

Isgur–Wise function and a new approach to potential model

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Considering the Cornell potential $V(r) = -\frac{4\alpha_s}{3r} + br + c$, we have revisited the Dalgarno's method of perturbation by incorporating two scales r^{short} and r^{long} as integration limit so that the perturbative procedure can be improved in a potential model. With the improved version of the wave function the ground state masses of the heavy–light mesons D , D_s , B , B_s and B_c are computed. The slopes and curvatures of the form factors of semileptonic decays of heavy–light mesons in both HQET limit and finite mass limit are calculated and compared with the available data.

Keywords: Quantum chromodynamics; Dalgarno's method; Isgur–Wise function.

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1. Introduction

The heavy hadron spectroscopy played a major role in the foundation of QCD. In last few years, it has sparked a renewed interest in the subject due to numerous data available from the B factories,¹ CLEO,² LHCb³ and the Tevatron.⁴ In more recent times, the discovery of $X - Y$ states⁵ as possible charmonium and bottonium hybrids have extended such study of the exotic heavy hadron spectroscopy. The most recent discoveries of the charmonium pentaquarks⁶ have further increase its importance. The simplest system of this area is the heavy–light and heavy–heavy hadrons.

In this paper, we will report a study of such heavy flavored mesons in a QCD potential model⁷ pursued in recent years. In the last few years, the experimental study of heavy–light and heavy–heavy mesons has renewed the theoretical interest toward Heavy Quark Effective Theory (HQET) and Isgur–Wise function.^{8–12}

The dynamics of the heavy quark meson is governed by the inter-quark potential. The properties of the heavy mesons are in rough approximation is described by

the Cornell potential, $V(r) = -\frac{4\alpha_s}{3r} + br + c$,¹³ which is a Coulomb-plus-linear nonrelativistic confinement potential. The first Coulomb term of the potential is consistent with one-gluon-exchange contribution for short distance. The second term generates the confinement in long distance. Both the potentials play decisive role in the quark dynamics and their separation is not possible. Besides there is no appropriate small parameter so that one of the potential within a perturbative theory can be made perturbative. The third term “ c ”¹⁴ which is a phenomenological constant needed to reproduce correct masses of heavy–light meson bound state.

In general, it is expected that a constant term “ c ” in the potential should not affect the wave function of the system while applying the perturbation theory. But in our previous work,¹⁵ it is seen that whether the term “ c ” is in parent or perturbed part of the Hamiltonian, it always appears in the total wave function which is inconsistent with the quantum mechanical idea that a constant term “ c ” in the potential can at best shift the energy scale, but should not perturb the wave function, i.e. a Hamiltonian H with such a constant and another H' without it should give rise to the same wave functions.

Due to this inconsistency or for the validation of the quantum mechanical idea while using perturbation theory like Dalgarno’s method^{16,17} in this work we have considered the scaling factor $c = 0$.

Also in this work both the short range and long range effects are tried to incorporate in the total wave function. Because in our earlier works,^{11,18,19} the properties of the mesons are studied considering the Coulombic part of the Cornell potential dominant over the linear part. On the other hand in Refs. 10, 20 and 21, the Schrödinger equation is solved by considering the linear part to be dominant over the Coulombic part.

However, it is well known that at short distance Coulomb potential plays a more dominant role than the linear confinement because while the former is inversely proportional to “ r ”, the later is linear. Similarly, for large distance the confinement takes over the Coulomb effect. Therefore, if the inter-quark separation “ r ” can be roughly divided into short distance (r^{short}) and long distance (r^{long}) effectively one of the potential will dominate over the other. In such situation confinement parameter (b) and the strong coupling parameter (α_s) can be considered as effective and appropriate small perturbative parameters.

This paper is organized as follows. In Sec. 2, we outline the formalism, while in Sec. 3 summarize the results for masses of various mesons and slope and curvature for Isgur–Wise function. Section 4 contains conclusion and comments.

2. Formalism

2.1. Dalgarno’s method of perturbation

The nonrelativistic two body Schrödinger equation¹⁷ is

$$H|\psi\rangle = (H_0 + H')|\psi\rangle = E|\psi\rangle, \quad (1)$$

so that the first-order perturbed eigenfunction $\psi^{(1)}$ and eigenenergy $W^{(1)}$ can be obtained using the relation

$$H_0\psi^{(1)} + H'\psi^{(0)} = W^{(0)}\psi^{(1)} + W^{(1)}\psi^{(0)}, \quad (2)$$

where

$$W^{(0)} = \langle \psi^{(0)} | H_0 | \psi^{(0)} \rangle, \quad (3)$$

$$W^{(1)} = \langle \psi^{(0)} | H' | \psi^{(0)} \rangle. \quad (4)$$

We calculate the total wave functions using Dalgarno’s method of perturbation for the potential

$$V(r) = -\frac{4\alpha_s}{3r} + br, \quad (5)$$

where $-\frac{4}{3}$ is due to the color factor, α_s is the strong coupling constant, r is the inter-quark distance, b is the confinement parameter (phenomenologically, $b = 0.183 \text{ GeV}^2$).²²

