Variational Estimation of the Wave Function at Origin for Heavy Quarkonium

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Abstract

The wave function at the origin (WFO) is an important quantity in studying many physical problems concerning heavy quarkonia. However, when one used the variational method with fewer parameters, in general, the deviation of resultant WFO from the “accurate” solution was not well estimated. In this paper, we discuss this issue by employing several potential forms and trial wave functions in detail and study the relation between WFO and the reduced mass.

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I. Introduction

Recently, the wave function at the origin for the S-wave bound state of a heavy quark-antiquark system once again attracts physicists’ attentions\cite{1,2}. This is because that it is not only a very important quantity for calculating spin state hyperfine splitting, but also crucial to evaluating the production and decay amplitude of the heavy quarkonium. Within the context of the non-relativistic potential model, Refs. \cite{1} and \cite{2} demonstrated the numerical results of WFO of the S-wave c\bar{c}, b\bar{c} and b\bar{b} systems and compared with those obtained in various "successful" potential models.

As well known, except the Coulomb and the harmonic oscillator potentials, there are few potentials which bound state problems can be analytically solved. For solving these non-analytically soluble bound state problems, one has to use approximations. Numerically solving Schrödinger equation is the most powerful method which can reach most required accuracy. But the numerical method has some defects, for instance, it cannot give analytical expressions for further discussion. Moreover, all numerical method for the central potential is only available for the $v(r)$ which has the singularity less than $\frac{1}{r^2}$ when $r$ approximate to 0, therefore, it definitely fails as $\frac{1}{r^3}$ exist in the potential. It is unfortunately, the case is encountered usually in calculating the fine-splitting of the P state.

The perturbative method is another approximation method which has most extensively been used. However, the practical applicability of the perturbative expansion in many cases is limited due to divergence, and the ranges of perturbation parameter values are usually restricted by the convergence requirements. Moreover, in the perturbation method, the treatment for wave functions is much more difficult than that for energy eigenvalues. As it was declared by MacClary and Byers \cite{4} that it is not simple to obtain the wave function correct to the order of $v^2/c^2$, because the perturbative correction to the wave function should be given by an infinite sum over all states of the nonrelativistic Hamiltonian. As an example, in the positronium case, this sum diverges because of the divergence of the potential at the origin. Besides, for the singular $\frac{1}{r^3}$ potential, the perturbative method is the one used most frequently yet. The splitting of the energy level is obtained by calculating an integral. However, as mentioned in Ref.\cite{5}, such a singular potential would lead to an exotic result which does not correspond to the real physics. Therefore, the meaning of the result given by the perturbative calculation is not evident actually.

Of course, as a physical state which can be measured in the experiment, there should
be a theoretically derived solution to match, as long as the employed model is correct. The
problem is how to get it. For instance, the energy levels of the triplet P states of the $c\bar{c}$
system must have definite measured values. In the theoretical calculation, due to the non-
soluble nonperturbative QCD effect, one has to rely on specific models. The non-relativistic
quark potential model is one of them. Under the tree diagram approximation and the non-
relativistic approximation, a potential term of $r^{-3}$ appears. This is simply because that even
in the perturbative framework, one does not collect (actuarially is not able to do so) all
the high order diagrams in the perturbative expansion and all the high order terms in the
non-relativistic reduction. Then the question is how to catch the major character of the real
physics.

There were lots of conscientious attempts have been made. It is noteworthy that in
Gupta’s papers $[6, 7]$, the non-relativistic reduction was performed with respect to the power
of $\vec{p}^2/E^2$ so that the singular $r^{-3}$ potential term can be avoided. Our recent study indicates
that the variational method can give some interesting sight to the singular $\frac{1}{r}$ problem.

As well known that the variational methods a widely employed approach. In principle,
by using this method one can leave the above mentioned problem alone and get the major
content of the real physics. We will discuss this issue in our successive paper $[8]$. In spite of
this, the variational method has more advantages. It can give an analytical expression of the
wave function. In particular, if there is only a single parameter in the trial wave function,
the resultant wave function has a simple form. Then it is very convenient in the practical
application and physical discussion.

The variational method has extensively been used and seems to be successful in many
aspects. Although most of works paid their attentions on seeking out accurate energy eigen-
values and seldom discussed the wave function, in particular WFO, Ref. $[9]$ simply discussed
the wave function by employing the multi-Gaussian trial wave function.

In many simple cases, the Gaussian-type or the exponential-type functions with a single-
parameter were taken as the trial wave function to discuss the ground or excited states. In
general, the accuracy of the resultant energy eigenvalues is satisfactory. However, by looking
at the wave function, one would find that although the resultant wave function sometimes
may not deviate much from the ”accurate” solution (usually it can be obtained by solving
the Schrödinger equation numerically) in the long-range part, but this deviation turns larger
and larger when $r \to 0$. 
In this work, we would study this problem in detail with various potentials which were used frequently in studying heavy quarkonia and put more emphasis on estimating WFO. The adopted trial wave functions were used in literatures except the last one.

