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Variational study of weakly coupled triply heavy baryons

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ABSTRACT: Baryons made of three heavy quarks become weakly coupled, when all the quarks are sufficiently heavy such that the typical momentum transfer is much larger than $\Lambda_{\rm QCD}$. We use variational method to estimate masses of the lowest-lying *bcc*, *ccc*, *bbb* and *bbc* states by assuming they are Coulomb bound states. Our predictions for these states are systematically lower than those made long ago by Bjorken, but still compatible with the known mass inequalities in QCD.

KEYWORDS: Heavy Quark Physics, QCD, Asymptotic Freedom, NLO Computations.

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1. Introduction

The field of heavy quark spectroscopy is experiencing a rapid renaissance, mainly propelled by the emergencies of several unusual charmonium resonances, of which X(3872), Y(4260)are the highlights [1]. Accompanied with these unexpected discoveries, progress has also been made steadily in the more traditional sector of charmonium spectroscopy, exemplified by the recent sightings of several long-awaited particles such as $\eta_c(2S)$, h_c , and particularly the doubly-charmed baryons such as Ξ_{cc}^+ , Ξ_{cc}^{++} . Precise knowledge of their properties will help to refine our present understanding of heavy quark dynamics [2].

After the tentative establishment of the doubly charmed baryons [3], one may naturally expects to fill the baryon family with the last missing member, *i.e.*, baryons composed entirely of heavy quarks, denoted the QQQ states in short. Being a baryonic analogue of heavy quarkonium, the triply-heavy baryons are of considerable theoretical interest, since they are free of light quark contamination and may serve as a clean probe to the interplay between perturbative and nonperturbative QCD.

One of the basic properties of these heaviest baryons in Nature is their masses, which will be the primary concern of this paper. In contrast with the spectra of the singlyheavy and doubly-heavy baryons, to which a vast number of literature based on either phenomenological approaches or lattice QCD simulations are dedicated, only sparse attention has been paid to the spectroscopy of triply-heavy baryons, perhaps mainly due to the lack of experimental incentive. The interest toward these baryons can be traced back to Bjorken, who first carried out a comprehensive studies on their properties two decades ago, particularly focusing on the discovery potential of the triply-charmed baryon state [4]. Reconstructing a QQQcandidate is a rather challenging job experimentally, since it is difficult to separate all the decay products emerging from the cascade decay chain $QQQ \rightarrow QQq \rightarrow Qqq$ from the copious hadronic background. Nevertheless, according to Bjorken, some semileptonic decay channels such as $\Omega_{ccc}^{++} \rightarrow \Omega^- + 3\mu^+ + 3\nu_{\mu}$, may offer a clean signature to trigger a *ccc* event.

Needless to say, the discovery potential of triply-heavy baryons also crucially depends on the production environment. Baranov and Slad have shown that the production cross sections for triply-charmed baryons at e^+e^- collider are too tiny to be practically relevant [5]. Gomshi-Nobary and Sepahvand have recently calculated the fragmentation functions of c and b evolving into various triply-heavy baryons, and estimated that the corresponding fragmentation probabilities vary in the range $10^{-7} \sim 10^{-4}$ [6]. They consequently estimated two largest cross sections, which are associated with producing Ω_{bcc} and Ω_{ccc} , to be about 2 and 0.3 nb in the forthcoming Large Hadron Collider (LHC) experiment with cuts of $p_T > 10$ GeV and |y| < 1. For an integrated luminosity of 300 fb⁻¹ (about one year of running at the LHC design luminosity $\mathcal{L} = 10^{34} \text{ cm}^2 \text{ s}^{-1}$), the amount of Ω_{bcc} and Ω_{ccc} yield can reach about 6×10^8 and 1×10^8 . It seems rather promising to establish these two states in such a large data sample.

Stimulated by the discovery possibility of triply-heavy baryons in near future, it is no longer of only academic interest to study their properties like mass spectra. Unfortunately, no predictions to the masses of triply heavy baryons from lattice QCD simulations have emerged yet (only the static three-quark potential has been measured [7, 8]), and one has to resort to other theoretical means at this moment.

Heavy quarkonium spectroscopy is traditionally the arena of phenomenological potential models, which in general incorporate a long-range confinement interaction [9-11](see also Godfrey's contribution in [2]). Nevertheless, recent advances in nonrelativistic effective field theories of QCD, particularly the effective theory dubbed potential NRQCD (pNRQCD), has started to put heavy quarkonium spectroscopy on a model-independent ground [12] (for a recent review, see [13]). A novel aspect of this effective field theory is that the interquark potential arises as the matching coefficients. In this language, different quarkonium states are categorized with respect to the relative magnitude between the typical momentum scale, mv, and the nonperturbative QCD scale, $\Lambda_{\rm QCD}$. In the case of $mv \gg \Lambda_{\rm QCD}$, the corresponding state is said to be *weakly coupled*, and the dynamics is largely dictated by the short-distance potential which can be calculated order by order in α_s , whereas the confinement potential is unimportant; in the other situation like $mv \sim \Lambda_{\rm QCD}$, the state is said to be strongly coupled since the potential is no longer calculable in perturbation theory, instead must be determined by nonperturbative methods such as lattice QCD. It is in the latter situation that a pNRQCD framework intimately resembles the phenomenological Cornell model.

Contrary to the traditional wisdom that the confinement potential is indispensable for any heavy quarkonium state, evidences are accumulating to hint that Υ , B_c may well be identified with the weakly-coupled system, whereas J/ψ lies in the borderline between the weak and strong couping regime, and the first few excited bottomonium states (far from the open flavor threshold) belong to the strongly-coupled system [13]. Numerous work involving higher order perturbative calculation of the mass spectrum seems to endorse the weak-coupling assignment of the lowest-lying heavy quarkonium states (for an incomplete list of work on perturbative computation of mass spectrum, see Ref. [14–19]).

In parallel with the formulation of pNRQCD for the quarkonium, Brambilla, Vairo and Rosch have recently laid down an analogous framework for triply-heavy baryons [20]. The effective Lagrangian has been written down for both weakly-coupled and strongly-coupled QQQ states, with some of the matching coefficients supplied. Among various possible applications of Ref. [20], exploring the mass spectra of QQQ states is the most straightforward to think of. This is the very goal of the present work. To make things more tractable, we will confine ourselves in this work to the weakly-coupled states only. The Ω_{ttt} , if exists, would be an ideal prototype for such a state. However, to be phenomenologically relevant, we have to stick to baryons made exclusively of bottom or charm. As in quarkonium, most probably only the ground states are amenable to a weak-coupling assignment. To be objective, due to weaker interquark color strength in a baryon than in a meson, and not so heavy charm and bottom masses, one cannot exclude the possibility that even the ground states might be strongly coupled.

Despite this disclaimer, we will proceed by assuming that the QQQ ground states are indeed the weakly-coupled system. In this work, we attempt to estimate the leading order contribution to the binding energy, therefore for this purpose, only the tree-level static interquark potential, *i.e.*, Coulomb potential, needs to be considered. Since rigorously solving a three-body Coulomb bound state problem is beyond our current ability, we have to resort to some sort of approximation method. Stimulated by success of the variational method in coping with few-body atomic system, we will invoke this simple but efficient approximation scheme to address our baryonic problem. For baryons containing simultaneously b and c, we will take advantage of the mass hierarchy $m_b \gg m_c$ to guide our variational analysis, just in analogy with that in the simple 3-body atomic system such as helium atom and the ionized hydrogen molecule, the physical picture becomes much more tractable by exploiting the fact $m_N \gg m_e$.

The rest of the paper is distributed as follows. In Section 2, we present a brief introduction to the most relevant features of the triply-heavy baryons in the weak-coupling regime. In Section 3, which is the main body of this work, we perform a detailed variational analysis to the binding energy of various QQQ ground states. Three different classes of triply-heavy baryons, *bcc*, *ccc* (*bbb*) and *bbc* states are treated separately, with the hierarchy $m_b \gg m_c$ utilized as a guidance for choosing proper trial states. Considerable amount of effort has been devoted to the *bbc* state, which is the most interesting case, but also most difficult to analyze. We have employed three different approaches to study this state and explored the implication of each approach in depth. Particularly the relevance of the compact diquark picture is discussed. In Section 4, we present our predictions to the masses of all the lowest-lying triply heavy baryons, and compare our results with other work. We summarize and present an outlook in Section 5.

2. Weakly coupled QQQ states

In this section we recapitulate the major aspects of weakly-coupled triply heavy baryons which are most relevant to this work. For more comprehensive discussion from the perspective of pNRQCD, we refer the interested readers to Ref. [20, 13].