For potential of type (5), one of the choice for parent and perturbed Hamiltonian is

$$H_0 = -\frac{4\alpha_s}{3r}$$

and

$$H' = br.$$

The total wave function (App. A) for this case is

$$\psi_I^{\text{total}}(r) = \frac{N}{\sqrt{\pi a_0^3}} \left[1 - \frac{1}{2} \mu b a_0 r^2 \right] \left(\frac{r}{a_0} \right)^{-\epsilon} e^{-\frac{r}{a_0}}, \quad (6)$$

where normalization constant is

$$N = \frac{1}{\left[\int_0^{r^{\text{short}}} \frac{4r^2}{a_0^3} \left[1 - \frac{1}{2} \mu b a_0 r^2 \right]^2 \left(\frac{r}{a_0} \right)^{-2\epsilon} e^{-\frac{2r}{a_0}} dr \right]^{\frac{1}{2}}}, \quad (7)$$

where the cutoff parameter r^{short} is used as integration limit for Coulomb as parent and linear as perturbation. Because here Coulomb part is considered to be dominant over the linear part for short distance and

$$a_0 = \left(\frac{4}{3} \mu \alpha_s \right)^{-1}, \quad (8)$$

$$\mu = \frac{m_q m_Q}{m_q + m_Q}, \quad (9)$$

m_q and m_Q are the masses of the light and heavy quark/antiquark respectively and μ is the reduced mass of the mesons and

$$\epsilon = 1 - \sqrt{1 - \left(\frac{4}{3}\alpha_s\right)^2} \quad (10)$$

is the correction for relativistic effect^{23,24} due to Dirac modification factor.

Similarly, the wave function up to $O(r^4)$ (App. B) for another choice of parent and perturbed Hamiltonian of (5), where

$$H_0 = br \quad (11)$$

and

$$H' = -\frac{4\alpha_s}{3r}, \quad (12)$$

is

$$\begin{aligned} \psi_{\text{II}}^{\text{total}}(r) = & \frac{N'}{r} [1 + A_0 r^0 + A_1(r)r + A_2(r)r^2 \\ & + A_3(r)r^3 + A_4(r)r^4] A_i[\rho_1 r + \rho_0] \left(\frac{r}{a_0}\right)^{-\epsilon}, \end{aligned} \quad (13)$$

where $A_i[r]$ is the Airy function²⁵ and N' is the normalization constant,

$$N' = \frac{1}{\left[\int_{r_{\text{long}}}^{r_0} 4\pi [1 + A_0 r^0 + A_1(r)r + A_2(r)r^2 + A_3(r)r^3 + A_4(r)r^4]^2 (A_i[\rho_1 r + \rho_0])^2 \left(\frac{r}{a_0}\right)^{-2\epsilon} dr \right]^{\frac{1}{2}}}. \quad (14)$$

The cutoff parameter r^{long} is used as integration limit because we have considered linear as parent and Coulomb as perturbation, where the linear part is considered to be dominant over the Coulomb part for long distance. The upper cutoff r_0 is used to make the analysis normalizable and convergent, because we have used Airy function as meson wave function. Later, we fixed r_0 to 1 Fermi²⁶ for our calculations.

The coefficients of the series solution as occurred in Dalgarno's method of perturbation are the function of α_s , μ , and b :

$$A_0 = 0, \quad (15)$$

$$A_1 = \frac{-2\mu \frac{4\alpha_s}{3}}{2\rho_1 k_1 + \rho_1^2 k_2}, \quad (16)$$

$$A_2 = \frac{-2\mu W^1}{2 + 4\rho_1 k_1 + \rho_1^2 k_2}, \quad (17)$$

$$A_3 = \frac{-2\mu W^0 A_1}{6 + 6\rho_1 k_1 + \rho_1^2 k_2}, \quad (18)$$

$$A_4 = \frac{-2\mu W^0 A_2 + 2\mu b A_1}{12 + 8\rho_1 k_1 + \rho_1^2 k_2}. \quad (19)$$

The parameters are

$$\rho_1 = (2\mu b)^{\frac{1}{3}}, \quad (20)$$

$$\rho_0 = -\left[\frac{3\pi(4n-1)}{8}\right]^{\frac{2}{3}}, \quad (21)$$

(in our case $n = 1$ for ground state)

$$k = \frac{0.355 - (0.258)\rho_0}{(0.258)\rho_1}, \quad (22)$$

$$k_1 = 1 + \frac{k}{r}, \quad (23)$$

$$k_2 = \frac{k^2}{r^2}, \quad (24)$$

$$W^1 = \int \psi^{(0)*} H' \psi^{(0)} d\tau, \quad (25)$$

$$W^0 = \int \psi^{(0)*} H_0 \psi^{(0)} d\tau. \quad (26)$$

2.2. Ground state masses of mesons

Masses of heavy flavored mesons in a specific potential model in the ground state can be obtained as:

$$M_P = m_{q/Q} + m_{\bar{q}/\bar{Q}} + \langle H \rangle, \quad (27)$$

where $m_{q/Q}$ is mass of light (or heavy) quark and $m_{\bar{q}/\bar{Q}}$ is mass of light (or heavy) antiquark constituting the meson bound state.

The above expression shows that to calculate the masses of mesons one needs to find $\langle H \rangle$, so that

$$\begin{aligned} \langle H \rangle &= \left\langle \frac{p^2}{2\mu} \right\rangle + \langle V(r) \rangle \\ &= 4\pi \int_0^\infty r^2 \psi^*(r) H \psi(r) dr \\ &= 4\pi \int_0^\infty r^2 \psi^*(r) \left(\frac{p^2}{2\mu} + V(r) \right) \psi(r) dr. \end{aligned} \quad (28)$$

To take into account both the Coulomb and linear parts of the potential we improve the above equation with the cutoff scales r^{short} and r^{long} as

$$\begin{aligned} \langle H \rangle = 4\pi & \left[\int_0^{r^{\text{short}}} r^2 \psi_I^*(r) \left(\frac{p^2}{2\mu} + V(r) \right) \psi_I(r) dr \right. \\ & \left. + \int_{r^{\text{long}}}^{r_0} r^2 \psi_{\text{II}}^*(r) \left(\frac{p^2}{2\mu} + V(r) \right) \psi_{\text{II}}(r) dr \right], \end{aligned} \quad (29)$$

where the wave functions $\psi_I(r)$ and $\psi_{\text{II}}(r)$ are defined in Eqs. (6) and (13), respectively.