The paper is organized as following. After the introduction, the variational method by using the single−parameter trial wave function is discussed in Sec.II. In Sec.III, variational calculation by employing multi-parameter trial wave functions is presented. The variational study on the 2S state of the $c\bar{c}$ system is further shown in Sec.IV, and in Sec.V, the relation between WFO and the reduced mass for various trial wave functions is investigated. In the last section, the discussion and conclusion are given.

II. Variational method with single−parameter trial wave function

There are many potential models which can fit the experimental spectra of the heavy quarkonia with certain accuracy. In the rest of the paper, we call them as "successful" potential models.

Within the framework of the non-relativistic potential model, the S-state wave function $\psi(r)$ of the heavy quarkonium satisfies the Schrödinger equation

$$H\psi(r) = -\frac{1}{2\mu} \Delta \psi(r) + V(r)\psi(r) = E\psi(r)$$

(1)

where $H$ is the Hamiltonian of the quarkonium, $V(r)$ denotes the central potential between quark and antiquark, $E$ represents the energy eigenvalue, and $\mu$ is the reduced mass. In general, one can numerically solve the Schrödinger equation to obtain $E$ and $\psi(r)$ simultaneously, and calculates $\psi(0)$ (WFO) in terms of the average value of $\frac{dV}{dr}$, i.e.

$$|\psi(0)|^2 = \frac{\mu}{2\pi} < \frac{dV}{dr} >$$

(2)

The values of the squared WFO for various "successful" potential models were listed in Refs. 1, 2. (note: $|R(0)|^2$ is equal to $4\pi|\psi(0)|^2$ in the Table 1 of Ref. 1.

To solve Eq.(1) by using the variational method, one needs to choose a suitable trial wave function $\psi(r; c)$ with $N$ independent parameters $\{c\} = \{c_1, c_2, \cdots, c_N\}$ first and then to seek out a set of parameters $\{c_0\} = \{c_{i0}, i = 1, 2, \cdots, N\}$ which minimizes the expectation value of Hamiltonian, namely

$$E(c) = < H > = \frac{<\psi(c)|H|\psi(c)>}{<\psi(c)|\psi(c)>}.$$  

(3)
The minimum value $E(c_0)$ gives an upper limit of the ground state energy. In the use of the variational method, one wishes to obtain $E(c_0)$ which is as close as possible to the "accurate" solution with the minimum number of parameters.

In this work, what we concern is how close to the "accurate" solution the resultant wave function can be, when $E(c_0)$ is satisfactorily close to the "accurate" energy eigenvalue. In particular, we would try to find the accuracy of WFO for various trial wave functions, which obviously affects the application of the variational method.

In this paper, we choose three most popular and "successful" models listed in Refs.[1, 2], so that the conclusion could be more general. These models are:

1. Cornell potential[10]:

$$V(r) = -\frac{4}{3} \alpha_s \frac{\alpha_s}{r} + kr,$$

with $\alpha_s = 0.39$, $k = 1/2.34^2(GeV)^2$ and the mass of $c$ quark $m_c = 1.84 GeV$.

2. Martin potential[11]:

$$V(r) = kr^{0.1},$$

with $k = 6.898$ and $m_c = 1.8 GeV$.

3. Logarithmic potential[12]:

$$V(r) = k\log(r),$$

with $k = 0.733$ and $m_c = 1.5 GeV$.

In this section, we choose the simplest trial wave function in which there is only one variational parameter to study the 1S state of $c\bar{c}$. The general form of such trial wave function is written as

$$\psi_{\text{trial}}(r) = N e^{-a r^b}$$

where

$$N = \left[ b \left( \frac{2a}{b} \right)^{\frac{3}{2}} \right]^{\frac{1}{b}}.$$

Indeed, $k$ in Eqs.(5) and (6) should have proper dimensions, but in our work, it is not important because they would be attributed into the normalization factors.
is the normalization constant, $a$ denotes the variational parameter which will be fixed by minimizing the expectation value of Hamiltonian and $b$ is the model parameter which determines the type of the trial wave function. In practice, we select following four trial wave functions:

(1). $b = 1$, namely $N e^{-a} r$ (hydrogen wave function or exponential wave function). It is the solution of the Coulomb potential model.

(2). $b = 2$, namely $N e^{-a} r^2$ (harmonic oscillator wave function or a Gaussian wave function).

(3). $b = \frac{3}{2}$, namely $N e^{-a} r^{3/2}$. This function was used by Gupta [6].

(4). $b = \frac{4}{3}$, namely $N e^{-a} r^{4/3}$. This is a newly proposed trial wave function, and we will pay more attention on it.

In order to fully understand the accuracies of the variational results in three different potential cases, we calculate four quantities by using four different trial wave functions and the corresponding "accurate" results by solving the Schrödinger equation numerically as well. These quantities are:

(1). the energy eigenvalue $E$ (note: we do not try to fit the experimental spectrum here, because it is not the aim of this work).

(2). average radius $<r>$.

(3). average value of the inversed radius $\langle \frac{1}{r} \rangle$.

