

Calculation of Wave Function at the Origin (WFO) for Heavy Mesons by Numerical Solving of the Schrodinger Equation

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Abstract—Many recent high energy physics calculations involving charm and beauty invoke wave function at the origin (WFO) for the meson bound state. Uncertainties of charm and beauty quark masses and different models for potentials governing these bound states require a simple numerical algorithm for evaluation of the WFO's for these bound states. We present a simple algorithm for this propose which provides WFO's with high precision compared with similar ones already obtained in the literature.

Keywords—Mesons, Bound states, Schrodinger equation, Non-relativistic quark model.

I. INTRODUCTION

STUDY of the bound states in high energy physics is an old argument. A relativistic approach was developed due to Bethe and Salpeter and the bound state equation is known as the Bethe-Salpeter equation (BSE). In this approach the constituents of the bound states are relativistic (even in its rest frame) and the solution to BSE provides a general wave function for the bound state. Such solutions are directly applied for calculation of different physical quantities.

Non-relativistic quantum mechanics (NRQM) has shown to be successful in many areas in low-energy physics.

Recently a new opportunity for application of non-relativistic methods has been opened in high energy physics. This happened mainly in the discovery of $\psi(3\text{GeV}/c^2)$ and $\Upsilon(10\text{GeV}/c^2)$ families of heavy neutral mesons. These are bound states of a massive quark and antiquark ($\bar{Q}Q$) moving non-relativistically. Application of the Schrodinger equation to study the spectroscopy of hadrons has achieved significant improvements [1].

The method of NRQM has been applied to wide variety of situations regarding heavy mesons among which we mention the determination of WFO's. This was partly due to the development of a new approach to study the heavy mesons bound states in which the amplitude for a specific process is calculated in terms of (WFO) for mesons bound states with charm and beauty constituents [2]. To be more explicit, it serves to calculate important physical quantities such as spin

state hyperfine splitting and production and decay amplitudes for heavy mesons [3]. Therefore need for the WFO's arise for the first time. This need was pronounced in the case of treating the bound states containing charm and beauty quarks. Since these quarks mass is much higher than the scale of strong interactions, they are assumed to be heavy so that the constituents could be treated non-relativistically. Interesting explicit examples for this are the states J/ψ [4], Υ [5] and B_c [6].

To find the WFO's for heavy meson bound state, different approaches have been made among which we mention the numerical solution of the Schrodinger equation and variational methods [7]. On the other hand to find the WFO's no matter what method we are using, we need inputs such as quark masses and the potential functions for which no unique value have been assigned. Therefore for an elaborate computational method is in order. Here we show that the Numerov algorithm is a more efficient and fast one to achieve this goal.

II. THE SCHRODINGER EQUATION

The Schrodinger equation for a two body system with reduced mass μ , the relative distance of the constituents \vec{r} , and with an interaction potential $V(\vec{r})$ has the following form

$$-\frac{\hbar^2}{2\mu} \nabla^2 \Psi_{nlm}(\vec{r}) + [V(\vec{r}) - E_{nl}] \Psi_{nlm}(\vec{r}) = 0 \quad (1)$$

Where $\Psi_{nlm}(\vec{r})$ is the Schrodinger wave function. For a central potential it is convenient to write

$$\Psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\theta, \phi) \quad (2)$$

Where $R_{nl}(r)$ is the radial wave function and $Y_{lm}(\theta, \phi)$ is a spherical harmonic. Here n is the principal quantum number, l and m are the orbital angular momentum and its projection.

The Schrodinger wave function is normalized, $\int d^3\vec{r} |\Psi_{nlm}(\vec{r})|^2 = 1$, so that $\int_0^\infty r^2 |R_{nl}(r)|^2 dr = 1$. It is readily seen that the radial wave function satisfies

$$-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R_{nl}(r) - \left[E_{nl} - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R_{nl}(r) = 0 \quad (3)$$

The radial equation can be put in formal correspondence with the one-dimensional Schrodinger equation by means of

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the substitution of $u_{nl}(r) \equiv rR_{nl}(r)$ which defines the reduced radial equation

$$u_{nl}''(r) + \frac{2\mu}{\hbar^2} \left[E_{nl} - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] u_{nl}(r) = 0 \quad (4)$$

Subject to the boundary conditions $u_{nl}(0) = 0$ and $u_{nl}'(0) = R_{nl}(0) = \sqrt{4\pi} \Psi_{nlm}(0)$. Equation (4) is identical to a one-dimensional equation for an effective potential given by $V(r) + l(l+1)\hbar^2 / 2\mu r^2$ except that the even parity solution are inconsistent with the above mentioned boundary conditions.

