}_{gluon}(\mathbf{p},\mathbf{k})=&-\frac{16\pi\alpha_s}{3}\frac{f}{\mathbf{k}^2}\Bigg[1+\frac{\mathbf{p}^2}{m_1m_2}-\frac{\mathbf{k}^2}{4m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\\&+\frac{i\mathbf{S}_1\cdot(\mathbf{k}\times\mathbf{p})}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\\&+\frac{i\mathbf{S}_2\cdot(\mathbf{k}\times\mathbf{p})}{4m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\\&-\frac{(\mathbf{S}_1\cdot\mathbf{S}_2)\mathbf{k}^2-(\mathbf{S}_1\cdot\mathbf{k})(\mathbf{S}_2\cdot\mathbf{k})}{4m_1m_2}\Bigg]\\&(\text{for } Aq\to Aq);\end{aligned} \tag{12}$$

$$\begin{aligned}V^{AS}_{gluon}(\mathbf{p},\mathbf{k})=&\frac{16\pi\alpha_s}{3}\frac{f}{2\sqrt{2}\mathbf{k}^2}\Bigg[\frac{i\mathbf{S}_2(\mathbf{k}\times\mathbf{p})}{m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\\&-\frac{(\mathbf{S}_1\cdot\mathbf{S}_2)\mathbf{k}^2-(\mathbf{S}_1\cdot\mathbf{k})(\mathbf{S}_2\cdot\mathbf{k})}{m_1m_2}\Bigg]\\&(\text{for } Aq\to Sq \text{ or } Sq\to Aq),\end{aligned} \tag{13}$$

where m_1 and m_2 are the masses of the light quark and the heavy diquark, respectively.

C. Ordering of operators

When we derive the scattering amplitude in the momentum space, all quantities are commutative. However, when we transform them into the QM operators and carry out a Fourier transformation to the configuration space, there exists an ordering problem in general.

For example, there can be four different orders for $\mathbf{p},\mathbf{p},g(r)$ where $g(r)$ is a function of $r(=|\mathbf{r}|)$[1] as

$$g(\mathbf{r})\hat{\mathbf{p}}^2,\quad \frac{1}{2}[g(\mathbf{r})\hat{\mathbf{p}}^2+\hat{\mathbf{p}}^2g(\mathbf{r})],\quad \hat{\mathbf{p}}\cdot g(\mathbf{r})\hat{\mathbf{p}},$$

$$\frac{1}{4}[g(\mathbf{r})\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\cdot g(\mathbf{r})\hat{\mathbf{p}}+\hat{\mathbf{p}}^2g(\mathbf{r})].$$

In general, the expression $g(r)\hat{\mathbf{p}}^2$ is not Hermitian because $g(r)$ and $\hat{\mathbf{p}}^2$ do not commute even though both are Hermitian operators. At present we only concern the S wave, so all angular-momentum-dependent terms do not exist and all quantities are only functions of radius r. But in our case as we take expectation value of $E(\lambda)=\langle R(\lambda)|H|R(\lambda)\rangle/\langle R(\lambda)|R(\lambda)\rangle$, the situation is worth some discussions.

$g(r)$ and $\hat{\mathbf{p}}^2$ or $\hat{p}_r^2$ do not commute with each other, but one can prove

$$\begin{aligned}&\langle R(r)|g(r)p_r^2|R(r)\rangle\\&=\int_0^\infty R(r)^*g(r)\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)R(r)r^2dr\\&=\int_0^\infty R(r)\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)(g(r)R(r))^*r^2dr,\end{aligned}$$

as long as $g(r)$ is less singular than $1/r$ and the phase of $R(r)$ is a constant. However, in our case of the effective potential, $g(r)$ can be the Coulomb piece and the Yukawa piece, which is as singular as $1/r$, therefore, the above equality does not hold.[2] Thus the hermiticity is broken in this case.

An alternative way to restore the hermiticity is to take a combination $\frac{1}{2}(g(r)p_r^2+p_r^2g(r))$ instead of $g(r)p_r^2$. However, as the form of $g(r)p_r^2$ is widely adopted in literature, we also list the numerical results evaluated with the ordering scheme $g(r)p_r^2$ in Table I for a comparison with the other three schemes.

In [8], only the scheme $\hat{\mathbf{p}}g(r)\hat{\mathbf{p}}$ is taken. In our work, we compare the different ordering schemes and our numerical results show that different schemes which retain the hermiticity would lead to different parametrizations, but the final measurable spectra are not very sensitive to the ordering (see the ordering 2 to 4 in Table I).