(4) the squared WFO $|\psi(0)|^2$.

For each calculated quantity $q$ we give a relative deviation $\delta q$, which is defined as

$$\delta q = \frac{q_{\text{var}} - q_{\text{true}}}{q_{\text{true}}}$$

where $q_{\text{var}}$ is the variational result and $q_{\text{true}}$ the "accurate" value.

In the case of the Cornell potential (4), kinetic energy $<T>$ and potential energy $<V>$ are:

$$<T> = \frac{(2a)^{\frac{7}{6}}b^2\Gamma(2 + \frac{1}{b})}{8\mu\Gamma(\frac{4}{b})},$$

(9)

$$<V> = -4(2a)^{\frac{7}{6}}\alpha_s\Gamma(\frac{2}{b}) + 3k\Gamma(\frac{4}{b})$$

(10)

Then we can obtain the expectation value of Hamiltonian and consequently an algebraic equation, which is used to determine $a$,

$$[3b^2\Gamma(2 + \frac{1}{b})]x^3 - [16\alpha_s\mu\Gamma(\frac{2}{b})]x^2 - 12k\mu\Gamma(\frac{4}{b}) = 0,$$
where \( x = (2a)^{1\over 3} \). It is very easy to solve this equation. If we rewrite it in the following form:

\[
A_3 x^3 + A_2 x^2 + A_0 = 0,
\]

(11)

the real solution of \( x \) can be expressed as:

\[
x_{\text{real}} = -\frac{A_2}{3A_3} + \frac{2^{1\over 3} A_2^2}{3A_3 B} + \frac{B}{3} \left( 2^{1\over 3} A_3^2 \right),
\]

(12)

where \( B = (B_0 + \sqrt{-4A_2^6 + B_0^2})^{1\over 4} \) and \( B_0 = -2A_3^3 - 27A_0 A_3^2 \).

In the case of Martin potential (5), the potential energy reads:

\[
\langle V \rangle = \frac{k \Gamma \left( \frac{3}{4} + \frac{1}{b} \right)}{(2a)^{\frac{3}{4} + \frac{1}{b}} \Gamma \left( \frac{3}{2} \right)}.
\]

(13)

Therefore, the equation for determining \( a \) is quite simple. The solution is

\[
a = \frac{1}{2} \left[ \frac{0.4 \mu k}{b^2 \Gamma(2 + \frac{1}{b})} \right]^{1\over 3}.
\]

(14)

In the case of logarithmic potential (6), by the similar procedure we obtain

\[
a = \frac{1}{2} \left[ \frac{4 \mu k}{b^2 \Gamma(2 + \frac{1}{b})} \right]^{1\over 2}.
\]

(15)

All the numerical results are listed in Tables 1.1 to 1.3. In order to make comparison, we write the corresponding "accurate" results in the table captions and list relative deviations in the corresponding tables.

Table 1.1

| \( b \) | \( E \) | \( \langle r \rangle \) | \( \langle r^2 \rangle \) | \( |\psi(0)|^2 \) |
|-------|-------|----------------|----------------|----------------|
| 1     | 0.272795 (0.059) | 1.7908 (0.049) | 0.8376 (0.036) | 0.197052 (0.61) |
| 2     | 0.280039 (0.087) | 1.7234 (0.069) | 0.7388 (-0.098) | 0.050403 (-0.57) |
| \( \frac{1}{2} \) | 0.259785 (0.0088) | 1.6989 (0.0049) | 0.7908 (-0.022) | 0.082911 (-0.29) |
| \( \frac{1}{3} \) | 0.257809 (0.0011) | 1.7083 (0.0006) | 0.8083 (-0.0002) | 0.103334 (-0.11) |

Table 1.2

The variational results with a single parameter trial function in the Martin potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: \( E(1S) = 7.5605 \text{ GeV} \), \( \langle r \rangle = 1.72332 \text{ GeV}^{-1} \), \( \langle \frac{1}{r} \rangle = 0.782946 \text{ GeV} \), \( |\psi(0)|^2 = 0.0778779 \text{ GeV}^3 \).
Table 1.3

The variational results with a single parameter trial function in the logarithmic potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: \( E(1S) = 0.730733 \text{ GeV}, \) \( < r > = 1.87535 \text{ GeV}^{-1}, \) \( < \frac{1}{r} > = 0.723538 \text{ GeV}, \) \( |\psi(0)|^2 = 0.0633063 \text{ GeV}^3. \)

| \( b \) | \( E \) | \( < r > \) | \( < \frac{1}{r} > \) | \( |\psi(0)|^2 \) |
|---|---|---|---|---|
| 1 | 7.5871 (0.0035) | 1.8606 (0.079) | 0.8064 (0.030) | 0.166933 (1.14) |
| 2 | 7.57509 (0.0019) | 1.7151 (-0.0048) | 0.7423 (-0.052) | 0.091445 (-0.34) |
| \( \frac{1}{2} \) | 7.5607 (3\( \times 10^{-5} \)) | 1.7194 (-0.0023) | 0.7814 (-0.0020) | 0.079984 (-0.027) |
| \( \frac{3}{4} \) | 7.5622 (0.0002) | 1.7415 (0.011) | 0.7928 (0.013) | 0.097596 (-0.25) |