To efficiently investigate the low energy properties of a tripled heavy baryon, such as binding energy, it is convenient to work with a low energy effective theory that focuses on the most relevant degrees of freedom. In a weakly-coupled QQQ state, the relevant low energy degrees of freedom are nonrelativistic heavy quarks and (ultrasoft) gluons with energy and momentum of order mv^2 , just like in a weakly-coupled quarkonium. All the high energy degrees of freedom, which can only appear in the virtual states, have been integrated out explicitly. One particularly important high energy mode is the (soft) gluons with momentum of order mv, whose effects are encoded in the low energy theory as the interquark potentials. Since we have $mv \gg \Lambda_{\rm QCD}$ in a weakly coupled state, the potentials can be determined in perturbation theory by matching procedure. There are infinite number of potentials, which are organized in expansions of 1/m. The most important potential is the $\mathcal{O}(1/m^0)$ (static) potential.

The explicit form of potentials depends on the overall color configuration of quarks. Three heavy quarks can be in either color singlet, octet or decuplet state. The color-singlet state represents the most important case, since it constitutes the leading Fock component of a baryon. The singlet static potential is well known,

$$V_{S}^{(0)} = -\frac{2\alpha_{s}}{3} \left(\frac{1}{|\mathbf{x}_{1} - \mathbf{x}_{2}|} + \frac{1}{|\mathbf{x}_{2} - \mathbf{x}_{3}|} + \frac{1}{|\mathbf{x}_{3} - \mathbf{x}_{1}|} \right) + \mathcal{O}(\alpha_{s}^{2}), \qquad (2.1)$$

where the color interaction between any pair of quarks is attractive. In general, in the color octet and decuplet configurations, some or all pairs of quarks will repel each other.

Thus far, the low energy effective theory is completely depicted by a set of uncoupled Schrödinger equations governing the motion of heavy quarks in different color configurations. The situation becomes more intriguing when ultrasoft gluons are included. Since the typical wavelength of ultrasoft gluons is much longer than the typical interquark distance, the gluon fields can be multipole expanded. Very much like the electromagnetic multipole transition in atoms, ultrasoft gluons can also induce chromo-electromagnetic multipole transition from one heavy quark color configuration to a different one. In particular, a chromo-electric dipole transition can occur between a color-singlet QQQ configuration to an octet one. The interaction between bound heavy quarks and vacuum gluonic fluctuations through this chromo-E1 operator, will generate the leading nonperturbative correction to mass of a triply-heavy baryon, as a manifestation of Lamb shift in QCD ¹. The magnitude of this nonperturbative correction depends on the relative size between mv^2 and $\Lambda_{\rm QCD}$. It is quite difficult to estimate this effect accurately, and we will not consider it further.

We end this section by commenting briefly on the solidity of the weak-coupling assignment to the lowest-lying triply heavy baryons that are of practical interest. As was

¹The analogous effect in quarkonium system, originally considered by Voloshin [21], has been extensively explored by many authors.

admitted in Introduction, since the interquark color strength in a baryon is only a half of the quark-antiquark color strength in a quarkonium, the typical dimension of a triply heavy baryon, say, Ω_{bbb} , is expected to be considerably fatter than that of Υ . One may worry that the wave function of the former could permeate deeply into the confinement region. Fortunately, as will be shown quantitatively in the forthcoming section, the interquark attraction is effectively enhanced due to the influence of the third quark, so the actual situation turns out to be considerably better than this pessimistic anticipation.

3. Variational estimate of binding energy

In this section, we attempt to estimate the binding energy of various QQQ ground states. Our starting point is the color-singlet hamiltonian:

$$H_S = -\frac{1}{2} \sum_{i=1}^{3} \frac{\nabla_i^2}{m_i} + V_S^{(0)} + \cdots, \qquad (3.1)$$

where the ellipsis stands for the higher-dimensional potentials suppressed by powers of 1/m. Because the purpose of this work is to calculate the leading $\mathcal{O}(\alpha_s^2)$ contribution, we will restrict to the lowest order static potential only.

To describe a bound state, we need first separate the relative motions of quarks from the center-of-mass motion in (3.1). There are infinite ways to perform this separation. A simple way is to replace the old coordinates by the center-of-mass coordinate plus two new coordinates defined as the positions of the quark 1, 2 relative to the quark 3:

$$\mathbf{X} = \frac{1}{\sum m_i} \sum_{i=1}^3 m_i \mathbf{x}_i,$$

$$\mathbf{r}_1 = \mathbf{x}_1 - \mathbf{x}_3,$$

$$\mathbf{r}_2 = \mathbf{x}_2 - \mathbf{x}_3.$$
(3.2)

In terms of these new coordinates, the hamiltonian (3.1) can be separated into

$$H_S = H_S^{\rm CM} + h_S \,, \tag{3.3}$$

where $H_S^{\text{CM}} = -\nabla_{\mathbf{X}}^2/(2\sum m_i)$ is the center-of-mass part, and the part governing the relative motion reads

$$h_S = -\frac{\nabla_{r_1}^2}{2m_{13}} - \frac{\nabla_{r_2}^2}{2m_{23}} - \frac{\nabla_{r_1} \cdot \nabla_{r_2}}{m_3} - \frac{2\alpha_s}{3} \left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_{12}}\right), \qquad (3.4)$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, $m_{ij} = (1/m_i + 1/m_j)^{-1}$ is the reduced mass of quark *i* and *j*. In such a coordinate system, the quark 3, sitting at the origin, is artificially singled out from two other quarks.

Our task then becomes solving the bound state problem defined in (3.4). In the following, we will use the variational method to estimate the corresponding binding energy of each type of QQQ ground states.



Figure 1: Sketch of the coordinate system used for the *bcc* state.

3.1 bcc

We start from the simplest case, the baryon made of one heavier bottom quark of mass M and two lighter charm quarks of mass m (throughout this section, we will use the notation $M \equiv m_b$ and $m \equiv m_c$).

It is convenient to choose a coordinate system as specified in (3.2), with b sitting at the origin. This coordinate system is sketched in Fig. 1. Subsequently, substituting $m_1 = m_2 = m$ and $m_3 = M$ into (3.4), the hamiltonian describing the internal motion of a singlet *bbc* state reads

$$h_S = -\frac{\nabla_1^2}{2m_{\rm red}} - \frac{\nabla_2^2}{2m_{\rm red}} - \frac{\nabla_1 \cdot \nabla_2}{M} - \frac{2\alpha_s}{3} \left(\frac{1}{r_1} + \frac{1}{r_2}\right) - \frac{2\alpha_s}{3} \frac{1}{r_{12}}, \qquad (3.5)$$

where $m_{\text{red}} = (1/m + 1/M)^{-1}$ is the reduced mass of c and b. Note in this choice of coordinates, the motion of b is embodied in the reduced mass and the operator $\nabla_1 \cdot \nabla_2/M$.

Let us first consider an ideal *bcc* state with $M/m \to \infty$. In this situation, the *b* quark just acts as a static color source, with two *c* quarks revolving around. This picture is very similar to that of the two-electron atoms such as H^- , He and Li^+ , where the nucleus is practically fixed in space, and two K-shell electrons orbit about it. Estimating the energy of the two-electron atoms is considered as a classical application of the variational method, which has been discussed virtually in every quantum mechanics textbook (e.g., see [22]).

Closely following the textbook treatment of helium, we may approximate the *bcc* ground state to be the one in which each of the *c* moves in the 1*s* orbital of an effective Coulomb potential, somewhat stronger than $-2\alpha_s/3r$. This is so because the attractive color interaction felt by each *c* due to *b* is strengthened due to the attraction exerted by another *c*. This is in opposite situation to *He*, where nuclear charge felt by each electron is partly screened due to the repulsion exerted by another electron.

In a physical *bcc* state, the hierarchy $M \gg m$ is much less perfect than that in a helium. Nevertheless, the above ansatz about the form of the ground state wave function still seems plausible. What we need is to take the motion of *b* into account. For notational simplicity, we will take the "baryonic" unit $m_{\rm red} = 2\alpha_s/3 = 1$, in which all the length and

energy scales are measured in the unit of the Bohr radius $(m_{\rm red} 2\alpha_s/3)^{-1}$ and Bohr energy $m_{\rm red} (2\alpha_s/3)^2$. We choose the spatial part of trial wave functions as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = f(r_1)f(r_2), \qquad (3.6)$$

where

$$f(r) = \frac{\lambda^{3/2}}{\sqrt{\pi}} e^{-\lambda r}$$
(3.7)

is the normalized 1s Coulomb wave function. Here λ is a variational parameter, which characterizes the effective color charge of b perceived by each of the c. Obviously, when the attractive interaction between two charm is turned off, λ would simply be 1. For the reason discussed earlier, we expect $\lambda > 1$ in our case, so that each c can be thought of moving on a squeezed 1s orbital. This is opposite to what is expected for a helium.