D. The potential in the configuration space

Finally, we have the full Hamiltonian

$$H=K+V, \tag{14}$$

where K is the kinetic part and the potential is

$$V=V_{gluon}+V_{conf}, \tag{15}$$

and

$$V_{conf}=V^V_{conf}+V^S_{conf}, \tag{16}$$

[1]Maybe, there could be more other schemes, but they are not reasonable, so we only discuss these four commonly adopted schemes.

[2]Detailed discussions and proof will be published in a separate work.

TABLE I. Binding energies and masses for doubly heavy baryons in different ordering schemes.

Type	Ordering 1		Ordering 2		Ordering 3		Ordering 4	
	e	M_B	e	M_B	e	M_B	e	M_B
$(ccq)(1/2)$	0.1158	3.7058	0.1231	3.7131	0.1370	3.7270	0.1170	3.7070
$(ccq)(3/2)$	0.2319	3.8219	0.2297	3.8197	0.2534	3.8434	0.2336	3.8236
$(ccs)(1/2)$	0.1278	3.8878	0.0109	3.7709	0.0351	3.7951	0.0581	3.8181
$(ccs)(3/2)$	0.2436	4.0036	0.1312	3.8912	0.1532	3.9132	0.1744	3.9344
$(cbq)(1/2)_S$	0.2063	7.0563	0.1807	7.0307	0.1978	7.0478	0.1863	7.0363
$(cbq)(1/2)_A$	0.1555	7.0055	0.1286	6.9786	0.1469	6.9969	0.1354	6.9854
$(cbq)(3/2)_A$	0.2317	7.0817	0.2066	7.0566	0.2233	7.0733	0.2117	7.0617
$(cbs)(1/2)_S$	0.2040	7.2240	0.0625	7.0825	0.0926	7.1126	0.1206	7.1406
$(cbs)(1/2)_A$	0.1529	7.1729	0.0092	7.0292	0.0406	7.0606	0.0693	7.0893
$(cbs)(3/2)_A$	0.2295	7.2495	0.0891	7.1091	0.1186	7.1386	0.1461	7.1661
$(bbq)(1/2)$	0.1813	10.3013	0.1424	10.2624	0.1623	10.2823	0.1524	10.2724
$(bbq)(3/2)$	0.2190	10.3390	0.1815	10.3015	0.2004	10.3204	0.1903	10.3103
$(bbs)(1/2)$	0.1794	10.4694	0.0265	10.3165	0.0589	10.3489	0.0896	10.3796
$(bbs)(3/2)$	0.2069	10.4969	0.0665	10.3565	0.0978	10.3878	0.1277	10.4177

where the superscripts V and S denote the vector and scalar parts of the confinement (see below), respectively. The single gluon exchange potential V_{gluon} has the following forms:

$$V_{gluon}=V'^{SS,AA,SA}_{gluon}+V_{spin}, \tag{17}$$

where the explicit forms of $V'^{SS,AA,SA}_{gluon}$ are given below and V_{spin} is the spin-spin coupling part whose coefficients are proportional to $\delta^3(r)$ and will be discussed in Sec. II F.

We have the following concrete forms of $V'^{SS,AA,SA}$:

$$\begin{aligned}V'^{SS}_{gluon}(r)=&-\frac{4\alpha_s}{3}\Bigg[\frac{A}{r}+\frac{A}{4m_1m_2}\left(\frac{1}{r}\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\frac{1}{r}\hat{\mathbf{p}}+\hat{\mathbf{p}}^2\frac{1}{r}\right)-\frac{\pi A}{m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\delta(\mathbf{r})-\frac{A}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\frac{\mathbf{S}_1\cdot\mathbf{L}}{r^3}+\frac{B'e^{-Cr}}{r}\\&+\frac{B'}{4m_1m_2}\left(\frac{e^{-Cr}}{r}\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\frac{e^{-Cr}}{r}\hat{\mathbf{p}}+\hat{\mathbf{p}}^2\frac{e^{-Cr}}{r}\right)+\frac{B'C^2}{4m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\frac{e^{-Cr}}{r}-\frac{B'}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\frac{(Cr+1)e^{-Cr}}{r^3}\mathbf{S}_1\cdot\mathbf{L}\\&+\frac{De^{-\Lambda r}}{r}+\frac{D}{4m_1m_2}\left(\frac{e^{-\Lambda r}}{r}\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\frac{e^{-\Lambda r}}{r}\hat{\mathbf{p}}+\hat{\mathbf{p}}^2\frac{e^{-\Lambda r}}{r}\right)+\frac{D\Lambda^2}{4m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\frac{e^{-\Lambda r}}{r}\\&-\frac{D}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\frac{(\Lambda r+1)e^{-\Lambda r}}{r^3}\mathbf{S}_1\cdot\mathbf{L}\Bigg],\quad(\text{for scalar-diquark}+q\ \text{ baryons}),\end{aligned} \tag{18}$$