2.3. Slope and curvature of Isgur–Wise function

Isgur, Wise, Georgi and others showed that in weak semileptonic decays of heavy–light mesons (e.g. B mesons to D or D^* mesons), in the limit $m_Q \rightarrow \infty$ all the form factors that describe these decays are expressible in terms of a single universal function of velocity transfer, which is normalized to unity at zero-recoil. This function is known as the Isgur–Wise function. It measures the overlap of the wave functions of the light degrees of freedom in the initial and final mesons moving with velocities v and v' respectively.

The Isgur–Wise functions are denoted by $\xi(Y)$, where $Y = v \cdot v'$ and $\xi(Y)|_{Y=1} = 1$ is the normalization condition at the zero-recoil point ($v = v'$).²⁷

The calculation of Isgur–Wise function is nonperturbative in principle and is performed for different phenomenological wave functions for mesons.^{11,21} This function depends upon the meson wave function and some kinematic factor as given below:

$$\xi(Y) = \int_0^\infty 4\pi r^2 |\psi(r)|^2 \cos(pr) dr, \quad (30)$$

where $\psi(r)$ is the wave function for light quark only and

$$\cos(pr) = 1 - \frac{p^2 r^2}{2} + \frac{p^4 r^4}{24} + \dots \quad (31)$$

with $p^2 = 2\mu^2(Y - 1)$.

Taking $\cos(pr)$ up to $O(r^4)$, we get,

$$\begin{aligned} \xi(Y) = & \int_0^\infty 4\pi r^2 |\psi(r)|^2 dr - \left[4\pi \mu^2 \int_0^\infty r^4 |\psi(r)|^2 dr \right] (Y - 1) \\ & + \left[\frac{2}{3} \pi \mu^4 \int_0^\infty r^6 |\psi(r)|^2 dr \right] (Y - 1)^2. \end{aligned} \quad (32)$$

In an explicit form, the Isgur–Wise function can be written as^{28,29}

$$\xi(Y) = 1 - \rho^2(Y - 1) + C(Y - 1)^2, \quad (33)$$

where $\rho^2 > 0$.

The quantity ρ^2 is the slope of the Isgur–Wise function which determines the behavior of Isgur–Wise function close to zero recoil point ($Y = 1$) and known as charge radius:

$$\rho^2 = \left. \frac{\partial \xi}{\partial Y} \right|_{Y=1}. \quad (34)$$

The second-order derivative is the curvature of the Isgur–Wise function known as convexity parameter:

$$C = \left. \frac{1}{2} \left(\frac{\partial^2 \xi}{\partial Y^2} \right) \right|_{Y=1}. \quad (35)$$

A precise knowledge of the slope and curvature of $\xi(Y)$ basically determines the Isgur–Wise function in the physical region. In HQET as proposed by Neubert,²⁸ the Isgur–Wise function at zero recoil point allows us to determine CKM element $|V_{cb}|$ ³⁰ for the semileptonic decays $B^0 \rightarrow D^* l \nu$ and $B^0 \rightarrow D l \nu$.

Now from Eqs. (32) and (33),

$$\rho^2 = 4\pi\mu^2 \int_0^\infty r^4 |\psi(r)|^2 dr, \quad (36)$$

$$C = \frac{2}{3}\pi\mu^4 \int_0^\infty r^6 |\psi(r)|^2 dr \quad (37)$$

and

$$\int_0^\infty 4\pi r^2 |\psi(r)|^2 dr = 1. \quad (38)$$

In this work, we improve the above equations for ρ^2 and C to

$$\rho^2 = 4\pi\mu^2 \left[\int_0^{r^{\text{short}}} r^4 |\psi_I(r)|^2 dr + \int_{r^{\text{long}}}^{r_0} r^4 |\psi_{II}(r)|^2 dr \right] \quad (39)$$

and

$$C = \frac{2}{3}\pi\mu^4 \left[\int_0^{r^{\text{short}}} r^6 |\psi_I(r)|^2 dr + \int_{r^{\text{long}}}^{r_0} r^6 |\psi_{II}(r)|^2 dr \right]. \quad (40)$$

Using these modified expressions for slope and curvature of Isgur–Wise function in Eq. (33), we have computed the results. In Eqs. (39) and (40), $\psi_I(r)$ and $\psi_{II}(r)$ are the wave functions as defined in (6) and (13), respectively.

Now to find the cutoffs r^{short} and r^{long} , we use the two choices of perturbative conditions:

Choice I: For Coulomb as parent and linear as perturbation

$$-\frac{4\alpha_s}{3r} > br. \quad (41)$$

Choice II: For linear as parent and Coulomb as perturbation

$$br > -\frac{4\alpha_s}{3r}. \quad (42)$$

Table 1. r^{short} and r^{long} in Fermi with $c = 0$ and $b = 0.183 \text{ GeV}^2$.

α_s -value	$r^{\text{short}} = r^{\text{long}}$ (Fermi)
0.39 (for charmonium scale)	0.332
0.22 (for bottomonium scale)	0.249

Table 2. Reduced masses of heavy–light mesons in GeV.