In the *He* ground state, two K-shell electrons must form a spin singlet to obey Fermi statistics, since its spatial wave function is symmetric under the interchange of two electrons. Due to the extra color degree of freedom carried by quarks, two *c* quarks in the *bcc* ground state must instead be a spin triplet. When combined with *b*, the lowest-lying *bcc* baryon can be either $J^P = \frac{1}{2}^+$ or $\frac{3}{2}^+$, which are degenerate up to $\mathcal{O}(m^2 \alpha_s^4/M)$ corrections due to the hyperfine splitting.

We now attempt to find the expression for the ground state energy, E. Taking the expectation value of h_S with the trial wave function in (3.6), after some effort one obtains

$$E = -\lambda^2 + 2\lambda(\lambda - 1) + \mathcal{J}, \qquad (3.8)$$

where

$$\mathcal{J} = -\frac{\lambda^6}{\pi^2} \iint d^3 r_1 d^3 r_2 \, \frac{e^{-2\lambda(r_1 + r_2)}}{r_{12}} = -\frac{5}{8}\lambda\,, \qquad (3.9)$$

measures the average potential energy stored between two charm quarks.

Note that the double integral involving the $\nabla_1 \cdot \nabla_2$ term vanishes, because of spherical symmetry possessed by the 1s wave functions. Thus, the effect of kinetic energy of b is fully taken into account by the reduced mass m_{red} .

The minimum of energy can be found by requiring $dE/d\lambda = 0$, which leads to

$$\lambda = \frac{21}{16}, \qquad (3.10)$$

indeed compatible with our expectation. The corresponding ground state energy is

$$E = -\left(\frac{21}{16}\right)^2 \longrightarrow -\left(\frac{7}{8}\right)^2 m_{\rm red} \,\alpha_s^2\,,\tag{3.11}$$

where the Bohr energy has been inserted in the last term, to recover the actual dimension of energy.

3.2 ccc

The triply charmed baryon states no longer have an atomic counterpart. On the other hand, the *ccc* ground state is highly constrained by symmetry. To have lowest energy, it necessarily possesses a totally symmetric spatial wave function. After the totally antisymmetric color wave function is included, Fermi statistics then demands that it must have $J^P = \frac{3}{2}^+$.

We again work with a coordinate system defined in (3.2), with one c, artificially denoted charm 3, fixed at the origin. The hamiltonian depicting the relative motion of three identical c can be obtained by making the replacement $M \to m$ in (3.5). We then have the reduced mass $m_{\rm red} = m/2$. To condense the notation, we will work with the "baryonic" unit, in which the corresponding hamiltonian becomes

$$h_S = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{\nabla_1 \cdot \nabla_2}{2} - \left(\frac{1}{r_1} + \frac{1}{r_2} + \frac{1}{r_{12}}\right).$$
(3.12)

We are attempting to seek a proper form for the trial wave function for ccc ground state. One simplest choice is motivated from that adopted for a bcc state. Let us temporarily imagine the charm 3 can be distinguished from the rest of two, then (3.6) constitutes a reasonable representation for such a state. Now coming back to a physical ccc state, to account for the indistinguishablity of c, we should fully symmetrize (3.6). With the spin part of wave function suppressed, the trial wave function then reads

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{f(r_1)f(r_2) + f(r_1)f(r_{12}) + f(r_{12})f(r_2)}{\sqrt{3(1+2T)}},$$
(3.13)

where f is the same as given in (3.7), and contains a variational parameter λ . One can check this wave function is symmetrical under the interchange of any two charm quarks. The Ψ is normalized by incorporating the overlap integral \mathcal{T} ,

$$\mathcal{T} = \frac{\lambda^6}{\pi^2} \iint d^3 r_1 d^3 r_2 \, e^{-\lambda(2r_1 + r_2 + r_{12})} = \frac{176}{243} \,. \tag{3.14}$$

Taking the expectation value of h_S in the trial state (3.13), after some straightforward manipulation, we end up with the expression

$$E = \frac{-\lambda^2 + 2\lambda(\lambda - 1) + \mathcal{J} - \lambda^2 \mathcal{T} + 2(\lambda - 1)\mathcal{P} - 4\mathcal{Q} + \mathcal{F} - \mathcal{G}}{1 + 2\mathcal{T}}, \qquad (3.15)$$

where \mathcal{J} has been given in (3.9), and

$$\mathcal{P} = \frac{\lambda^{6}}{\pi^{2}} \iint d^{3}r_{1}d^{3}r_{2} \frac{e^{-\lambda(2r_{1}+r_{2}+r_{12})}}{r_{1}} = \frac{68}{81}\lambda,$$

$$\mathcal{Q} = \frac{\lambda^{6}}{\pi^{2}} \iint d^{3}r_{1}d^{3}r_{2} \frac{e^{-\lambda(2r_{1}+r_{2}+r_{12})}}{r_{2}}$$

$$= \frac{\lambda^{6}}{\pi^{2}} \iint d^{3}r_{1}d^{3}r_{2} \frac{e^{-\lambda(2r_{1}+r_{2}+r_{12})}}{r_{12}} = \frac{16}{27}\lambda.$$

$$\mathcal{F} = \frac{\lambda^{6}}{\pi^{2}} \iint d^{3}r_{1}d^{3}r_{2} e^{-\lambda(2r_{1}+r_{2})}\nabla_{2}^{2}e^{-\lambda r_{12}} = -\frac{112}{243}\lambda^{2},$$

$$\mathcal{G} = \frac{\lambda^{6}}{\pi^{2}} \iint d^{3}r_{1}d^{3}r_{2} e^{-\lambda(r_{1}+r_{2})}\nabla_{1}\cdot\nabla_{2} e^{-\lambda(r_{1}+r_{12})} = \frac{56}{243}\lambda^{2}.$$
(3.16)



Figure 2: Sketch of the coordinate system adopted for the *bbc* state.

Note the exchange integrals \mathcal{P} , $\mathcal{Q} \mathcal{F}$ and \mathcal{G} arise from the symmetrization effect, which are absent in the expression for the energy of the *bcc* baryon, (3.8). In particular, \mathcal{G} , the double integral involving $\nabla_1 \cdot \nabla_2$, no longer vanishes this time.

Substituting the results of these integrals into (3.15), we obtain

$$E = -\frac{2\,595}{952}\lambda + \frac{531}{595}\lambda^2\,. \tag{3.17}$$

The optimum can be found by variational principle,

$$\lambda = \frac{4\,325}{2\,832} \approx 1.527\,,\tag{3.18}$$

and

$$E = -\frac{3\,741\,125}{1\,797\,376} \longrightarrow -0.925\,m_{\rm red}\,\alpha_s^2\,,\tag{3.19}$$

where the normal unit is recovered in the last entity.

It is interesting to compare the results we have got for the *bcc* and *ccc* ground states. First lowering the *b* mass in a *bcc* state down to *m*, we get a fictitious *ccc* state with one *c* distinguishable from the other two. Comparing (3.19) and (3.11), we immediately find the symmetrization effect tends to lower the energy. Moreover, by comparing (3.18) and (3.10), we find the symmetrization effect also tends to compress the bound state size more.

For actual *bcc* and *ccc* states, we find $E_{\Omega_{ccc}} > E_{\Omega_{bcc}}$ (note m_{red} in two cases are different), which implies that charm quarks in Ω_{bcc} are more tightly bound than in Ω_{ccc} . This is consistent with the general expectation that a bound state with constitutes of vastly disparate masses is more stable than that with equal-mass constitutes, say, a hydrogen atom is more stable than a positronium.

3.3 bbc

We finally turn to baryons made of two heavier b quarks and a lighter c quark. This type of baryon is more complicated than the preceding two, because the effective potential felt by c is no longer spherically-symmetric, but merely axially-symmetric.