III. Trial functions with two, three and four parameters

The trial wave function with two or more variational parameters may have various forms. The most straightforward one is to multiply Eq.(7) by a polynomial of \( r \), namely

\[
\psi(r) = (c_0 + c_1 r + c_2 r^2 + \cdots + c_n r^n) e^{-a r^b}, \tag{16}
\]

where \( a \) and \( c_1, c_2, \cdots, c_n \) are variational parameters, and \( c_0 \) can be fixed by the normalization condition. Using the standard procedure discussed above, we calculate the above mentioned four quantities in terms of the trial wave functions with two, three and four parameters in the three potential cases and four \( b \) value cases. The numerical results are listed in Tables 2.1–2.3, 3.1–3.3 and 4.1–4.3, respectively.

Table 2.1

The variational results with the two-parameter trial wave function in the Cornell potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: \( E(1S) = 0.257526 \text{ GeV}, \) \( < r > = 1.7073 \text{ GeV}^{-1}, \) \( < \frac{1}{r} > = 0.80848 \text{ GeV} \) and \( |\psi(0)|^2 = 0.116054 \text{ GeV}^3. \)

| \( b \) | \( E \) | \( < r > \) | \( < \frac{1}{r} > \) | \( |\psi(0)|^2 \) |
|---|---|---|---|---|
| 1 | 0.265416 (0.031) | 1.7562 (0.029) | 0.8296 (0.026) | 0.158048 (0.36) |
| 2 | 0.271382 (0.054) | 1.7098 (0.0015) | 0.7585 (-0.062) | 0.065156 (-0.44) |
| \( \frac{1}{2} \) | 0.258738 (0.0047) | 1.6991 (0.0043) | 0.7959 (-0.016) | 0.091133 (-0.22) |
| \( \frac{3}{4} \) | 0.257624 (0.0004) | 1.7080 (0.0004) | 0.8088 (0.0003) | 0.108602 (-0.064) |

Table 2.2
The variational results with the two-parameter trial wave function in the Martin potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: $E(1S) = 7.5605 \, \text{GeV}$, $< r > = 1.72332 \, \text{GeV}^{-1}$, $< \frac{1}{r} > = 0.782946 \, \text{GeV}$, $|\psi(0)|^2 = 0.0778779 \, \text{GeV}^3$.

| $b$ | $E$ | $< r >$ | $< \frac{1}{r} >$ | $|\psi(0)|^2$ |
|-----|-----|---------|----------------|----------------|
| 1   | 7.56173 (0.0001) | 1.7337 (0.0060) | 0.7847 (0.0022) | 0.069440 (-0.11) |
| 2   | 7.56873 (0.0011) | 1.7110 (-0.0007) | 0.7569 (-0.033) | 0.064430 (-0.17) |
| $\frac{1}{b}$ | 7.56068 ($2 \times 10^{-6}$) | 1.7213 (-0.0012) | 0.7830 ($4 \times 10^{-5}$) | 0.082579 (0.060) |
| $\frac{1}{b}$ | 7.56054 ($5 \times 10^{-6}$) | 1.7222 (-0.0006) | 0.7832 (0.0001) | 0.0785065 (-0.0081) |

Table 2.3

The variational results with the two-parameter trial wave function in the logarithmic potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: $E(1S) = 0.730733 \, \text{GeV}$, $< r > = 1.87535 \, \text{GeV}^{-1}$, $< \frac{1}{r} > = 0.7246 (0.0015)$, $|\psi(0)|^2 = 0.0633063 \, \text{GeV}^3$.

| $b$ | $E$ | $< r >$ | $< \frac{1}{r} >$ | $|\psi(0)|^2$ |
|-----|-----|---------|----------------|----------------|
| 1   | 0.731264 (0.0007) | 1.88523 (0.0053) | 0.7246 (0.0015) | 0.058204 (-0.081) |
| 2   | 0.740704 (0.014) | 1.8587 (-0.0089) | 0.6968 (-0.037) | 0.050334 (-0.21) |
| $\frac{1}{b}$ | 0.731022 (0.0004) | 1.8707 (-0.0025) | 0.7233 (-0.0017) | 0.064733 (0.050) |
| $\frac{1}{b}$ | 0.730798 ($9 \times 10^{-6}$) | 1.8741 (-0.0007) | 0.7236 (0.0001) | 0.064889 (0.025) |

Table 3.1

The variational results with the three-parameter trial wave function in the Cornell potential case. The values listed in parentheses are relative deviations. The "accurate" results are: $E(1S) = 0.257526 \, \text{GeV}$, $< r > = 1.7073 \, \text{GeV}^{-1}$, $< \frac{1}{r} > = 0.8086 (0.0001)$, $|\psi(0)|^2 = 0.116054 \, \text{GeV}^3$.