$$\begin{aligned}V'^{AA}_{gluon}(r)=&-\frac{4\alpha_s}{3}\Bigg[\frac{A}{r}+\frac{A}{4m_1m_2}\left(\frac{1}{r}\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\frac{1}{r}\hat{\mathbf{p}}+\hat{\mathbf{p}}^2\frac{1}{r}\right)-\frac{\pi A}{m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\delta(\mathbf{r})-\frac{A}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\frac{\mathbf{S}_1\cdot\mathbf{L}}{r^3}\\&-\frac{A}{4m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{\mathbf{S}_2\cdot\mathbf{L}}{r^3}-\frac{A}{4m_1m_2}\frac{S_{12}}{r^3}+\frac{B'e^{-Cr}}{r}+\frac{B'}{4m_1m_2}\left(\frac{e^{-Cr}}{r}\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\frac{e^{-Cr}}{r}\hat{\mathbf{p}}+\hat{\mathbf{p}}^2\frac{e^{-Cr}}{r}\right)\\&+\frac{B'C^2}{4m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\frac{e^{-Cr}}{r}-\frac{B'}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\frac{(Cr+1)e^{-Cr}}{r^3}\mathbf{S}_1\cdot\mathbf{L}\\&-\frac{B'}{4m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{(Cr+1)e^{-Cr}}{r^3}\mathbf{S}_2\cdot\mathbf{L}-\frac{B'}{12m_1m_2}\end{aligned}$$

$$\times\frac{C^2r^2+3Cr+3}{r^3}e^{-Cr}S_{12}+\frac{B'}{6m_1m_2}\frac{C^2e^{-Cr}}{r}\mathbf{S}_1\cdot\mathbf{S}_2+\frac{De^{-\Lambda r}}{r}+\frac{D}{4m_1m_2}\left(\frac{e^{-\Lambda r}}{r}\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}\frac{e^{-\Lambda r}}{r}\hat{\mathbf{p}}+\hat{\mathbf{p}}^2\frac{e^{-\Lambda r}}{r}\right)$$

$$+\frac{D\Lambda^2}{4m_1}\left(\frac{1}{2m_1}+\frac{1}{m_2}\right)\frac{e^{-\Lambda r}}{r}-\frac{D}{2m_1}\left(\frac{1}{m_1}+\frac{2}{m_2}\right)\frac{(\Lambda r+1)e^{-\Lambda r}}{r^3}\mathbf{S}_1\cdot\mathbf{L}-\frac{D}{4m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{(\Lambda r+1)e^{-\Lambda r}}{r^3}\mathbf{S}_2\cdot\mathbf{L}$$

$$-\frac{D}{12m_1m_2}\frac{\Lambda^2r^2+3\Lambda r+3}{r^3}e^{-\Lambda r}S_{12}+\frac{D}{6m_1m_2}\frac{\Lambda^2e^{-\Lambda r}}{r}\mathbf{S}_1\cdot\mathbf{S}_2\Bigg],\quad (\text{for axial-vector-diquark}+q\ \text{ baryons}), \tag{19}$$

$$V'^{SA}_{gluon}(r)=-\frac{4\alpha_s}{3}\Bigg[\frac{A}{2\sqrt{2}m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{\mathbf{S}_2\cdot\mathbf{L}}{r^3}+\frac{A}{2\sqrt{2}m_1m_2}\frac{S_{12}}{r^3}+\frac{B'}{2\sqrt{2}m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{(Cr+1)e^{-Cr}}{r^3}\mathbf{S}_2\cdot\mathbf{L}$$

$$+\frac{B'}{6\sqrt{2}m_1m_2}\frac{C^2r^2+3Cr+3}{r^3}e^{-Cr}S_{12}-\frac{B'}{3\sqrt{2}m_1m_2}\frac{C^2e^{-Cr}}{r}\mathbf{S}_1\cdot\mathbf{S}_2+\frac{D}{2\sqrt{2}m_2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\frac{(\Lambda r+1)e^{-\Lambda r}}{r^3}\mathbf{S}_2\cdot\mathbf{L}$$