To make the symmetry between two b quarks manifest, we may adopt a more appropriate coordinate system other than (3.2). Letting $m_1 = m_2 = M$, $m_3 = m$, we define the following new coordinates:

$$\mathbf{X} = \frac{M(\mathbf{x}_1 + \mathbf{x}_2) + m\mathbf{x}_3}{2M + m},$$

$$\mathbf{R} = \mathbf{x}_1 - \mathbf{x}_2,$$

$$\mathbf{r} = \mathbf{x}_3 - \frac{\mathbf{x}_1 + \mathbf{x}_2}{2}.$$
(3.20)

Note now the coordinate origin coincides with the middle point between two b quarks. The geometry of these new coordinates can be clearly visualized in Fig. 2. Substituting (3.20) into the original hamiltonian (3.1), we find that the part of hamiltonian responsible for the internal motion is

$$h_S = -\frac{\nabla_R^2}{2M_{\rm red}} - \frac{2\alpha_s}{3}\frac{1}{R} - \frac{\nabla_r^2}{2m_{\rm red}} - \frac{2\alpha_s}{3}\left(\frac{1}{r_1} + \frac{1}{r_2}\right), \qquad (3.21)$$

where $M_{\text{red}} = M/2$, $m_{\text{red}} = (1/m + 1/2M)^{-1}$ are the reduced masses, and $r_1 = |\mathbf{r} - \frac{\mathbf{R}}{2}|$, $r_2 = |\mathbf{r} + \frac{\mathbf{R}}{2}|$.

A nuisance may deserve some caution before we move on further. Two strong coupling constants in (3.21) have been tacitly assumed to be evaluated at the same renormalization scale μ . This procedure seems incompatible with our intuition that the first α_s should be affiliated with a scale $\sim 1/\langle R \rangle$, and the second one with a different scale $\sim 1/\langle r \rangle$, where $\langle R \rangle$ and $\langle r \rangle$ represent the typical values of R and r_i , respectively. When M and m are widely separated, $\langle R \rangle \ll \langle r \rangle$ is expected, and this recipe will miss the contributions of large logarithm $\ln(\langle r \rangle / \langle R \rangle)$, no matter which value of μ is chosen. The symptom encountered in this equal- α_s ansatz is a typical shortcoming of lowest-order perturbative calculation in a multi-scale problem, and one in principle can ameliorate its prediction by appealing to renormalization group equation to resum the large logarithms of the form $\alpha_s^n \ln^{n-1}(\langle r \rangle / \langle R \rangle)$. Fortunately, for a physical *bbc* baryon, M is only three times larger than m, $\langle R \rangle$ and $\langle r \rangle$ likely don't differ much, hence we don't need worry much about this nuisance.

In the following, we will treat the *bbc* ground state with three different approaches: point-like diquark approximation, Born-Oppenheimer approximation, and variational method.

3.3.1 Point-like diquark approximation

In a fictitious world where M is many orders of magnitude heavier than m, the physical picture simplifies enormously. The influence of c to the motion of very heavy b can be safely neglected. Consequently, two b quarks in the bbc ground state form a 1s spin-triplet state. The very compact Bohr radius of b, cannot be resolved by c which is orbiting from far away. Thus from the perspective of c, the bb cluster is just like a point particle. To distribute itself in the lowest energy, the c is revolving around this point particle in the corresponding 1s orbital. Being in $\overline{3}$ color state, this compact diquark may be identified with a heavy antiquark. In this sense, the bbc ground state is analogous to the heavy quarkonium B_c .

In passing, it is worth mentioning that the doubly heavy baryons, such as bbq states, fit into this compact diquark picture to a better extent than the bbc state, because the average distance between q and diquark in the former, $\sim 1/\Lambda_{\rm QCD}$, is considerably larger than the average distance between c and diquark in the latter, $\sim 1/(m\alpha_s)$. Properties of doubly-heavy baryons was first studied within a compact diquark picture long ago in HQET language [23]. Some refinement to this picture, which invokes the nonrelativistic EFT of QCD to describe the internal excitation of the diquark, has recently come out [20, 24].

The form of (3.21) is particularly convenient to accommodate the compact diquark picture ². Because $\langle R \rangle \ll \langle r \rangle$ in this case, one may approximate r_1 and r_2 by r, the color potential felt by c then becomes $-4\alpha_s/3r$, as if it is due to a heavy antiquark sitting at the origin. Eq. (3.21) then collapses into two separate hamiltonians, one governing the internal motion of the diquark, the other governing the motion of c in a central Coulomb potential. The energy of the *bbc* ground state is then simply the sum

$$E = -\frac{1}{2}M_{\rm red} \left(\frac{2}{3}\alpha_s\right)^2 - \frac{1}{2}m_{\rm red} \left(\frac{4}{3}\alpha_s\right)^2.$$
(3.22)

For a physical bbc state, the mass hierarchy between b and c is far from ideal, so the usefulness of this oversimplified approximation is doubtful.

3.3.2 Born-Oppenheimer approximation

We now seek an alternative method that explicitly incorporates the effect of finite diquark size. First observe that an ideal *bbc* state bears some similarities with the simplest molecule, the H_2^+ ion, in the sense that both are three-body bound states held together by Coulomb force, and both contain two heavy particles and one much lighter particle. Motivated by this similarity, one may wonder whether some well-known method developed to analyze H_2^+ can be transplanted here.

A standard tactics to cope with diatomic molecules, such as the H_2^+ ion, is Born-Oppenheimer approximation (*adiabatic* approximation). This method was originally motivated by the strong separation of time scales between electronic and nuclear motion, which is mainly a consequence of the hierarchy $m_e \ll m_N$. The recipe of this method is that, to solve molecular problem, one first determines the electronic eigenstates at fixed nuclear positions, then takes the corresponding electronic energy as an effective potential, in conjunction with the internuclear Coulomb potential to describe the nuclear motion.

There is a caveat, however. Despite the aforementioned similarities, one should realize there is one fundamental difference between H_2^+ and the *bbc* state, that is, the internuclear Coulomb interaction is repulsive, whereas the Coulomb interaction between *b* is attractive. This difference in turn results in drastically distinct properties of H_2^+ and an ideal *bbc* state. As a result, success of adiabatic approximation to the former does not automatically guarantee that it can be taken for granted for the latter.

To better orientate ourselves, it is instructive to recall first how an adiabatic picture arises from the H_2^+ ground state [22]. A snapshot of this simplest molecule is that, two

²For pedagogical purpose, in the following two α_s in (3.21) will be simply taken equal even in the limit $M/m \to \infty$.

nuclei slowly vibrate about some equilibrium positions with small amplitude, whereas the electron flies around much more swiftly. The vibrational nuclear motion is a consequence of the balance between internuclear Coulomb repulsion and an effective attractive interaction induced by the electron. A crucial fact is that the typical period of nuclear motion is much $(\sim \sqrt{m_N/m_e})$ longer than that of electronic motion. It is thus a good approximation to regard nuclei as frozen when considering the electronic motion, consequently the electron will distribute itself in the ground state of this static nuclear potential. Moreover, the electron can be regarded as responding instantaneously to the change of nuclear arrangement, therefore it follows the nuclear motion *adiabatically*, which implies that it can always remain in the corresponding ground state for each nuclear configuration.

In contrast, an ideal bbc state bears a completely different structure. As we have known, this state is characterized by a compact diquark picture. The pull exerted by cagain induces an effective attractive interaction between two b quarks. However, when superimposed on the attractive Coulomb interaction, it helps, though with a rather minor impact, to push two b closer. The only agent to prevent a complete collapsing is the kinetic energy of b. It is interesting to compare the overwhelmingly dominant role enjoyed by the kinetic energy of b with the insignificant role played by the nuclear kinetic energy in H_2^+ .

Based on the point-like diquark picture, one can show that b is confined in a region about m/M smaller than c, the typical velocities of b and c are about equal ($\sim \alpha_s$), and the typical kinetic energy of b is about M/m larger than that of c. Obviously, notions such as "fast c" and "slow b" are simply misnomers. Moreover, uncertainty principle tells that the typical orbiting period of b is much ($\sim M/m$) shorter than that of c. As a result, c can hardly follow the fuzzy pace of b, let alone to readjust itself instantaneously to the ground state for a particular configuration of b. In sharp contrast with H_2^+ , the bbc state exhibits a completely anti-adiabatic nature.