Meson	Reduced mass (μ) (GeV)
$D(c\bar{u}/c\bar{d})$	0.276
$D_s(c\bar{s})$	0.368
$B(u\bar{b}/d\bar{b})$	0.314
$B_s(s\bar{b})$	0.440
$B_c(\bar{b}c)$	1.180

From (41) and (42), we can find the bounds on r up to which choices I and II are valid. Choice I gives the cutoff on the short distance $r_{\text{max}}^{\text{short}} < \sqrt{\frac{4\alpha_s}{3b}}$ and choice II gives the cutoff on the long distance $r_{\text{min}}^{\text{long}} > \sqrt{\frac{4\alpha_s}{3b}}$.

We make $r^{\text{short}} = r^{\text{long}} = \sqrt{\frac{4\alpha_s}{3b}}$ for our analysis, otherwise unless they are identical, the addition of two counterparts (linear part and Coulomb part) either overestimate or underestimate the calculated values of quantities which involves the integration over 0 to r^{short} and r^{long} to r_0 .³¹

In Table 1, we show the bounds on r^{short} and r^{long} in Fermi which yields exact/most restrictive upper bounds of the quantities to be calculated.

3. Results

We calculate the masses of various heavy–light mesons using Eq. (27) and the obtained results are compared with the experimental data³² in Table 3. We have used Mathematica version 7.0.0 to compute the results.

The input parameters in the numerical calculations used are $m_u = 0.336 \text{ GeV}$, $m_s = 0.483 \text{ GeV}$, $m_c = 1.55 \text{ GeV}$, $m_b = 4.95 \text{ GeV}$ and $b = 0.183 \text{ GeV}^2$ and α_s values 0.39 and 0.22 for charmonium and bottomonium scale, respectively, are same with the previous work.^{15,31}

With these values, the reduced masses (μ) of the mesons using Eq. (9) are shown in Table 2.

Our results for B mesons are found to be more agreement with experimental data than D mesons.

In Tables 4 and 5, we find slope (ρ^2 and ρ'^2) and curvature (C and C') using modified Eqs. (39) and (40), respectively.

Table 3. Masses of heavy–light mesons in GeV.

α_s	Meson	$r^S = r^L$ (Fermi)	Mass (M_P) (GeV)	Experimental mass (GeV) (Ref. 32)
0.39	$D(c\bar{u}/c\bar{d})$	0.332	2.378	1.869 ± 0.0016
	$D_s(c\bar{s})$		2.500	1.968 ± 0.0033
0.22	$B(u\bar{b}/d\bar{b})$	0.249	5.798	5.279 ± 0.0017
	$B_s(s\bar{b})$		5.902	5.366 ± 0.0024
	$B_c(\bar{b}c)$		6.810	6.277 ± 0.006

 Table 4. Values of ρ^2 and C in this present work and other works in the limit $m_Q \rightarrow \infty$.

	ρ^2	C
Present work	1.176	0.180
Other work		
Le Youanc <i>et al.</i> ³⁴	≥ 0.75	0.47
Rosner ³⁵	1.66	2.76
Mannel ³⁶	0.98	0.98
Pole ansatz ³⁷	1.42	2.71
Ebert <i>et al.</i> ³⁸	1.04	1.36

 Table 5. Values of slope (ρ'^2) and curvature (C') of the form factor of heavy meson decays in this present work and previous work with finite mass correction.

	Meson	ρ'^2	C'
Present work	$D(c\bar{u}/c\bar{d})$	0.911	0.106
	$D_s(c\bar{s})$	1.318	0.228
	$B(u\bar{b}/d\bar{b})$	1.110	0.260
	$B_s(s\bar{b})$	1.722	0.721
	$B_c(c\bar{b})$	4.646	6.074
Previous work ^{11,33}	$D(c\bar{u}/c\bar{d})$	1.136	5.377
	$D_s(c\bar{s})$	1.083	3.583
	$B(u\bar{b}/d\bar{b})$	128.28	5212
Previous work ³⁰	$B_s(s\bar{b})$	112.759	4841
	$B_c(c\bar{b})$	5.45	31.39

The numerical results for ρ^2 and C in the Isgur–Wise limit is shown in Table 4, where we consider the limit where the mass of active quark/antiquark (in this case b -quark) is infinitely heavy ($m_Q/m_{\bar{Q}} \rightarrow \infty$) and the reduced mass μ becomes that of the light quark/antiquark ($m_q/m_{\bar{q}}$) (in this case u -quark). We have also compared our results with the predictions of other theoretical models.^{34–38}

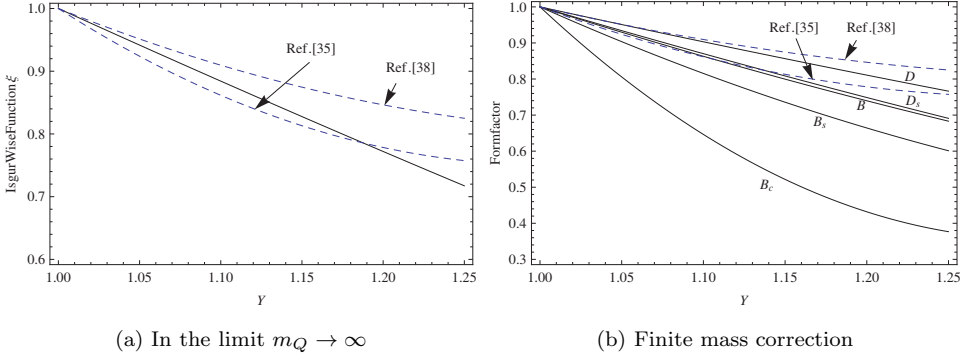


Fig. 1. Variation of form factor with Y in the Isgur–Wise limit is represented in (a) and that of finite mass correction is represented in (b).