| $b$ | $E$ | $< r >$ | $< \frac{1}{r} >$ | $|\psi(0)|^2$ |
|-----|-----|---------|----------------|----------------|
| 1   | 0.257834 (0.0012) | 1.7096 (0.0013) | 0.8096 (0.0014) | 0.108931 (-0.061) |
| 2   | 0.257908 (0.0015) | 1.7063 (-0.0006) | 0.8059 (-0.0032) | 0.105760 (-0.089) |
| $\frac{1}{b}$ | 0.257665 (0.0005) | 1.7073 ($-4 \times 10^{-7}$) | 0.8078 (-0.0008) | 0.105696 (-0.089) |
| $\frac{1}{b}$ | 0.257623 (0.0004) | 1.7079 (0.0004) | 0.8086 (0.0001) | 0.108278 (-0.067) |

Table 3.2

The variational results with the three-parameter trial wave function in the Martin potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: $E(1S) = 7.5605 \, \text{GeV}$, $< r > = 1.72332 \, \text{GeV}^{-1}$, $< \frac{1}{r} > = 0.782946 \, \text{GeV}$, $|\psi(0)|^2 = 0.0778779 \, \text{GeV}^3$.

| $b$ | $E$ | $< r >$ | $< \frac{1}{r} >$ | $|\psi(0)|^2$ |
|-----|-----|---------|----------------|----------------|
| 1   | 7.56082 ($4 \times 10^{-5}$) | 1.7264 (0.0008) | 0.7843 (0.0017) | 0.070081 (-0.10) |
| 2   | 7.56077 ($4 \times 10^{-5}$) | 1.7203 (-0.0002) | 0.7848 (-0.0023) | 0.090033 (0.16) |
| $\frac{1}{b}$ | 7.56050 ($6 \times 10^{-5}$) | 1.7233 ($5 \times 10^{-5}$) | 0.7829 ($-3 \times 10^{-5}$) | 0.077090 (-0.010) |
| $\frac{1}{b}$ | 7.56069 ($2 \times 10^{-5}$) | 1.7236 (-0.0002) | 0.7818 (0.0014) | 0.081307 (-0.044) |
The variational results with the three-parameter trial wave function in the logarithmic potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: \(E(1S) = 0.730733 \text{ GeV}, \quad <r> = 1.78535 \text{ GeV}^{-1}, \quad \langle \frac{1}{r} \rangle = 0.723538 \text{ GeV}, \quad |\psi(0)|^2 = 0.0633063 \text{ GeV}^3.\)

| \(b\) | \(E\) | \(<r>\) | \(<\frac{1}{r}>\) | \(|\psi(0)|^2\) |
|-----|------|------|--------|--------|
| 1   | 0.730759 (4 \times 10^{-5}) | 1.8762 (0.0004) | 0.7236 (8 \times 10^{-6}) | 0.065321 (0.032) |
| 2   | 0.730996 (0.0003) | 1.8757 (0.0002) | 0.7245 (-0.0014) | 0.072312 (0.14) |
| \(\frac{1}{2}\) | 0.73088 (0.0002) | 1.8745 (-0.0004) | 0.7240 (0.0006) | 0.0676953 (0.069) |
| \(\frac{3}{2}\) | 0.730796 (9 \times 10^{-5}) | 1.8743 (-0.0006) | 0.7238 (0.0004) | 0.0651086 |

The variational results with the four-parameter trial function in the Cornell potential case. The values listed in parentheses are relative deviations. The "accurate" results are: \(E(1S) = 0.257526 \text{ GeV}, \quad <r> = 1.7073 \text{ GeV}^{-1}, \quad \langle \frac{1}{r} \rangle = 0.8086 (0.0002) \text{ GeV}^3.\)

| \(b\) | \(E\) | \(<r>\) | \(<\frac{1}{r}>)\ | \(|\psi(0)|^2\) |
|-----|------|------|--------|--------|
| 1   | 0.257599 (0.0003) | 1.7093 (0.0012) | 0.806 (0.0002) | 0.114842 (-0.010) |
| 2   | 0.257667 (0.0005) | 1.7021 (0.0003) | 0.8096 (-0.0014) | 0.106024 (-0.037) |
| \(\frac{1}{2}\) | 0.257566 (0.0005) | 1.7068 (-0.0003) | 0.8077 (-0.0010) | 0.106024 (-0.037) |
| \(\frac{3}{2}\) | 0.257581 (0.0002) | 1.7074 (6 \times 10^{-5}) | 0.8085 (5 \times 10^{-5}) | 0.0791203 (0.016) |