The above negative argument seems to persuade us to give up adiabatic approximation in analyzing an ideal *bbc* state, since the orthodox picture on which this method is based is badly violated. Ironically, this method practically does yield correct result for this state. The reason can be traced as follows. We have argued that it is difficult for c to react quickly to the rapid change of configurations of b. It simply gets confused. However, the really important point is, what c can see is only a smeared bb cluster which is well localized in a small region, it doesn't care about the details going on inside this cluster. What c can do is to distribute itself in the ground state of the Coulomb potential due to a remote $\overline{3}$ color source. This is of course nothing but the point-like diquark picture. Born-Oppenheimer method takes the energy eigenvalue of c in static configurations of b as effective potential for b. For an ideal bbc state, only the value of this effective potential at very small separation of b is relevant, which is just the 1s energy of c in the Coulomb potential of an antiquark. Following the Born-Oppenheimer procedure, the motion of b is described by a new potential, which is the original Coulomb potential shifted up by this tiny constant. One then readily reproduces the correct answer, (3.22), for the ground state energy.

It is now clear that Born-Oppenheimer approximation practically works for an ideal *bbc* state because of very compact diquark size. But we certainly are more interested in

the physical bbc state. Since m and M are not widely separated in this case, there is no more strong separation of time scales, this approximation thus is not expected to yield accurate result in the first place. Nevertheless, since this method takes the finite diquark size effect into consideration, which is relevant for a physical bbc state, we will take a practical attitude, applying it to this state to watch what results will come out.

Let us now concretely analyze the *bbc* state following Born-Oppenheimer method. To start, we first approximate the full wave function Ψ as

$$\Psi(\mathbf{R}, \mathbf{r}) \approx \Phi(\mathbf{R}) \varphi(\mathbf{R}, \mathbf{r}), \qquad (3.23)$$

where φ represents the charm ground state for a static configuration of b, and Φ stands for the amplitude to find b in this configuration when c is in the state φ .

In the Born-Oppenheimer ansatz, we need first determine the lowest eigenstate φ by solving the Schrödinger equation

$$\left[-\frac{\nabla_r^2}{2m_{\rm red}} - \frac{2\alpha_s}{3}\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\right]\varphi(\mathbf{R}, \mathbf{r}) = \varepsilon(R)\varphi(\mathbf{R}, \mathbf{r}).$$
(3.24)

Since the positions of b explicitly enter the potential, the energy eigenvalue ε depends on R.

This is exactly the same problem as one encounters in H_2^+ , to determine the electronic ground state at fixed nuclear positions, therefore we can follow the standard treatment [25]. Solving (3.24) rigorously is unfeasible, one commonly appeals to variational method. A reasonable form taken for the trial wave function is a linear combination of 1s charm states centered on each of b quarks. A variational parameter λ is included in the 1s trial state to characterize the effective color charge of b perceived by c. Taking the indistinguishableness of b into account, the trial wave function of c takes the form

$$\varphi(\mathbf{R}, \mathbf{r}) = \frac{f(r_1) \pm f(r_2)}{\sqrt{2\left(1 \pm \mathcal{S}(\lambda, R)\right)}}, \qquad (3.25)$$

where f is given in (3.7). To keep our notation simple, we have chosen to work with the lighter "baryonic" unit $m_{\rm red} = 2\alpha_s/3 = 1$. The overlap integral is incorporated to make φ normalized,

$$\mathcal{S}(\lambda,R) = \frac{\lambda^3}{\pi} \int d^3 r \, e^{-\lambda \left(r_1 + r_2\right)} = \left[1 + \lambda R + \frac{\lambda^2 R^2}{3}\right] \, e^{-\lambda R} \,. \tag{3.26}$$

The wave function φ must be either symmetric or antisymmetric upon interchange of two b ($\mathbf{R} \to -\mathbf{R}$), so that the corresponding bb pair, if in relative *s*-wave, must be either a spin triplet or singlet in line with Fermi statistics. When combined with c, the former configuration corresponds to a *bbc* state with $J^P = \frac{3}{2}^+$ or $\frac{1}{2}^+$, and the latter corresponds to a state with $J^P = \frac{1}{2}^-$. As is well known in H_2^+ , the antisymmetric configuration has higher energy level than the symmetric one. Since we are only interested in the *bbc* ground state, we will discard the state with odd parity.



Figure 3: λ and effective potential as functions of R, determined by the variational calculus (solid line). All the numbers are given in the lighter "baryonic" unit. In the lower half plot, the dashed curve represents the function given in (3.29), which is hardly distinguishable from the actual one.

We thus choose the symmetric one in (3.25). Multiplying both sides of (3.24) by the corresponding φ^* , integrating over **r**, one finds that the charm energy reads [25]

$$\varepsilon(R) = -\frac{\lambda^2}{2} + \frac{\lambda(\lambda - 1) - \mathcal{C}(\lambda, R) + (\lambda - 2)\mathcal{E}(\lambda, R)}{1 + \mathcal{S}(\lambda, \mathcal{R})}.$$
(3.27)

The classical interaction integral \mathcal{C} and exchange integral \mathcal{E} are given by

$$\mathcal{C}(\lambda, R) = \frac{\lambda^3}{\pi} \int d^3 r \, \frac{e^{-2\lambda r_1}}{r_2} = \frac{1}{R} \left[1 - (1 + \lambda R) \, e^{-2\lambda R} \right] ,$$

$$\mathcal{E}(\lambda, R) = \frac{\lambda^3}{\pi} \int d^3 r \, \frac{e^{-\lambda (r_1 + r_2)}}{r_2} = \lambda \left(1 + \lambda R \right) e^{-\lambda R} .$$
(3.28)

To locate the minimum of (3.27) at a given R, we resort to the condition $\partial \varepsilon / \partial \lambda |_R = 0$. The analytical expression for the optimum, if can be worked out, would be very cumbersome, so we are content with providing numerical solutions only. The optimized λ and ε as functions of R are shown in Fig. 3. In digression, we would like to mention that a trick adopted by some texts (for example, [25]), which aims to facilitate finding the optimum, is mathematically inconsistent, therefore we have refrained from using it.

Fig. 3 illustrates some expected features of charm ground state in a static configuration of b. At R = 0, the bb diquark shrinks to a point, the color charges double, so we have $\lambda = 2$ and $\varepsilon = -2^2/2 = -2$. This is exactly what we would expect by replacing a point-like diquark with an antiquark. As R gets large, c will be essentially localized with one of the b, forming a 1s state, and the influence of the other b becomes negligible. To put in a quantitative way, at large R, the effective charge $\lambda \approx 1$, and the energy of c is the 1s energy plus the potential energy between c and the other b, that is, $\varepsilon \approx -1/2 - 1/R$.

In the Born-Oppenheimer ansatz, the charm energy plays the role of effective potential for b. To expedite our analysis, it is convenient to have an analytic formula that mimics the actual $\varepsilon(R)$, which is known only numerically. We find the following parameterization,

$$\varepsilon_{\rm fit}(R) = -0.5 - \frac{1.5}{1 + 0.586 R^{1.421}},$$
(3.29)

represents a good fit to the actual one, with error less than one percent provided that R is not too large. As already pointed out, due to the compact diquark nature of a *bbc* state, only the knowledge in small R range affects the bound state property.

The remaining task is to determine Φ , with the effective potential taken as input. In Born-Oppenheimer approximation, the motion of *b* is simply governed by the following Schrödinger equation³:

$$\left[-\frac{\nabla_R^2}{2} - \frac{1}{R} + \kappa \left\{-0.5 - 1.5 \left[1 + 0.586 \left(\kappa R\right)^{1.421}\right]^{-1}\right\}\right] \Phi(\mathbf{R}) = E \Phi(\mathbf{R}), \quad (3.30)$$

where $\kappa \equiv m_{\rm red}/M_{\rm red}$. For convenience, we have switched to the heavier "baryonic" unit $M_{\rm red} = 2\alpha_s/3 = 1$. Note κ plays the role of scale conversion factor.

This equation can be solved numerically once κ is specified. Consequently, the energy of the baryon ground state, E, can be identified with the eigenvalue of the corresponding 1s state. The dependence of E on κ in a wide range is shown in Fig. 4. As is expected, at small κ , the energy predicted from this approach does coincide with the one from the point-like diquark approximation. Technically, this can be understood by examining (3.30) in the limit $\kappa \to 0$, in which the effective potential reduces to a constant -2κ . As discussed before, the underlying reason should be attributed to the fact that for small κ , only the value of the effective potential near R = 0 is relevant.

In short, the lesson we have learned is that, even though Born-Oppenheimer approximation is not theoretically justified for an ideal *bbc* state, this procedure still leads to correct results because of the compact diquark nature of this state.