$$+\frac{D}{6\sqrt{2}m_1m_2}\frac{\Lambda^2r^2+3\Lambda r+3}{r^3}e^{-\Lambda r}S_{12}-\frac{D}{3\sqrt{2}m_1m_2}\frac{\Lambda^2e^{-\Lambda r}}{r}\mathbf{S}_1\cdot\mathbf{S}_2\Bigg],$$

$$(\text{for mixing between scalar-diquark}+q\ \text{ and axial-vector-diquark}+q\ \text{ baryons}), \tag{20}$$

where

$$B'\equiv\frac{B}{1-\dfrac{C^2}{\Lambda^2}},\quad D\equiv-(A+B').$$

E. The confinement part

The confinement part of the potential is fully due to the nonperturbative QCD effects and is not derivable in any established theoretical framework. So far, one can only postulate its form and determine the concerned parameters by fitting data.

The most commonly adopted confinement form is the linear potential $V^0_{conf}=ar+b$ at the leading order, where a,b are the parameters in the linear confinement potential, which will be determined in the variational method (see Sec. III). It can be split into scalar and vector pieces which may lead to different relativistic corrections. Since its source is obscure so far, one cannot decide the fraction of each piece. But in general, it can be written as [8]

$$V^{S0}_{conf}(r)=\kappa(ar+b), \tag{21}$$

$$V^{V0}_{conf}(r)=(1-\kappa)(ar+b), \tag{22}$$

where we have introduced a parameter κ to describe the fractions of scalar and vector pieces. In later numerical calculations, we will employ several typical values of κ.

The resultant confinement potentials with all relativistic corrections are

$$V^S_{conf}(r)=V^{S0}_{conf}(r)-\frac{1}{2m_1^2}\mathbf{p}V^{S0}(r)\mathbf{p}+\frac{1}{8m_1^2}\nabla^2V^{S0}(r)$$
$$-\frac{1}{2m_1^2}\frac{V'^{S0}(r)}{r}\mathbf{S}_1\cdot\mathbf{L}-\frac{1}{2m_2^2}\frac{V'^{S0}(r)}{r}\mathbf{S}_2\cdot\mathbf{L}, \tag{23}$$

$$V^V_{conf}(r)=V^{V0}_{conf}(r)-\frac{1}{4m_1}\left(\frac{1}{2\mu}+\frac{1}{2m_2}-\frac{1+\kappa}{m_1}\right)\nabla^2V^{V0}(r)$$
$$+\frac{1}{m_1m_2}\mathbf{p}V^{V0}(r)\mathbf{p}+\frac{1}{m_1}\left(\frac{1+\kappa}{\mu}-\frac{1}{2m_1}\right)$$
$$\times\frac{V'^{V0}(r)}{r}\mathbf{S}_1\cdot\mathbf{L}-\frac{1}{2m_2^2}\frac{V'^{V0}(r)}{r}\mathbf{S}_2\cdot\mathbf{L}$$
$$+\frac{2(1+\kappa)}{3m_1m_2}\nabla^2V^{V0}(r)\mathbf{S}_1\cdot\mathbf{S}_2+\frac{1+\kappa}{3m_1m_2}$$
$$\times\left(\frac{V'^{V0}(r)}{r}-V''^{V0}(r)\right)S_{12}, \tag{24}$$

where

$$S_{12}\equiv\frac{3}{r^2}(\mathbf{S}_1\cdot\mathbf{r})(\mathbf{S}_2\cdot\mathbf{r})-\mathbf{S}_1\cdot\mathbf{S}_2.$$

Obviously, in the S wave with which we are concerned in this work, the contribution of the tensor S_{12} is 0.

F. The spin-spin interaction with coefficient proportional to the δ function

The formulas directly derived by assuming the diquark structure cannot be applied to evaluate the spin-spin coupling as discussed above. Since V^{SA} cannot be handled in the framework of the static quantum mechanics, we omit the contents concerning V^{SA}, but only deal with V^{SS} and V^{AA}. The coefficients of the operator $\mathbf{S}_1\cdot\mathbf{S}_2$ are proportional to the δ function, namely it is only significant for the small distance between the light quark and the diquark. However, as the distance becomes so small, the light quark would no longer see the diquark as a whole object, but as two separate heavy quarks. It means that the interaction term $g(M_D)\delta^3(|\mathbf{r}|)\mathbf{S}_1\cdot\mathbf{S}_2$, where $g(M_D)$ is a function of the diquark mass M_D, is not properly presented and this issue was not discussed in the earlier literature [3].