However, in a generalized way, we can also check the flavor dependence of the form factor in heavy meson decays. We calculate the slope (ρ'^2) and curvature (C') of form factor of semileptonic decays in finite mass limit with the flavor dependent correction. In Table 5, we compare our present results with the previous work.^{11,33} The results in this work clearly shows an improvement of the previous analysis.

The variation of Isgur–Wise function $\xi(Y)$ with Y in the Isgur–Wise limit is shown in Fig. 1(a) (using Table 4), where the mass of the b -quark is considered to be infinitely heavy and the reduced mass μ is 0.336 GeV (mass of u or d -quark/antiquark). In a similar way, we draw the graph of Fig. 1(b) (using Table 5) for finite mass and flavor dependent correction. Also for comparison the results of Refs. 35 and 38 are plotted in both the graphs.

To draw the graphs as shown in Fig. 1, we have used Eqs. (39) and (40) in (33). $\xi(Y)$ is found to have expected fall with $Y = v \cdot v'$. It is also seen from the figure that the computed results are well within the other model values.^{35,38}

4. Discussion and Conclusion

We have calculated the values of masses and convexity parameter of the Isgur–Wise function considering the scaling factor “ c ” as zero. One of the important point about this work is that we have given equal fitting to both the Coulomb and linear parts of the Cornell potential unlike in the previous analysis.^{10,11,18–21,30,33} Also our calculations provide a measure of the slope and curvature of the form factors with finite mass corrections. We can say that the modification induced by mass effect is not so significant. Furthermore, the consideration of the finite mass correction changes the results only slightly (significantly for $B(u\bar{b}/d\bar{b})$ meson). However, for the mesons where light quark/antiquark is not so light compared to the heavy quark/antiquark, the finite mass limit do show a very strong dependence on the spectator quark mass; for example we can see $B_c(c\bar{b})$ meson (Table 5).

Our calculated values of masses of mesons are found to be in good agreement with the experimental data (Table 3). Also the calculated values of slope and

curvature of Isgur–Wise function in this work are well within the limit of other theoretical values (Table 4). However, the re-evaluation of the model with a nonzero scaling factor with the satisfaction of the quantum mechanical idea is currently under study.

Let us conclude this paper with a comment that the relativity is by no means negligible for heavy–light systems. Such effects do not merely lead to a Dirac modification factor as used in this work, but also have other significant effects as have been studied in various relativistic treatments of the problem.³⁸ In spite of the phenomenological success of the present model, it falls short of such expectation.

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Appendix A. Wave Function for Coulomb ($-\frac{4\alpha_s}{3r}$) as Parent and Linear (br) as Perturbation

The first-order perturbed eigenfunction $\psi^{(1)}$ and first-order eigenenergy $W^{(1)}$ using quantum mechanical perturbation theory (Dalgarno’s method) can be obtained using the relation

$$H_0\psi^{(1)} + H'\psi^{(0)} = W_0\psi^{(1)} + W^{(1)}\psi^{(0)}, \quad (\text{A.1})$$

where

$$W^{(1)} = \langle \psi^{(0)} | H' | \psi^{(0)} \rangle \quad (\text{A.2})$$

$$= \int \psi_{100}^* H' \psi_{100} d\tau. \quad (\text{A.3})$$

For Cornell potential (5), we consider

$$H_0 = -\frac{4\alpha_s}{3r} \quad (\text{A.4})$$

and

$$H' = br. \quad (\text{A.5})$$

From (A.1) we obtain

$$(H_0 - W^{(0)})\psi^{(1)} = (W^{(1)} - H')\psi^{(0)}. \quad (\text{A.6})$$

Putting

$$A = \frac{4\alpha_s}{3}, \quad (\text{A.7})$$

we obtain

$$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{A}{r}, \quad (\text{A.8})$$

$$W^{(0)} = E = \frac{\mu A^2}{2} \quad (\text{A.9})$$

and

$$\psi^{(0)}(r) = \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}, \quad (\text{A.10})$$

where $\psi^{(0)}$ is the unperturbed wave function in the zeroth-order of perturbation and a_0 is given by Eq. (8).

Taking $\hbar^2 = 1$,

$$\begin{aligned} (\text{A.6}) \Rightarrow \left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{A}{r} - E\right)\psi^{(1)} &= (W^{(1)} - br) \frac{1}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} \\ \Rightarrow \left(\nabla^2 + \frac{2\mu A}{r} - \mu^2 A^2\right)\psi^{(1)} &= (br - W^{(1)}) \frac{2\mu}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}} \\ \Rightarrow \left(\nabla^2 + \frac{2}{a_0 r} - \frac{1}{a_0^2}\right)\psi^{(1)} &= (br - W^{(1)}) \frac{2\mu}{\sqrt{\pi a_0^3}} e^{-\frac{r}{a_0}}. \end{aligned} \quad (\text{A.11})$$

Let

$$\psi^{(1)} = (br)R(r), \quad (\text{A.12})$$

then

$$(\text{A.11}) \Rightarrow \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \frac{2}{a_0 r} - \frac{1}{a_0^2}\right)(br)R(r) = D(br - W^{(1)})e^{-\frac{r}{a_0}}, \quad (\text{A.13})$$

where we put

$$D = \frac{2\mu}{\sqrt{\pi a_0^3}}. \quad (\text{A.14})$$

Now

$$\frac{d}{dr}(brR(r)) = bR(r) + br \frac{dR}{dr}, \quad (\text{A.15})$$

$$\frac{d^2}{dr^2}(brR(r)) = 2b \frac{dR}{dr} + br \frac{d^2 R}{dr^2}. \quad (\text{A.16})$$