As κ increases, the average diquark size becomes comparable with the typical distance between c and b. In this situation, neither point-like diquark approximation nor Born-Oppenheimer approximation is expected to make reliable prediction. Nevertheless, since the latter approach explicitly incorporates the effect of finite diquark size, we may expect it is closer to the truth than the former. As one can discern in Fig. 4, the prediction of E from the latter approach becomes incrementally higher than that from the former as κ increases. This is compatible with our expectation. The larger κ is, the more relevant the contribution of the effective potential at large separation of b becomes. Since ε monotonically increases

³To arrive at this formula, one has dropped two additional terms containing $\nabla_R \varphi$ (see [22] for detailed derivation). This procedure is partly justified by the fact $\nabla_R \varphi \ll \nabla_R \Phi$ as expected from the compact diquark picture. Although a rigorous mathematical proof is absent, we invoke the fact that this procedure makes correct prediction for an ideal *bbc* state as an evidence for its validity.

with R, starting from -2κ (see Fig. 3), thus as κ increases, the E predicted by the Born-Oppenheimer approximation becomes increasingly higher than the one predicted by the point-like diquark approximation.

3.3.3 One-step variational estimate

We have shown that both the point-like diquark approximation and Born-Oppenheimer approximation render correct predictions for an ideal bbc state. However, there is no *a priori* reason to expect them to work satisfactorily for a physical bbc state, where *m* and *M* are not so widely separated. A useful indicator is the ratio of the average diquark dimension to the typical distance between *c* and *b*, which is roughly

$$\frac{\langle R \rangle}{\langle r \rangle} \sim \kappa \approx \frac{2M_{J/\Psi}}{M_{\Upsilon}} \approx 0.6.$$
 (3.31)

Because of poor separation between $\langle R \rangle$ and $\langle r \rangle$, a more general approach is called for to analyze the physical *bbc* state.

In the following we will employ the third method, dubbed one-step variational estimate. It takes basically the same variational ansatz as used for the *bcc* and *ccc* system. However, due to more complex nature of the *bbc* system, two variational parameters have been introduced. The term one-step implies that the ground state energy as well as the full wave function are determined in a single step, in contrast with Bohr-Oppenheimer procedure, in which one determines the wave functions of c and b in two successive steps. On general ground, one expects this method is more accurate than the other two, inasmuch as it is based entirely on the variational principle and no other approximation is invoked. As long as the trial wave function is reasonably chosen, we expect it will render reliable prediction even when κ is not small.

For notational convenience, we adopt the heavier "baryonic" unit $M_{\rm red} = 2\alpha_s/3 = 1$ here. The hamiltonian (3.21) then simplifies to

$$h_{S} = -\frac{\nabla_{R}^{2}}{2} - \frac{1}{R} - \frac{1}{\kappa} \left(\frac{\nabla_{r}^{2}}{2} + \frac{\kappa}{r_{1}} + \frac{\kappa}{r_{2}} \right) , \qquad (3.32)$$

where the scale conversion factor is included in the c sector.

We first need to guess a proper form for the trial wave function Ψ . It is natural to follow the ansatz of (3.23), to express Ψ in a quasi-separable form $\Phi(\mathbf{R}) \varphi(\mathbf{R}, \mathbf{r})$, where Φ represents the *b* wave function, and φ denotes the *c* wave function, which may be taken the same as (3.25). This form of trial wave function clearly embodies the point-like diquark picture in the $\kappa \to 0$ limit. Since φ has incorporated the effects of finite diquark size, this choice of trial wave function seems reasonable also for large κ . We take the trial wave function for the *bbc* ground state explicitly to be

$$\Psi(\mathbf{R},\mathbf{r}) = \frac{1}{\sqrt{2\left(1+\overline{\mathcal{S}}\right)}} \frac{\delta^{3/2}}{\sqrt{\pi}} \frac{(\kappa\lambda)^{3/2}}{\sqrt{\pi}} e^{-\delta R} \left(e^{-\kappa\lambda r_1} + e^{-\kappa\lambda r_2}\right), \qquad (3.33)$$

with the spin wave function suppressed. λ and δ are variational parameters. Note Ψ is symmetric under the reflection $\mathbf{R} \to -\mathbf{R}$, as it should be for the ground state. The wave



Figure 4: The energy of the *bbc* ground state (in the heavier "baryonic" unit) as function of $m_{\rm red}/M_{\rm red}$. Three curves are generated by implementing three different approximation schemes. The dot-dashed line has the functional form $E = -\frac{1}{2} - 2\kappa$, as can be inferred from (3.22).

function is normalized by incorporating the overlap integral

$$\overline{\mathcal{S}} = \frac{\delta^3}{\pi} \int d^3 R \, e^{-2\delta R} \, \mathcal{S}(\kappa\lambda, R) = \frac{16\,\delta^3 \left(2\delta^2 + 5\delta\kappa\lambda + 4\kappa^2\lambda^2\right)}{(2\delta + \kappa\lambda)^5} \,, \tag{3.34}$$

where S is given in (3.26).

The physical implication of λ is the same as in Born-Oppenheimer ansatz, which describes the effective charge of *b* perceived by *c*, except here it is taken as a constant instead of a function of *R*. This simplification seems plausible, at least for small κ . As noticed before, the typical time scale characterizing the change of configurations of *b* is in general shorter than that of *c*, consequently *c* only sees smeared trajectories of *b*. When considering the impact of *b* on *c*, it is reasonable to average its effects over different configurations of *b*. This averaging procedure will lead to a constant value of λ .

The new parameter, δ , is introduced simultaneously to characterize the impact of c on the geometry of the diquark. It would simply equal 1 in the limit $\kappa \to 0$, when the influence of c becomes completely negligible.

Taking the expectation value of h_S , (3.32), in the trial state Ψ , (3.33), after some straightforward manipulation, we obtain

$$E = -\frac{\delta^2}{2} - \frac{\kappa\lambda^2}{2} - \frac{\kappa^2\lambda^2}{8} + \left[\delta(\delta - 1)(1 + \overline{\mathcal{X}}) + \kappa\left[\lambda\left(\lambda - 1\right) - \overline{\mathcal{C}} + (\lambda - 2)\overline{\mathcal{E}}\right] + \frac{\kappa^2\lambda}{4}\left(\lambda + \overline{\mathcal{E}} - 4\,\delta\,\overline{\mathcal{Y}}\right)\right]/(1 + \overline{\mathcal{S}}).$$
(3.35)



Figure 5: Dependence of two optimized variational parameters λ , δ on the mass ratio $m_{\rm red}/M_{\rm red}$.

The parameters in (3.35) are given by

$$\kappa \overline{\mathcal{C}} = \frac{\delta^3}{\pi} \int d^3 R \, e^{-2\delta R} \, \mathcal{C}(\kappa\lambda, R) = \frac{\delta\kappa\lambda \left(\delta^2 + 3\delta\kappa\lambda + \kappa^2\lambda^2\right)}{\left(\delta + \kappa\lambda\right)^3},$$

$$\kappa \overline{\mathcal{E}} = \frac{\delta^3}{\pi} \int d^3 R \, e^{-2\delta R} \, \mathcal{E}(\kappa\lambda, R) = \frac{16\,\delta^3\kappa\lambda \left(\delta + 2\kappa\lambda\right)}{\left(2\delta + \kappa\lambda\right)^4},$$

$$\delta \overline{\mathcal{X}} = \frac{\delta^3}{\pi} \int d^3 R \, e^{-2\delta R} \, \frac{\mathcal{S}(\kappa\lambda, R)}{R} = \frac{4\,\delta^3 \left(4\delta^2 + 8\delta\kappa\lambda + 5\kappa^2\lambda^2\right)}{\left(2\delta + \kappa\lambda\right)^4},$$

$$\kappa \overline{\mathcal{Y}} = \frac{\delta^3}{\pi} \int d^3 R \, e^{-2\delta R} \, \mathcal{Y}(\kappa\lambda, R) = \frac{4\,\delta^3\kappa\lambda \left(2\delta + 5\kappa\lambda\right)}{\left(2\delta + \kappa\lambda\right)^5}.$$
(3.36)

where \mathcal{C}, \mathcal{E} are given in (3.28), and

$$\mathcal{Y}(\lambda, R) = \frac{\lambda^3}{\pi} \int d^3 r \, e^{-\lambda(r_1 + r_2)} \, \nabla_R \, R \cdot \nabla_R \, r_1 = \frac{R}{6} \, \mathcal{E}(\lambda, R) \,. \tag{3.37}$$

It is interesting to note that the contribution of the charm energy, which is previously computed in Born-Oppenheimer procedure, (3.27), is also subsumed in (3.35) in a similar format. Besides this, (3.35) also incorporates terms that have been neglected in Born-Oppenheimer approximation, such as $\overline{\mathcal{Y}}$ (see the comment in Footnote 3).