The variational results with the four-parameter trial wavefunction in the Martin potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: \(E(1S) = 7.5605 \text{ GeV}, \quad <r> = 1.72332 \text{ GeV}^{-1}, \quad \langle \frac{1}{r} \rangle = 0.782946 \text{ GeV}^3.\)

| \(b\) | \(E\) | \(<r>\) | \(<\frac{1}{r}>)\ | \(|\psi(0)|^2\) |
|-----|------|------|--------|--------|
| 1   | 7.56051 (1 \times 10^{-6}) | 1.7233 (-2 \times 10^{-6}) | 0.7830 (2 \times 10^{-6}) | 0.0791203 (0.016) |
| 2   | 7.56068 (2 \times 10^{-6}) | 1.7192 (-0.0024) | 0.7852 (0.0029) | 0.0860623 (0.11) |
| \(\frac{1}{2}\) | 7.56051 (1 \times 10^{-6}) | 1.7226 (-0.0004) | 0.7830 (8 \times 10^{-6}) | 0.0779022 (0.0003) |
| \(\frac{3}{2}\) | 7.56051 (1 \times 10^{-6}) | 1.7232 (-8 \times 10^{-6}) | 0.7831 (0.0001) | 0.0779022 (0.0003) |

The variational results with the four-parameter trial wave function in the logarithmic potential case. The values listed in parentheses are relative deviations. The "accurate" solutions are: \(E(1S) = 0.730733 \text{ GeV}, \quad <r> = 1.78535 \text{ GeV}^{-1}, \quad \langle \frac{1}{r} \rangle = 0.723538 \text{ GeV}, \quad |\psi(0)|^2 = 0.0633063 \text{ GeV}^3.\)

| \(b\) | \(E\) | \(<r>\) | \(<\frac{1}{r}>)\ | \(|\psi(0)|^2\) |
|-----|------|------|--------|--------|
| 1   | 0.730757 (6 \times 10^{-5}) | 1.876 (0.0005) | 0.7234 (-0.0001) | 0.0633063 (-0.0036) |
| 2   | 0.730913 (0.0002) | 1.87499 (-0.0002) | 0.72366 (-0.0002) | 0.069062 (-0.10) |
| \(\frac{1}{2}\) | 0.730738 (7 \times 10^{-5}) | 1.8754 (4 \times 10^{-6}) | 0.7236 (0.0001) | 0.06408 (0.017) |
| \(\frac{3}{2}\) | 0.730732 (1 \times 10^{-5}) | 1.8754 (2 \times 10^{-6}) | 0.7236 (0.0004) | 0.0629413 (-0.0058) |
Another possible type of trial wave function with multi-parameters can be chosen in the form of the superposition of two or more above mentioned trial wave functions with different \( b \) or \( a \) values, respectively. We give an example in the following. From the resultant \( |\psi(0)|^2 \) in Tables 1.1–1.3, it is easy to see that in the exponential-type trial wave function \((b = 1)\) case, \( |\psi(0)|^2 \) values are larger than ”accurate” ones (the deviation is positive), while in the other three trial wave function cases \((b = 2, 3/2, \text{ and } 4/3)\), the corresponding results are less than ”accurate” ones (negative deviation). Therefore, one can compromise the deviations by combining two different types of trial wave functions with which the positive and negative deviations appear, respectively. After testing various combinations, we find that the results are similar to those by using three parameters in the last section. In fact, this new trial wave function has three variational parameters too. In the following, we list two specific combinations and corresponding results.

The first example is the mixture of a exponential-type wave function and a Gaussian wave function, i.e.

\[
R(r) = c_1 e^{-\frac{r}{a}} + c_2 e^{-\frac{a^2 r^2}{2}}.
\]

(17)

For the Cornell potential, the relative deviation of energy is 0.002 and the relative deviation of squared WFO is 0.099.

The second example is the mixture of an exponential-type function and a Gupta’s function, i.e.

\[
R(r) = c_1 e^{-\frac{r}{a}} + c_2 e^{-a_1 r^3}.
\]

(18)

For the Cornell potential the relative deviation of energy is 0.00015 and the relative deviation of squared WFO is 0.025.

Apparently, with the same number of variational parameters, these combined trial wave function can give better description on both energy and WFO.

IV. 2S state of \( c\bar{c} \)

Based on the results of the 1S state, it is easy to discuss the 2S state. We first select a normalized trial wave function which is orthogonal to the 1S wave function. It can be a single-parameter or multi-parameter function. But we find that it is quite difficult to obtain a highly accurate WFO. In order to make sense, we demonstrate two examples.
The first example is that we take the $1S$ trial wave function as

$$R_{1S}(r) = N e^{-a r^{3/2}},$$  \quad (19)$$

where $N$ is the normalization constant and $a$ is determined by the variational method. Then we choose the $2S$ trial wave function to be

$$R_{2S}(r) = (c_0 + c_1 r + c_2 r^2 ) e^{-a r^{3/2}},$$  \quad (20)$$

where $a$ takes the same value as that in $R_{1S}(r)$. By considering the orthonormal condition, only one parameter remains free. This parameter can be fixed by the variational method. The obtained results show that the relative deviation of energy is 0.004, while the relative deviation of the squared WFO of the $2S$ state is 0.25.

Moreover, if we take

$$R_{2S}(r) = (c_0 + c_1 r + c_2 r^2 + c_3 r^3 ) e^{-a r^{3/2}},$$  \quad (21)$$

there are two variational parameters in the trial wave function. The resultant relative deviations of energy and squared WFO turn to be 0.0009 and 0.11, respectively.