Using (A.15) and (A.16) in (A.13), we obtain

$$\begin{aligned} br \frac{d^2 R}{dr^2} + 2b \frac{dR}{dr} + \frac{2}{r} bR(r) + \frac{2}{r} br \frac{dR}{dr} \\ + \frac{2}{a_0 r} brR(r) - \frac{1}{a_0^2} brR(r) = D(br - W^{(1)})e^{-\frac{r}{a_0}}. \end{aligned} \quad (\text{A.17})$$

Putting

$$R(r) = F(r)e^{-\frac{r}{a_0}}, \quad (\text{A.18})$$

$$\frac{dR}{dr} = F'(r)e^{-\frac{r}{a_0}} - \frac{1}{a_0}F(r)e^{-\frac{r}{a_0}}, \quad (\text{A.19})$$

$$\frac{d^2R}{dr^2} = F''(r)e^{-\frac{r}{a_0}} - \frac{2}{a_0}F'(r)e^{-\frac{r}{a_0}} + \frac{1}{a_0^2}F(r)e^{-\frac{r}{a_0}}, \quad (\text{A.20})$$

$$\begin{aligned} (\text{A.17}) &\Rightarrow br \left\{ F''(r) - \frac{2}{a_0}F'(r) + \frac{1}{a_0^2}F(r) \right\} + 2b \left\{ F'(r) - \frac{1}{a_0}F(r) \right\} + \frac{2b}{r}F(r) \\ &\quad + 2bF'(r) - \frac{2b}{a_0}F(r) + \frac{2b}{a_0}F(r) - \frac{1}{a_0^2}brF(r) = D(br - W^{(1)}) \\ &\Rightarrow brF''(r) + \left\{ 4b - \frac{2b}{a_0}r \right\} F'(r) + \left\{ \frac{2b}{r} - \frac{2b}{a_0} \right\} F(r) = D(br - W^{(1)}). \end{aligned} \quad (\text{A.21})$$

Let

$$F(r) = \sum_{n=0}^{\infty} A_n r^n, \quad (\text{A.22})$$

then

$$F'(r) = \sum_{n=0}^{\infty} nA_n r^{n-1} \quad (\text{A.23})$$

and

$$F''(r) = \sum_{n=0}^{\infty} n(n-1)A_n r^{n-2}. \quad (\text{A.24})$$

$$\begin{aligned} (\text{A.21}) &\Rightarrow br \sum_{n=0}^{\infty} n(n-1)A_n r^{n-2} + \left\{ 4b - \frac{2b}{a_0}r \right\} \sum_{n=0}^{\infty} nA_n r^{n-1} \\ &\quad + \left\{ \frac{2b}{r} - \frac{2b}{a_0} \right\} \sum_{n=0}^{\infty} A_n r^n = D(br - W^{(1)}) \\ &\Rightarrow \left\{ b \sum_{n=0}^{\infty} n(n-1)A_n + 4b \sum_{n=0}^{\infty} nA_n + 2b \sum_{n=0}^{\infty} A_n \right\} r^{n-1} \\ &\quad - \left\{ \frac{2b}{a_0} \sum_{n=0}^{\infty} nA_n + \frac{2b}{a_0} \sum_{n=0}^{\infty} A_n \right\} r^n = D(br - W^{(1)}). \end{aligned} \quad (\text{A.25})$$

Equating the coefficients of r^{-1} on both sides of the above identity (A.25)

$$2bA_0 = 0,$$

since $b \neq 0$, therefore

$$\Rightarrow A_0 = 0. \tag{A.26}$$

Equating the coefficients of r^0 on both sides of the identity (A.25),

$$4bA_1 + 2bA_1 - \frac{2b}{a_0}A_0 = -DW^{(1)}$$

$$\Rightarrow A_1 = -\frac{DW^{(1)}}{6b}. \tag{A.27}$$

Equating the coefficients of r^1 on both sides of the identity (A.25),

$$2bA_2 + 8bA_2 + 2bA_2 - \frac{2b}{a_0}A_1 - \frac{2b}{a_0}A_1 = Db.$$

Using (A.27) and (A.26),

$$A_2 = \frac{D}{12} - \frac{DW^{(1)}}{18ba_0}. \tag{A.28}$$

Equating the coefficients of r^2 on both sides of the identity (A.25),

$$6bA_3 + 12bA_3 + 2bA_3 - \frac{4b}{a_0}A_2 - \frac{2b}{a_0}A_2 = 0. \tag{A.29}$$

Using (A.27) and (A.28),

$$A_3 = \frac{D}{40a_0} - \frac{DW^{(1)}}{60ba_0^2}. \tag{A.30}$$

Equating the coefficients of r^3 on both sides of the identity (A.25),

$$12bA_4 + 16bA_4 + 2bA_4 - \frac{2b}{a_0}3A_3 - \frac{2b}{a_0}A_3 = 0.$$

Using (A.28) and (A.30),

$$A_4 = \frac{D}{150a_0^2} - \frac{DW^{(1)}}{225ba_0^3}. \tag{A.31}$$

From (A.22)

$$F(r) = A_0r^0 + A_1r^1 + A_2r^2 + A_3r^3 + A_4r^4 + \dots. \tag{A.32}$$

Now from (A.12), (A.18) and (A.32),

$$\psi^{(1)}(r) = brF(r)e^{-\frac{r}{a_0}} \tag{A.33}$$

$$= br(A_0r^0 + A_1r^1 + A_2r^2 + A_3r^3 + A_4r^4 + \dots)e^{-\frac{r}{a_0}}$$

$$= \{A_0(br) + A_1(br^2) + A_2(br^3) + A_3(br^4) + A_4(br^5) + \dots\}e^{-\frac{r}{a_0}}. \tag{A.34}$$