The minimum of (3.35) can be found by enforcing $\partial E/\partial \lambda|_{\delta} = \partial E/\partial \delta|_{\lambda} = 0$. It is rather difficult to derive analytic expressions for these optima, hence we resort to numerical method to determine them. Subsequently, the energy of *bbc* ground state as function of κ , juxtaposed with predictions made by two other approaches, is shown in Fig. 4. The optimized values of λ and δ as functions of κ are shown in Fig. 5. As is expected, the energy predicted from this approach coincides with those from the other two in the $\kappa \to 0$ limit. The technical reason is easily traceable. Note all the integrals in (3.35) simplify greatly in this limit, e.g., \overline{S} , $\overline{\mathcal{X}} \approx 1$, and \overline{C} , $\overline{\mathcal{E}} \approx \lambda$. Neglecting higher order terms, Eq. (3.35) then reduces to

$$E = -\frac{\delta^2}{2} + \delta(\delta - 1) + \kappa \left[-\frac{\lambda^2}{2} + \lambda(\lambda - 2) \right] + \mathcal{O}(\kappa^2).$$
(3.38)

The optima $\delta = 1$, $\lambda = 2$ can be trivially inferred, and the corresponding energy is exactly the same as (3.22), which was first derived in the point-like diquark approximation.

Fig. 5 illustrates some anticipated features of a *bbc* state. As κ grows, this state starts to depart from the simple point-like diquark picture, and the effect of finite diquark size becomes increasingly important. It can be clearly observed that δ ascends in a slower pace than λ descends. This is compatible with the expectation that the impact of *c* on *b* is less important than the impact of *b* on *c*.

One interesting observation from Fig. 4 is that Born-Oppenheimer approximation renders rather close prediction to that from the variational approach, virtually in all κ range. The reason is perhaps that those terms dropped by Born-Oppenheimer procedure turn out to be insignificant in this case. In any rate, this approximation scheme is not expected to work so well when κ gets large. It is worth mentioning that, when analyzing baryon mass spectra using phenomenological potential model, Fleck and Richard have also found this scheme yields rather accurate results [26]. They have attributed it to a lore that asserts "Born-Oppenheimer approximation works always better than expected".

We end this section by pointing out an interesting finding. In the complicated expression for E, (3.35), the last two terms nearly cancel with each other in virtually all the range of κ , once the optimized values of λ and δ are used. We thus achieve a great simplification:

$$E \approx -\frac{\delta^2}{2} - \kappa \frac{\lambda^2}{2}. \tag{3.39}$$

This approximate formula works surprisingly well. It deviates from the actual one by 3 % in maximum in the range $\kappa < 1$. If one restricts to the smaller range $\kappa < 0.8$, the error of this formula is less than 1 %.

Without a deeper understanding, one might simply regard the success of (3.39) as a fortuitous coincidence. If taken seriously, it seems to indicate that the point-like diquark picture might be useful even at large κ . It will yield the right answer, if one pretends that the color potential between two *b* quarks is $-\delta/R$, and the *bb* diquark perceived by *c* is equivalent to an antiquark carrying the color charge λ .

4. Phenomenology

In this section, we will assemble the knowledge gleaned in the preceding section to estimate masses of various lowest-lying triply heavy baryons. We then compare our results with other work in literature, and discuss corresponding implications.

It should be first realized that our predictions will be sensitive to the input of heavy quark masses. Therefore, it is important to specify an appropriate quark mass scheme to lessen arbitrariness. Since our working assumption is the weak-coupling regime, it is most consistent to express the heavy quark pole mass in terms of the masses of lowest-lying quarkonia, J/Ψ and Υ , assuming they are the weakly coupled system. At order α_s^2 , we can write m_c and m_b as

$$m_{c} = \frac{M_{J/\Psi}}{2} \left[1 + \frac{2 \alpha_{s}^{2}(\mu)}{9} \right] ,$$

$$m_{b} = \frac{M_{\Upsilon}}{2} \left[1 + \frac{2 \alpha_{s}^{2}(\mu)}{9} \right] .$$
(4.1)

We will take the physical values $M_{J/\psi} = 3.097$ GeV, $M_{\Upsilon} = 9.460$ GeV as input.

We are now at a position to express the masses of tripled-heavy baryons in perturbative expansion. We start from Ω_{bcc} . Using the result of (3.11), we find

$$M_{\Omega_{bcc}} = m_b + 2m_c + E$$

= $\frac{M_{\Upsilon}}{2} + M_{J/\Psi} + \left[\frac{2}{9}M_{J/\psi} + \frac{1}{9}M_{\Upsilon} - \left(\frac{7}{8}\right)^2 \frac{M_{J/\Psi}M_{\Upsilon}}{2(M_{J/\Psi} + M_{\Upsilon})}\right] \alpha_s^2(\mu)$
= $\frac{M_{\Upsilon}}{2} + M_{J/\Psi} \left[1 + 0.273 \alpha_s^2(\mu)\right].$ (4.2)

In expressing the reduced mass, we simply replace m_c with half of $M_{J/\Psi}$, and m_b with half of M_{Υ} . This simplified procedure induces an error of order α_s^4 to the baryon mass, thus legitimate at present $\mathcal{O}(\alpha_s^2)$ accuracy.

The masses of baryons made of three identical quarks can be estimated in a similar manner. With the input from (3.19), we infer the Ω_{ccc} mass to be

$$\begin{split} M_{\Omega_{ccc}} &= 3m_c + E \\ &= \frac{3M_{J/\psi}}{2} \left[1 + \left(\frac{2}{9} - \frac{0.925}{6} \right) \alpha_s^2(\mu) \right] \\ &= \frac{3M_{J/\psi}}{2} \left[1 + 0.068 \, \alpha_s^2(\mu) \right] \,, \end{split}$$
(4.3)

and the Ω_{bbb} mass can be obtained by making obvious replacement.

For the *bbc* state, we have attempted three different approaches to estimate the binding energy. Since the one-step variational estimate is believed to be most reliable, we will adopt its prediction (though Born-Oppenheimer approximation yields a close result, as disclosed in Fig. 4). First we need specify the value of κ , the ratio of two reduced quark masses. It can be approximated as

$$\kappa \approx \frac{4M_{J/\Psi}}{M_{J/\Psi} + 2M_{\Upsilon}} = 0.563\,,\tag{4.4}$$

and the error brought in by this procedure is assumed to be negligible.

The optima can be determined numerically from (3.35) by variational ansatz:

$$\delta = 1.137, \qquad \lambda = 1.603, \tag{4.5}$$

with the corresponding energy

$$E = -1.363 \longrightarrow -1.363 M_{\text{red}} \left(\frac{2\alpha_s}{3}\right)^2, \qquad (4.6)$$

where we have inserted the Bohr energy of b quark in the last entity.

Piecing everything together, we obtain

$$M_{\Omega_{bbc}} = 2m_b + m_c + E$$

= $\frac{M_{J/\Psi}}{2} + M_{\Upsilon} + [M_{J/\psi} + (2 - 1.363)M_{\Upsilon}] \frac{\alpha_s^2(\mu)}{9}$
= $\frac{M_{J/\Psi}}{2} + M_{\Upsilon} [1 + 0.107 \alpha_s^2(\mu)].$ (4.7)

So far we have treated each of triply-heavy baryons separately, it is not yet clear whether there is any connection among them. Interestingly, there is a mass convexity inequality relating different baryon states, which arises from general reasoning in QCD [27]. To our interest, such an inequality demands

$$M_{\Omega_{bbc}} \le 2 M_{\Omega_{bcc}} - M_{\Omega_{ccc}} \,. \tag{4.8}$$

The underlying assumption of this theorem is universal interquark potential. Taking α_s in (4.2), (4.3) and (4.7) to be equal, we readily verify that our predictions based on variational ansatz are indeed compatible with this QCD theorem.