Similar to the $1S$ state trial wave function, if we take a trial wave function with four parameters, the resultant relative deviation of the squared WFO of the $2S$ state is less than 0.05.

V. Relationship between WFO and reduced mass

There were lots of discussions concerning the relation between WFO and the reduced mass in the heavy quarkonium system \cite{1,2}. Because the variational method can give the analytical expression of the wave function, consequently the exact value of WFO, the approximate relation between WFO and the reduced mass can be obtained. For example, if the trial wave function with parameter $a$ for the $1S$ state, Eq.(7), is chosen, the squared WFO can be written as

$$|\psi(0)|^2 = N^2 = \frac{b (2a)^{3/2}}{4\pi \Gamma(3b/2)}.$$  \quad (22)$$

In the Martin potential case, substituting (14) into (22), we obtain

$$|\psi(0)|^2 = \frac{b}{4\pi \Gamma(3/2)} \left[ \frac{0.4k\Gamma(3.1)}{b^2 \Gamma(2 + \frac{3}{b})} \mu \right]^\frac{3}{2}.$$  \quad (23)$$
This relation is similar to that given by the simple scaling arguments for the power-law potential, namely

$$|\psi(0)|^2 \sim \mu^{\frac{3}{2}+\nu}. \quad (24)$$

When $\nu = 0.1$, Eqs.(23) and (24) coincide with each other. It clearly shows that although the variational method is an approximation, it retains the main characteristics of the solution. This observation encourages us to apply the variational method to the estimation of WFO.

As shown in Table 1.1, when $b = \frac{3}{2}$, the squared WFO of the 1S state of $c\bar{c}$ has the least deviation(0.027). By taking $m_b = 5.174 GeV$ [11], one obtains 0.361475 for the squared WFO of the 1S state of $b\bar{b}$. In the $B_c$ meson case, the calculated reduced mass is 1.3336 GeV, and the squared WFO of the 1S state is 0.140547. The resultant relative deviations of WFO for both $b\bar{b}$ and $B_c$ are 0.027 which is the same as that for $c\bar{c}$.

In the logarithmic potential case, the similar treatment leads to

$$|\psi(0)|^2 = \frac{b}{4\pi\Gamma\left(\frac{3}{2}\right)} \left[ \frac{4k\Gamma\left(\frac{2}{b}\right)}{b^2\Gamma(2+\frac{1}{b})} \right] \mu^{\frac{3}{2}}. \quad (25)$$

It is easy to see that the relation between WFO and the reduced mass $\mu$ is consistent with that obtained from the scaling arguments for the power-law potential with $\nu = 0$.

Again in the single-parameter trial wave function with $b = \frac{3}{2}$ case, one finds the least deviation. By taking $m_c = 1.5 GeV$ and $m_b = 4.906 GeV$ [12], the squared WFOs of the 1S states of $J/\psi$, $\Upsilon$ and $B_c$ are 0.062492, 0.36964 and 0.118462, and the corresponding relative deviations are about 0.013, respectively. This is a quite satisfactory and encouraging observation.

In the Cornell potential case, by employing the single-parameter trial wave function with $a$ given in Eq.(12), one can carry out a similar discussion. The obtained relation between the squared WFO and the reduced mass is much more complicated than that in Eqs.(23) and (25). We omit the detailed expression in the text but give following two interesting results, which are computed by taking $b = \frac{4}{3}$ and the relative deviation within 10%.

(1). The curve of $|\psi(0)|^2$ as the function of the reduced mass $\mu$ has the similar behavior as those in the former two cases. When $\mu = 0.2$ – 3.0 GeV, the function $f(\mu) \sim \mu^{2.2}$ can fit the curve very well. This corresponds to $\nu = -0.65$ in Eq.(24).

(2). If we take $m_c = 1.84$ GeV and $m_b = 5.17$ GeV [11], the conjecture of Eq. (8) in Ref.[1]
\[ |\psi_{bc}(0)|^2 \simeq |\psi_{cc}(0)|^{1.3} |\psi_{bb}(0)|^{0.7} \]

holds within 2.5%.

**VI. Conclusion and discussion**

In this paper, we carefully studied the variational method, especially in determining the binding energies, wave functions at the origin, average radii and etc. of the quarkonium. Retaining generality as much as possible, we employ several "successful" potential models to analyze. By comparing the numerical results obtained in terms of the variational method with those by solving Schrödinger equation numerically, we present the relative deviations by employing different trial wave functions with single- or multi-parameters in various potential models.

In the variational method with fewer parameters, even the calculated binding energies and some transition matrix elements are accurate enough, it is not easy to obtain a very accurate WFO. Because of the phenomenological requirements, a certain accuracy is requested. Thus, one of our aims is to seek for a possible and simpler way to solve this problem.