Now applying (A.26)–(A.28), (A.30)–(A.34),

$$\begin{aligned} \psi^{(1)}(r) = & \left[-\frac{DW}{6b}(br^2) + \left\{ \frac{D}{6} \left(\frac{1}{2} - \frac{W}{3ba_0} \right) \right\} (br^3) \right. \\ & \left. + \left\{ \frac{D}{20a_0} \left(\frac{1}{2} - \frac{W}{3ba_0} \right) \right\} (br^4) + \left\{ \frac{D}{75a_0^2} \left(\frac{1}{2} - \frac{W}{3ba_0} \right) \right\} (br^5) \right] e^{-\frac{r}{a_0}}. \end{aligned} \quad (\text{A.35})$$

Again from (A.2)

$$\begin{aligned} W^{(1)} = & \int \psi_{100}^* H' \psi_{100} d\tau = \frac{1}{\pi a_0^3} \int_0^\infty (br)r^2 e^{-\frac{2r}{a_0}} dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \\ = & \frac{4\pi}{\pi a_0^3} \int_0^\infty (br^3) e^{-\frac{2r}{a_0}} dr = \frac{4}{a_0^3} \left[b \frac{6a_0^4}{16} \right] = \frac{3}{2} ba_0. \end{aligned} \quad (\text{A.36})$$

Hence

$$\frac{1}{2} - \frac{W}{3ba_0} = 0. \quad (\text{A.37})$$

Therefore, (A.35) reduces to

$$\psi^{(1)}(r) = \left[-\frac{DW}{6b}(br^2) \right] e^{-\frac{r}{a_0}} = -\frac{1}{2\sqrt{\pi a_0^3}} \mu ba_0 r^2 e^{-\frac{r}{a_0}}. \quad (\text{A.38})$$

The total wave function is thus

$$\psi^{\text{total}} = \psi^{(0)} + \psi^{(1)} = \frac{1}{\sqrt{\pi a_0^3}} \left[1 - \frac{1}{2} \mu ba_0 r^2 \right] e^{-\frac{r}{a_0}}. \quad (\text{A.39})$$

Considering relativistic effect the above equation becomes

$$\psi^{\text{total}}(r) = \frac{N}{\sqrt{\pi a_0^3}} \left[1 - \frac{1}{2} \mu ba_0 r^2 \right] \left(\frac{r}{a_0} \right)^{-\epsilon} e^{-\frac{r}{a_0}}. \quad (\text{A.40})$$

Appendix B. Wave Function for Linear (br) as Parent and Coulomb ($-\frac{4\alpha_s}{3r}$) as Perturbation

Here we take br as parent and $-\frac{4\alpha_s}{3r}$ as perturbation so that

$$H_0 = -\frac{\hbar^2}{2\mu} \nabla^2 + br \quad (\text{B.1})$$

with

$$H' = -\frac{4\alpha_s}{3r}. \quad (\text{B.2})$$

To find the unperturbed wave function corresponding to H_0 we employ the radial Schrödinger equation for potential br for ground state,

$$-\frac{1}{2\mu} \left[\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + br \right] R(r) = ER(r), \quad (\text{B.3})$$

where $R(r)$ is the radial wave function. We introduce $u(r) = rR(r)$ and the dimensionless variable

$$\rho(r) = (2\mu b)^{\frac{1}{3}}r - \left(\frac{2\mu}{b^2}\right)^{\frac{1}{3}}E. \quad (\text{B.4})$$

Equation (B.3) then reduces to

$$\frac{d^2u}{d\rho^2} - \rho u = 0. \quad (\text{B.5})$$

The solution of this second-order homogeneous differential equation contains linear combination of two types of Airy's functions $\text{Ai}[r]$ and $\text{Bi}[r]$. The nature of the Airy's function reveals that

$$\text{Ai}[r] \rightarrow 0 \quad \text{and} \quad \text{Bi}[r] \rightarrow \infty \quad \text{as} \quad r \rightarrow \infty.$$

So, it is reasonable to reject the $\text{Bi}[r]$ part of the solution.

The unperturbed wave function²¹ for ground state is

$$\psi^{(0)}(r) = \frac{N_0}{r} \text{Ai}[\rho_1 r + \rho_0], \quad (\text{B.6})$$

where N_0 is the normalization constant and $\rho_1 = (2\mu b)^{1/3}$. ρ_0 is the zero of the Airy function, such that $\text{Ai}[\rho_0] = 0$. ρ_0 has the explicit form as mentioned in Eq. (21).

The first-order perturbed eigenfunction $\psi^{(1)}$ can be calculated using relation (A.6).

Then taking $\hbar^2 = 1$,

$$(\text{A.6}) \Rightarrow \left(-\frac{\hbar^2}{2\mu}\nabla^2 + br - E\right)\psi^{(1)} = \left(W^{(1)} + \frac{4\alpha_s}{3r}\right)\psi^{(0)}(r). \quad (\text{B.7})$$

In terms of the radial wave function the above equation can be expressed as

$$\left[\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) - 2\mu(br - E)\right]R(r) = -2\mu\left(W^{(1)} + \frac{4\alpha_s}{3r}\right)\frac{1}{r}\text{Ai}[\rho]. \quad (\text{B.8})$$