Strictly, we should obtain the three-body wave function from a much more complicated framework, such as the Faddeev equation, but it is too difficult. Instead, we will employ a simple phenomenological means to deal with this problem.

The term $g(M_D)\delta^3(|\mathbf{r}|)$ which would be in the form $-2\pi A/3m_qM_D(\mathbf{S_1}\cdot\mathbf{S}_2)\delta^3(\mathbf{r})$ in the diquark picture should be replaced by

$$V_{spin}=g(m_{Q'})\delta^3(|\mathbf{r}-\mathbf{r}_2'|)\mathbf{S}_1\cdot\mathbf{S}_2' +g(m_{Q''})\delta^3(|\mathbf{r}-\mathbf{r}_2''|)\mathbf{S}_1\cdot\mathbf{S}_2'', \tag{25}$$

where $g(M_D),g(m_{Q'}),g(m_{Q''})$ are functions of the masses of diquark, heavy quarks 1 and 2, respectively, (as noted, they have the same expression) and $\mathbf{r}-\mathbf{r}_2',\mathbf{r}-\mathbf{r}_2''$ are distance vectors between the light quark and the concerned heavy quarks Q' and Q'', respectively. We also have

$$g(m_Q)\propto\frac{1}{m_qm_Q},$$

where m_Q is the mass of the heavy quark in the meson. Since more significant effects only occur at $|\mathbf{r}-\mathbf{r}_2'|\to 0$ or $|\mathbf{r}-\mathbf{r}_2''|\to 0$, we can make the decomposition and each term deals with the interaction between the light quark and only one of the heavy quarks while another acts as a spectator.

In our strategy, we take $V'^{SS,AA}_{gluon}+V_{conf}$ as the 0th order potential and then treat V_{spin} as a perturbation. For the *S*-wave case, the tensor S_{12} does not contribute, so only $\mathbf{S}_1\cdot\mathbf{S_2}$ is responsible for the splitting of states.

Taking the spin-spin interaction as perturbation, these two terms would result in an extra contribution as

$$\Delta E_{spin}=g(m_{Q'})\langle\mathbf{S}_1\cdot\mathbf{S}_2'\rangle|\Psi_{qQ'}(0)|^2+g(m_{Q''}) \times\langle\mathbf{S}_1\cdot\mathbf{S}_2''\rangle|\Psi_{qQ''}(0)|^2, \tag{26}$$

where each term is proportional to the square of the wave function at origin $|\Psi_{qQ}(0)|^2$. Since the spectator heavy quark does not participate in the interaction [similar to the parton model in deep inelastic scattering], its wave function can be normalized away.

In analog to the analysis of Falk *et al.* [5], $|\Psi_{qQ}(0)|^2$ can be associated with the square of the wave function of the corresponding meson $\overline{q}Q(q\overline{Q})$. $\overline{q}Q$ constitutes a color singlet, while qQ remains as a color $\overline{3}-$triplet. This difference would cause a color factor to $|\Psi_{qQ}(0)|^2$. The authors of Ref. [5] suggested that in a hydrogenlike potential the wave function at origin $\Psi(0)$ is proportional to $(C_F\alpha_s)^{3/2}$. Since $\Psi(0)$ is mainly determined by the Coulomb part of the potential, a suppression factor 1/8 appears in $|\Psi_{qQ}|^2$ compared to $|\Psi_{\overline{q}Q}(0)|^2$ as $\overline{q}Q$ resides in a color singlet and qQ exists in a color-anti-triplet $\overline{3}$.

Indeed, for an *S*-wave meson, the splitting between M and M^* is only caused by the spin-spin interaction, so we can use the mass splittings $M_{D^*}-M_D, M_{B^*}-M_B, M_{D_s^*}-M_{D_s}$ as inputs to obtain the corresponding values for the baryons.

Substituting this relation into ΔE_{spin} we have

$$\Delta E_{spin}=\langle\mathbf{S}_1\cdot\mathbf{S}_2'\rangle_B\left(\frac{M^*_{M'}-M_{M'}}{8\langle\mathbf{S}_1\cdot\mathbf{S}_2'\rangle_M}\right) +\langle\mathbf{S}_1\cdot\mathbf{S}_2''\rangle_B\left(\frac{M^*_{M''}-M_{M''}}{8\langle\mathbf{S}_1\cdot\mathbf{S}_2''\rangle_M}\right), \tag{27}$$

where M' and M'' are the corresponding mesons and the subscripts B and M denote that the matrix elements of the spin coupling are taken for the baryon and meson, respectively. Meanwhile we need to keep the total spin of the two-heavy-quark system (diquark)

$$\mathbf{S}_2'+\mathbf{S}_2''=\mathbf{S}_2$$

to be 0 (scalar) or 1 (axial vector) as a constraint. Thus the matrix elements $\langle\mathbf{S}_1\cdot\mathbf{S}_2'(\mathbf{S}_2'')\rangle$ can be calculated straightfowardly.