We first study the single-parameter trial wave function case. The results shown in Tables 1.1-1.3 indicate that for the Cornell potential, the trial wave function with \( b = \frac{4}{3} \), i.e. \( \psi(r) = N e^{-a} r^4 \), can give the least relative deviation of squared WFO. The value of the deviation is about 0.11 which is not accurate enough, although the relative deviation of energy already reaches \( 10^{-3} \). For the Martin and the logarithmic potentials, the situations are better. When \( b = \frac{3}{2} \), one obtains the least values of 0.027 and 0.013 for the relative deviations of squared WFO, respectively, while the corresponding relative deviations of energy reach \( 10^{-4} \) and \( 10^{-5} \), respectively.

The accuracy of variational results can be improved when the number of the variational parameters are increased. This is true in general. If one adopts more than four variational parameters, he may expect very high accuracy for energy, but not always for WFO. It is much more difficult to further improve the accuracy of WFO than that of energy. The resultant accuracy of WFO seriously depends on the choice of the trial wave function. Sometimes as the number of parameters increases, the accuracy of WFO deteriorates, while the accuracy of energy is much more improved. Of course, in this case, the variational calculation becomes much more tedious and difficult.
The trial wave function with a single variational parameter is most convenient for use. If the accuracy of 10% for WFO in the Cornell potential case is tolerable, $\psi(r) = N e^{-a r^{\frac{4}{3}}}$ would be the best choice for the $1S$ state trial wave function. For the Martin and logarithmic potentials, $\psi(r) = N e^{-a r^{\frac{4}{3}}}$ is the most appropriate trial wave function for the $1S$ state, and the corresponding WFOs have quite satisfactory accuracies. In particular, these forms can give very simple and reasonable relations between WFO and the reduced mass, which agree with those deduced from the general arguments for power-law potentials. However, the requested accuracy of squared WFO in the system concerned is generally lower than $2 - 3\%$, and the trial wave functions with a single parameter cannot provide this accuracy. For instance, one indicated in Ref.\[13\] that the estimated decay constant in Ref.\[14\], where a single-parameter harmonic oscillator trial wave function was employed in solving the Schrödinger equation in the Cornell potential case, may not be reliable, although the computed transitions and energy are quite reasonable.

Here we would like to point out that to solve the Hamiltonian (Eq.(77) in Ref.\[15\])

$$H^{(1)} = -\frac{1}{m} \Delta - \frac{C_F \alpha_s}{r} - \frac{C_F \beta_0 \alpha_s^2}{2\pi} \ln \frac{r}{\mu},$$

the exponential-type trial wave function with a single parameter (Eq.(79) in \[15\])

$$f_b(r) = \frac{2}{b^2} e^{-\frac{r}{b}}$$

was employed in the variational framework. The paper reported that because the resultant energy agreed with the "accurate" value up to an order of $O(\alpha_s^4)$, Eq.(26) could be an appropriate trial wave function. Then, the resultant WFO would be accurate enough to serve their main goal. However, our estimation shows that by using various parameters given in Eq.(26) (take $\mu = m$ in Eq.(27)), the relative deviations of squared WFO are about 0.40 and 0.18 for $\tilde{c}\tilde{c}$ and $\tilde{b}\tilde{b}$, respectively. These results would lead to improper theoretical predictions for the quantities which are closely related to WFO.

As the conclusion we can draw, for the binding energy, most of trial wave functions, even with a single-parameter, can result a solution with a satisfactory accuracy. However, this is not always true for WFO. To obtain a reliable value of WFO, one has to adopt not only an appropriate trial wave function form for a specific potential, but also the proper number of variational parameters in the function. Our finding indicates that for a specific potential form and a not very higher accuracy of WFO, one can always find out a relatively simpler and more reliable trial wave function with an appropriate number of parameters. However, the form of the trial wave function strongly depends on the potential. In general, there is
no universal rule to determine the form and the number of the parameters of the trial wave function.

On the other hand, our study shows that if one chooses Eq.(16) as the trial wave function, when the potential is flatter at the large \( r \), the higher power terms, namely the higher configuration mixing, should be considered so that the higher accuracy of WFO can be reached. Moreover, the results by using Eqs.(17) and (18) indicate that if several components of the trial wave function can compromise the descriptions of the asymptotic behaviors of the potential at the short- and long-ranges, respectively, the trial wave function would have the simplest form and can provide higher accuracies for both binding energy and WFO. Namely, the trial wave function is more efficient. Usually, when a four-parameter trial wave function is chosen, in the commonly used potential cases, the accuracies of the energy and WFO can reach \( 10^{-4} \sim 10^{-6} \) and \( 10^{-2} \sim 10^{-3} \), respectively.

As mentioned in the introduction, the variational method should further be studied. Now, if the potential is not very singular, namely would not cause the divergence in solving Schrödinger equation, we find the way to construct an efficient trial wave function to get the more accurate binding energy and WFO. Then the next step is to study that if the potential is very singular, say more singular than \( 1/r^3 \), how the bound state problem can be solved and the real physics can be obtained by using the variational method, and whether the obtained result in this method corresponds to reality. These discussion is shown in our next paper [8].

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