Let

$$R(r) = \frac{1}{r}F(r)\text{Ai}[\rho] = \frac{1}{r}F(r)\text{Ai}[\rho_1 r + \rho_0], \quad (\text{B.9})$$

so that

$$\frac{dR}{dr} = -\frac{1}{r^2}F(r)\text{Ai}[\rho] + \frac{1}{r}F'(r)\text{Ai}[\rho] + \frac{\rho_1}{r}F(r)\text{Ai}'[\rho], \quad (\text{B.10})$$

$$\begin{aligned} \frac{d^2R}{dr^2} &= \frac{2}{r^3}F(r)\text{Ai}[\rho] - \frac{2}{r^2}F'(r)\text{Ai}[\rho] - \frac{2\rho}{r^2}F(r)\text{Ai}'[\rho] \\ &+ \frac{1}{r}F''\text{Ai}[\rho_1] + \frac{2\rho_1}{r}F'(r)\text{Ai}'[\rho] + \frac{\rho_1^2}{r}F(r)\text{Ai}''[\rho]. \end{aligned} \quad (\text{B.11})$$

Now we introduce the identity

$$\text{Ai}'[\rho] = \frac{d\text{Ai}(\rho)}{d\rho} = Z(\rho)\text{Ai}(\rho), \quad (\text{B.12})$$

so that

$$\text{Ai}''(\rho) = Z^2(\rho)\text{Ai}(\rho) + Z'(\rho)\text{Ai}(\rho). \quad (\text{B.13})$$

Then Eq. (B.8) becomes

$$\begin{aligned} F''(r) + 2\rho_1 F'(r)Z(\rho) + \rho_1^2[Z^2(\rho) + Z'(\rho)]F(r) - 2\mu(br - E)F(r) \\ = -\frac{4\alpha_s}{3} \frac{2\mu}{r} - 2\mu W^{(1)}. \end{aligned} \quad (\text{B.14})$$

Assuming

$$Z(\rho) = \frac{k_1(r)}{r}$$

and

$$Z^2(\rho) + Z'(\rho) = \frac{k_2(r)}{r^2},$$

$$\begin{aligned} (\text{B.14}) \Rightarrow F''(r) + 2\rho_1 F'(r) \frac{k_1(r)}{r} + \rho_1^2 F(r) \frac{k_2(r)}{r^2} - 2\mu(br - E)F(r) \\ = -\frac{4\alpha_s}{3} \frac{2\mu}{r} - 2\mu W^{(1)}. \end{aligned} \quad (\text{B.15})$$

Now using (A.22)–(A.24), the above equation (B.15) becomes

$$\begin{aligned} n(n-1) \sum_n A_n r^{n-2} + 2\rho_1 l \sum_n A_n r^{n-1} \frac{k_1}{r} + \rho_1^2 \sum_n A_n r^n \frac{k_2}{r^2} \\ - 2\mu(br - E) \sum_n A_n r^n = -\frac{4\alpha_s}{3} \frac{2\mu}{r} - 2\mu W^{(1)}, \end{aligned} \quad (\text{B.16})$$

$$\begin{aligned} \Rightarrow \left[n(n-1) \sum_n A_n + 2\rho_1 n \sum_n A_n k_1 + \rho_1^2 \sum_n A_n k_2 \right] r^{n-2} \\ - 2\mu b \sum_n A_n r^{n+1} + 2\mu E \sum_n A_n r^n = -\frac{4\alpha_s}{3} \frac{2\mu}{r} - 2\mu W^{(1)}. \end{aligned} \quad (\text{B.17})$$

Now equating the coefficients of r^{-2} from the above equation (B.17),

$$\rho_1^2 A_0 k_2 = 0 \Rightarrow A_0 = 0. \quad (\text{B.18})$$

Equating the coefficients of r^{-1} of (B.17),

$$2\rho_1 A_1 k_1 + \rho_1^2 A_1 k_2 = -2\mu \frac{4\alpha_s}{3} \Rightarrow A_1 = \frac{-2\mu \frac{4\alpha_s}{3}}{2\rho_1 k_1 + \rho_1^2 k_2}. \quad (\text{B.19})$$

Equating the coefficients of r^0 of (B.17),

$$\begin{aligned} 2A_2 + 4\rho_1 A_2 k_1 + \rho_1^2 A_2 k_2 + 2\mu E A_0 = -2\mu W^{(1)} \\ \Rightarrow A_2 = \frac{-2\mu W^{(1)}}{2 + 4\rho_1 k_1 + \rho_1^2 k_2}. \end{aligned} \quad (\text{B.20})$$

Equating the coefficients of r^1 of (B.17),

$$6A_3 + 6\rho_1 A_3 k_1 + \rho_1^2 A_3 k_2 - 2\mu b A_0 + 2\mu E A_1 = 0$$

$$\Rightarrow A_3 = \frac{-2\mu E A_1}{6 + 6\rho_1 k_1 + \rho_1^2 k_2}. \quad (\text{B.21})$$

Equating the coefficients of r^2 of (B.17),

$$12A_4 + 8\rho_1 A_4 k_1 + \rho_1^2 A_4 k_2 - 2\mu b A_1 + 2\mu E A_2 = 0$$

$$\Rightarrow A_4 = \frac{-2\mu E A_2 + 2\mu b A_1}{12 + 8\rho_1 k_1 + \rho_1^2 k_2}. \quad (\text{B.22})$$

Using (A.32), the perturbed wave function will be

$$\psi^{(1)}(r) = \frac{1}{r} [A_0 r^0 + A_1 r^1 + A_2 r^2 + A_3 r^3 + A_4 r^4 + \dots] \text{Ai}[\rho_1 r + \rho_0]. \quad (\text{B.23})$$

Now considering up to $O(r^4)$ with relativistic effect the total wave function is thus

$$\psi^{\text{total}}(r) = \frac{N'}{r} [1 + A_0 r^0 + A_1 r^1 + A_2 r^2 + A_3 r^3 + A_4 r^4] \text{Ai}[\rho_1 r + \rho_0] \left(\frac{r}{a_0}\right)^{-\epsilon}. \quad (\text{B.24})$$

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