Obviously, for the cc or bb diquark system, the common factors can be pulled out, so the result would be the same as treating the diquark as a whole object, but for the bc system, $g(m_{Q'})\neq g(m_{Q''})$ and $|\Psi_{qQ'}(0)|\neq|\Psi_{qQ''}(0)|$, the two components in V_{spin} would make different contributions.

It is noticed that there are no data for B_s^* yet, we cannot directly input experimental value for $M_{B_s^*}$ into our calculation. As noted, the function in front of $\mathbf{S}_1\cdot\mathbf{S}_2'^{(\prime\prime)}$ is inversely proportional to m_qm_Q and the data also tell us that the mass splittings of B^* and B is about 45.7 MeV, and is 142.12 MeV for D and D^*, their ratio is roughly 45.7/142.12 $\approx m_c/m_b\sim$1.55/4.88 which are the masses adopted in [3] and this work. This is consistent with what we learned from our derivation. Therefore we can assume that

$$M_{B_s^*}-M_{B_s}=\frac{m_c}{m_b}(M_{D_s^*}-M_{D_s}).$$

It is noted that the wave functions of B and D mesons at the origin are only related to the reduced masses which tend to be the mass of the light quark, so $|\Psi_B(0)|\approx|\Psi_D(0)|$.

III. THE NUMERICAL RESULTS

We employ the variational method to evaluate the spectra. In a previous paper we discussed the accuracy of the method [12], so here we omit all details.

A. The parameters α_s, a, and b

As noticed, the relativistic effects are serious because of the existence of a light quark. Unlike the heavy quarkonium, such as $J/\psi,\Upsilon$ etc., truncation of the nonrelativistic expansion where we only keep the order up to $\mathbf{p}^2/m^2$, is not a good approximation. However, we can partly compensate these effects by attributing the uncertainties to the potential parameters which are not directly measurable. In other words, in the process of fitting data of mesons containing a light quark, such as $B^{(*)}$, we have attributed the unknown factors into the phenomenological parameters, then later when we use the set of parameters to evaluate the spectra of baryons containing two heavy quarks and a light quark, the nonperturbative QCD effects and the relativistic influence are effectively included. Obviously in this case, if one uses the parameters obtained by fitting the data for heavy quarkonia, the errors are uncontrollable. Here we choose to use the data for $B^{(*)}$ to obtain α_s, a and b. When we use the variational method to obtain the parameters, we retain all the relativistic corrections in the potential for $B^{(*)}$ mesons.

B. Spectra of the baryons

Then we turn to calculate the spectra of the baryons containing two heavy quarks, in terms of the variational method. The expectation value of H is

$$E(\lambda)=\langle H\rangle=\frac{\langle R(\lambda)|H|R(\lambda)\rangle}{\langle R(\lambda)|R(\lambda)\rangle}, \tag{28}$$

where $R(\lambda)$ is a trial function. Then minimizing $E(\lambda)$ as

$$\frac{dE(\lambda)}{d\lambda}=0,$$

we obtain the λ value. In the expression H is the Hamiltonian $K+V'^{SS,AA}_{gluon}$, while V_{spin} is taken as the perturbation.

The advantage of using the variational method is obvious, that is, we are able to treat all terms simultaneously. In the perturbation method where large relativistic corrections are dealt with perturbatively, remarkable errors for the baryons which contain not only two heavy quarks but also a light one, emerge due to the ill treatment. On the contrary, the ambiguities can be avoided in our approach.

In the following we list the parameters to be used for numerical computation.