There also exists another inequality, which relates the masses of baryons and mesons [28, 29]. This is derived from the assumption that the quark-quark potential in a baryon is a half of the quark-antiquark potential in a meson, which is *de facto* satisfied in Coulomb bound states. To our purpose, this inequality reads

$$M_{\Omega_{bbc}} \ge \frac{M_{\Upsilon}}{2} + M_{B_c} \,. \tag{4.9}$$

To make a consistent examination of this relation, we need treat B_c also as a weaklycoupled state, which is believed to be the case [17]. Following the preceding procedure, we can express the B_c mass as

$$M_{B_c} = \frac{M_{\Upsilon}}{2} + \frac{M_{J/\Psi}}{2} + \left[M_{\Upsilon} + M_{J/\psi} - \frac{4M_{J/\Psi}M_{\Upsilon}}{M_{J/\Psi} + M_{\Upsilon}} \right] \frac{\alpha_s^2(\mu)}{9} \\ = \frac{M_{J/\Psi}}{2} + \frac{M_{\Upsilon}}{2} \left[1 + 0.076 \,\alpha_s^2(\mu) \right].$$
(4.10)

One can promptly check that this inequality also holds in our case.

A simple variant of (4.9) is to specify all the quarks to be of a single flavor [28]:

$$M_{\Omega_{ccc}} \ge \frac{3M_{J/\psi}}{2} \,. \tag{4.11}$$

Our prediction in (4.3) indeed respects this requirement.

To make quantitative estimates for the baryon masses, we need specify at which scale the strong coupling constant should be evaluated. In principle, physical observables should

	Bjorken [4]	This work	Vijande $et \ al \ [30]$
Ω_{bcc}	8.200 ± 0.090	7.98 ± 0.07	—
Ω_{ccc}	4.925 ± 0.090	4.76 ± 0.06	4.632
Ω_{bbb}	14.760 ± 0.180	14.37 ± 0.08	—
Ω_{bbc}	11.480 ± 0.120	11.19 ± 0.08	—

Table 1: Predictions for the masses of lowest-lying triply-heavy baryons from various work. All the masses are given in unit of GeV. In the entries for Ω_{bcc} and Ω_{bbc} , the $J^P = \frac{1}{2}^+$ and $J^P = \frac{3}{2}^+$ partners are not distinguished since the hyperfine splitting has been neglected.

be independent of the choice of μ , once the all-order perturbative expansion has been worked out. In practice, since what we have so far is only the leading order perturbative correction, our predictions are unavoidably sensitive to the choice of μ . To reduce the scale ambiguity optimally, we should take μ in proximity to the characteristic momentum transfer scale in a given QQQ state.

It is an empirical fact that the typical momentum transfer scales in J/ψ , B_c and Υ are about 0.9, 1.2 and 1.5 GeV, respectively. One might expect that the corresponding scale in the QQQ states would be considerably lower than that in their quarkonium counterparts. Encouragingly, as we have learned in Sec. 3, the effective color strength between a pair of quarks gets enhanced due to the presence of the third quark. As a result, the actual wave function is more compressed than naively expected. Therefore, it is not unreasonable to choose the scale for a QQQ state close to the one typically taken for its $Q\overline{Q}$ counterpart. We assign $\mu = 1.2$ GeV in the mass formula for Ω_{bcc} , Ω_{bbb} and Ω_{bbc} , with a corresponding $\alpha_s = 0.43$; for Ω_{ccc} , we take $\mu = 0.9$ GeV, with $\alpha_s = 0.59$. To compensate for our ignorance in uncalculated higher order corrections, we estimate the uncertainty in each mass prediction to be the leading $\mathcal{O}(\alpha_s^2)$ correction multiplied by another factor of α_s ⁴.

Our predictions to the masses of various QQQ ground states, together with those made by other authors [4, 30], which employ some phenomenological confinement potentials, are compiled in Table 1. The apparent discrepancy between the predictions of the Ω_{ccc} mass by Bjorken and by Vijande *et al*, which is as large as 300 MeV, might reflect the large uncertainty inherent in phenomenological approaches⁵. In contrast, our predictions are based on the perturbation theory, being systematically improvable, suffer less arbitrariness.

It can be readily recognized that Bjorken's predictions are systematically higher than ours. Note the variational method by default underestimates the binding energy, and a more accurate weak-coupling analysis will predict even lower masses for QQQ ground states, hence further enlarging this disagreement.

Note that the $\mathcal{O}(\alpha_s^2)$ corrections in (4.2), (4.3) and (4.7) are all positive, so as we lower down μ , which is meant to be the characteristic momentum scale, our predictions will shift upwards, getting close to Bjorken's predictions. When μ descends further and becomes

⁴Note in this work we have completely ignored the nonperturbative mass corrections due to ultrasoft gluons. Therefore the actual error should be larger than what are quoted in Table 1.

⁵Note the very low Ω_{ccc} mass predicted by Vijande *et al* violates the mass inequality (4.11).

comparable with Λ_{QCD} , our method breaks down and one enters the strong-coupling regime. In a sense, Bjorken's results can be considered as arising from a strong-coupling analysis.

The future experiments and lattice QCD simulations will decide which prediction is closer to the reality, consequently nature of the QQQ ground states may be revealed.

5. Summary and outlook

The theme of this work is to estimate the masses of various lowest-lying triply heavy baryon states, with the assumption that they are weakly-coupled system, analogous to Υ , B_c and J/ψ . Our philosophy is exactly the same as that assumed in those work dedicated to calculate the lowest-lying quarkonia masses using perturbative QCD [14–19], despite the fact that tackling the 3-body problem is technically more challenging than tackling the 2-body problem.

For our purpose, it is important to make a sound estimate for the binding energy of a nonrelativistic three heavy quark system, which is bound by short-distance interquark potentials that are organized by powers of α_s and 1/M. Due to our incapability of rigorously solving 3-body problem, we have invoked the variational method as an approximation scheme to analyze various QQQ ground states. As a first step, we have estimated the most important piece, *i.e.*, the $\mathcal{O}(\alpha_s^2)$ contribution to the binding energy, with only the tree-level static potential incorporated.

For the variational method to be accurate, it is important to choose a reasonable form of trial states. In view of this, different triply-heavy baryon states, the *bcc*, *ccc* (*bbb*) and *bbc* states, have been analyzed separately, each supplied with a different trial wave function motivated by the symmetry consideration and the presence of hierarchy $m_b \gg m_c$. Inspired by the similarity between our baryonic system and the three-body atomic system, some guidances have been taken from the familiar textbook treatment of helium atom and the ionized hydrogen molecule. Among various QQQ states, the *bbc* state is the most interesting one but most challenging to analyze. We have carried out a detailed study for this state, employing several different approaches. The implications of different approaches are elucidated, and in particular the relevance of the compact diquark picture has been discussed.

Masses of various QQQ ground states derived from our formalism are compatible with those well-known mass inequalities in QCD. Our quantitative predictions, which is based on the weak-coupling treatment, are systematically lower than Bjorken's, which may instead be viewed as resulting from a strong-coupling analysis. It leaves for future experiments and lattice QCD simulation to decide the nature of the lowest-lying triply heavy baryons, whether to be weakly coupled or strongly coupled.

Besides the ability to estimate the masses, our analysis also provide some reasonable knowledge about the quark wave functions. This will be useful, for example, in estimating the hyperfine splittings in the *bcc* and *bbc* states. One important byproduct of this knowledge is that a reasonable value of the *wave function at the origin* can be inferred. Like in a heavy quarkonium, this quantity is one of the basic characteristics of a triply-heavy baryon state, and is of some phenomenological interest. For instance, this value is a crucial input for reliably calculating the fragmentation function for the QQQ states [6].

It will be valuable if some powerful numerical methods developed to tackle the 3body problem, e.g., choosing more complicated form of trial wave functions other than the simple exponential one adopted in this work, or employing the *hyperspherical expansion method* [31], are utilized to check the accuracy of our results⁶. Based on our experiences in few-body atomic problem, we expect that the uncertainty in our simple variational analysis should be small. The most important point is that, however, any improved mass predictions for the weakly-coupled QQQ ground states starting from the hamiltonian (3.4) will be *lower* than ours by default, which in turn will reinforce, instead of weaken, the key conclusion of this work, that the mass predictions based on weak-coupling analysis will be systematically *lower* than those based on the consistent strong-coupling analysis, e.g., Bjorken's predictions.

One apparent improvement on this work is in prospect. As stressed several times before, we have only incorporated the tree-level static potential in this work, so that our predictions suffer from considerable scale dependence. The perturbative matching calculation for the one-loop static potential and tree-level $O(1/m^2)$ potentials is straightforward. It will be useful to implement their contributions into our variational framework.

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⁶Nevertheless, taking the simple exponential trial wave functions is much more advantageous if one wishes to compute the higher order perturbative corrections since its simplicity allows one to obtain the (quasi)analytic expressions, as is evident in Sec. 3. In general it will be rather cumbersome for the alternative numerical methods to deal with more singular higher-dimensional potentials.

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