The values for A,B,C in Eq. (6) are

$$A=1.00,\quad B=-1.00,\quad C=3.11\ \text{GeV},\quad \Lambda=2.86\ \text{GeV},\quad \text{for the } cc \text{ diquark;}$$

$$A=1.00,\quad B=-1.00,\quad C=8.30\ \text{GeV},\quad \Lambda=6.45\ \text{GeV},\quad \text{for the } bc \text{ diquark;}$$

$$A=1.00,\quad B=-1.00,\quad C=5.09\ \text{GeV},\quad \Lambda=4.33\ \text{GeV},\quad \text{for the } bb \text{ diquark.}$$

The masses of the diquarks should be calculated with the b and c quark masses as inputs. The constituent quark masses and the heavy diquark masses have the following values [3]:

$$m_u=m_d=0.33\ \text{GeV},\quad m_s=0.5\ \text{GeV},\quad m_c=1.55\ \text{GeV},\quad m_b=4.88\ \text{GeV},$$

$$M_{cc}=3.26\ \text{GeV},\quad M_{bc}=6.52\ \text{GeV},\quad M_{bb}=9.79\ \text{GeV}.$$

It is noted that the bb and cc diquark must be axial vectors, but bc can be either a scalar or an axial vector, the mass splitting between the scalar and axial vector bc diquarks can be neglected in practical calculations. The heavy diquark masses were also obtained in the BS equation approach [6] and their values are very close to those in [3]. The numerical results from these two sets of diquark masses undergo little changes.

The baryon spectra are calculated and the results are given in Tables I and II, in units of GeV. In Table I, we choose $\kappa=-1$ for the confinement potential which is consistent with that used in Ref. [8], and list results corresponding to various ordering schemes. In Table II, we change the κ values in the confinement potential and use the ordering scheme 2, i.e., $\hat{\mathbf{p}}g(\mathbf{r})\hat{\mathbf{p}}$.

In Table I, $q=u$ or d, ''ordering 1'' means $g(r)\hat{\mathbf{p}}^2$, where $\alpha_s=0.23,a=0.11,b=-0.13$; ''ordering 2'' means $\frac{1}{2}[g(r)\hat{\mathbf{p}}^2+\hat{\mathbf{p}}^2g(r)]$ where $\alpha_s=0.46,a=0.12,b=-0.31$; ''ordering 3'' is for $\hat{\mathbf{p}}g(r)\hat{\mathbf{p}}$ with $\alpha_s=0.41,a=0.09,b=-0.21$; ''ordering 4'' means $[g(r)\hat{\mathbf{p}}^2+2\hat{\mathbf{p}}g(r)\hat{\mathbf{p}}+\hat{\mathbf{p}}^2g(r)]/4$ with $\alpha_s=0.23,a=0.11,b=-0.27$. The subscript A and S stand for axial vector and scalar, respectively. e is the binding energy and M_B is the baryon mass with unit GeV. In the calculations, $\kappa=-1$.

TABLE II. Binding energies and masses for doubly heavy baryons with different κ values.

Type	$\kappa=0$	$\kappa=0.5$	$\kappa=1.0$
$(ccq)(1/2)$	$e=0.1423,\ M_B=3.7323$	$e=0.1619,\ M_B=3.7519$	$e=0.1474,\ M_B=3.7374$
$(ccq)(3/2)$	$e=0.2605,\ M_B=3.8505$	$e=0.2792,\ M_B=3.8692$	$e=0.2674,\ M_B=3.8574$
$(ccs)(1/2)$	$e=0.0258,\ M_B=3.7858$	$e=0.0368,\ M_B=3.7968$	$e=-0.0176,\ M_B=3.7424$
$(ccs)(3/2)$	$e=0.1459,\ M_B=3.9059$	$e=0.1563,\ M_B=3.9163$	$e=0.1057,\ M_B=3.8657$
$(cbq)(1/2)_S$	$e=0.2101,\ M_B=7.0601$	$e=0.2303,\ M_B=7.0803$	$e=0.2209,\ M_B=7.0709$
$(cbq)(1/2)_A$	$e=0.1584,\ M_B=7.0084$	$e=0.1790,\ M_B=7.0290$	$e=0.1681,\ M_B=7.0181$
$(cbq)(3/2)_A$	$e=0.2359,\ M_B=7.0859$	$e=0.2559,\ M_B=7.1059$	$e=0.2467,\ M_B=7.0967$
$(cbs)(1/2)_S$	$e=0.0876,\ M_B=7.1076$	$e=0.0981,\ M_B=7.1181$	$e=0.0453,\ M_B=7.0653$
$(cbs)(1/2)_A$	$e=0.0347,\ M_B=7.0547$	$e=0.0454,\ M_B=7.0654$	$e=-0.0091,\ M_B=7.0109$
$(cbs)(3/2)_A$	$e=0.1141,\ M_B=7.1341$	$e=0.1245,\ M_B=7.1445$	$e=0.0724,\ M_B=7.0924$
$(bbq)(1/2)$	$e=0.1747,\ M_B=10.2947$	$e=0.1969,\ M_B=10.3169$	$e=0.1872,\ M_B=10.3072$
$(bbq)(3/2)$	$e=0.2134,\ M_B=10.3334$	$e=0.2353,\ M_B=10.3553$	$e=0.2266,\ M_B=10.3466$
$(bbs)(1/2)$	$e=0.0536,\ M_B=10.3436$	$e=0.0650,\ M_B=10.3550$	$e=0.0112,\ M_B=10.3012$
$(bbs)(3/2)$	$e=0.0934,\ M_B=10.3834$	$e=0.1046,\ M_B=10.3946$	$e=0.0523,\ M_B=10.3423$

In Table II, for the confinement potential $V^S_{conf}=\kappa(ar+b), V^A_{conf}=(1-\kappa)(ar+b)$, we have for $\kappa=0$, the fitted $\alpha_s=0.44, a=0.14, b=-0.37$; for $\kappa=0.5$, the fitted $\alpha_s=0.5, a=0.14, b=-0.37$; for $\kappa=1$, the fitted $\alpha_s=0.73, a=0.16, b=0.45$. Here we use the ordering scheme 3, i.e., $\hat{\mathbf{p}}g(r)\hat{\mathbf{p}}$.

IV. CONCLUSION AND DISCUSSION

When we evaluate the spectra of baryons which contain two heavy quarks, the diquark picture is in general reasonable, but there are several serious problems which we should deal with carefully.

First, effective vertices $DD'g$ where D and D' are scalar or axial vector diquarks and g is gluon must be derived and the obtained form factors describe the spatial dispersion of the diquark objects. We derive the form factors at the vertices based on the BS equation and we can keep their explicit k^2 dependence which leads to an extra Yukawa-type term in the potential.

Secondly, we investigate the ordering problem which is brought up by the Fourier transformation with respect to the exchanged momentum $\mathbf{k}$ and the momentum $\mathbf{p}$. We find that various ordering schemes can lead to different parametrizations for the effective α_s, a, and b, which are not directly measurable. However, we also notice that the final results deviate from each other by about a few of tens MeV as long as the hermiticity is respected (ordering 2 to 4 in Table I), but if the operator determined by the ordering scheme is not Hermitian, the deviation from others is obvious (about 100 MeV) (see the ordering 1 in Table I).

Because the relativistic effects are very serious in the case where a light flavor is involved, the variational method is superior to the perturbative method. To reduce the uncertainties and errors brought up by the truncation of the nonrelativistic expansion, we use the $B^{(*)}$ data, where a light quark is moving around the heavy b quark, as inputs to obtain suitable parametrization. As hoped, most of those uncertainties can be alleviated.

Since the $\delta^3(r)\mathbf{S}_1\cdot\mathbf{S}_2$ term in the potential might violate the diquark picture, we separate out this piece from the others and we take it as a perturbation, then deal with it in a phenomenological approach.

Even though the diquark picture is believed to work in this case and the derived form factors further improves the situation, there still exists small deviation from reality, including the diquark masses. This should be further investigated.

Finally, as we pointed out above, although the mixing term which is derived in QFT is not trivially zero, when we sandwich it among the quantum states, we have

$$\langle\psi(1/2,A,l=0)|V^{(SA)}_{gluon}|\psi(1/2,S,l=0)\rangle$$

$$=\langle\psi(1/2,A,l=1)|V^{(SA)}_{gluon}|\psi(1/2,S,l=1)\rangle\equiv 0. \qquad (29)$$

The matrix elements are absolutely zero. This is because in the framework of nonrelativistic quantum mechanics there are no creation and annihilation operators as in QFT, consequently, we can only deal with elastic scattering. The mixing between $\psi(1/2,A)$ and $\psi(1/2,S)$ refers to a change of spin or particle identity, so cannot appear in QM even though we know such mixing must exist and may play important roles to hadron spectra. For example, in a completely different area of the hadron spectroscopy, the mixing between glueball and quarkonium is known to be very important or even crucial to phenomenology, but we cannot evaluate it in the potential model. We will further study these mixing effects in our future work [13].

The *B* factory and other facilities of high-energy experiments may provide data on baryons which containe two heavy quarks. Once the data are available, we may readjust our input parameters and make further predictions on the spectra and other characters of the baryons, and we can also testify the validity of the diquark picture and the nonrelativistic potential model.

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