III. SOLVING THE SCHRODINGER EQUATION NUMERICALLY

Most of the important physical differential equation could be written in the form of linear equation of second order [8]

$$\frac{d^2y}{dx^2} + K^2(x)y = S(x) \quad (5)$$

Where $S(x)$ brings in inhomogeneity and $K^2(x)$ is a real function.

We choose the Numerov algorithm for solution of the above equation. Using Taylor expansion method, the first derivative of y may be put into the following form

$$y'(x) = \frac{y(x+h) - y(x-h)}{2h} + \frac{h^2}{6} y'''(x) + O(h^4) \quad (6)$$

Similarity for the second derivative one finds

$$y''(x) = \frac{y(x+h) - 2y(x) + y(x-h)}{h^2} + \frac{h^2}{12} y^{IV}(x) + O(h^4) \quad (7)$$

So that both the first and second derivatives are represented by 3-points expressions involving the central point and one point on either side. Now using (5) and (7) we obtain the following recursion relation

$$y_{n+1} = \frac{2y_n - y_{n-1} - \frac{h^2}{12} [10K_n^2 y_n + K_{n-1}^2 y_{n-1}]}{1 + \frac{h^2}{12} K_{n+1}^2} + \frac{h^2}{12} (S_{n+1} - 2S_n + S_{n-1}) \quad (8)$$

Solving this linear equation for either y_{n+1} or y_{n-1} provides a recursion relation for integrating either forward or backward in x with a local error of $O(h^6)$. Note that this method is one order more accurate than the fourth order Runge-Kutta method, which might be used to integrate the problem as two coupled first order equations. The Numerov scheme is also more efficient as each step requires the computation of

K^2 and S at only the lattice points.

For the propose of this work we have obtained a recursion relation for the first derivative of y . Using (6) it reads as

$$y'_n = \frac{y_{n+1} - y_{n-1}}{2h} + \frac{h}{12} [K_{n+1}^2 y_{n+1} - K_{n-1}^2 y_{n-1}] - \frac{h}{12} [S_{n+1} - S_{n-1}] \quad (9)$$

Now we write (4) in the following form

$$u_{nl}''(r) + w_{nl}(r)u_{nl}(r) = 0 \quad (10)$$

We note that this equation is in the form of (5) with $S(x) = 0$ and

$$K^2 = w_{nl}(r) = \frac{2\mu}{\hbar^2} [E_{nl} - V(r)] - \frac{l(l+1)}{r^2} \quad (11)$$

The recursion relation for (10) by Numerov method is obtained as

$$u_{i+1} = \frac{2u_i - u_{i-1} - \frac{h^2}{12} [10w_i u_i + w_{i-1} u_{i-1}]}{1 + \frac{h^2}{12} w_{i+1}} \quad (12)$$

Where I is a free index. Thus given the values of u at $i-1$ and I , its value can be computed at $i+1$ and so on. Therefore only two values are needed to start the method. With substitution

$$\begin{aligned} r &\rightarrow r_i = i * h \\ u(r) &\rightarrow u(r_i) \equiv u_i \\ w(r) &\rightarrow w(r_i) \equiv w_i \end{aligned} \quad (13)$$

The equation (9) for $u(r)$ becomes

$$u'_i = \frac{u_{i+1} - u_{i-1}}{2h} + \frac{h}{12} [w_{i+1} u_{i+1} - w_{i-1} u_{i-1}] \quad (14)$$

To proceed we need to specify $w_{nl}(r)$ for which the necessary form of the potential function should be specified.

IV. THE POWER-LAW AND LOGARITHMIC POTENTIAL

First we introduce the quantization condition form which the energy eigenvalues may be obtained. One-dimensional motion in an arbitrary non-singular potential for a particle of energy E moving between x_1 and x_2 a reasonable choice of the Schrodinger wave function leads to the following quantization condition

$$\int_{x_1}^{x_2} dx P(x) = \left(m + \frac{1}{2}\right) \pi \hbar \quad ; \quad m = 0, 1, 2, \dots \quad (15)$$

Where

$$P(x) = [2\mu(E - V(x))]^{\frac{1}{2}} \quad (16)$$

Equation (15) represents a condition which specifies the values of E in (16) that can lead to bound states.

The one-dimensional discussion carries over directly to S-wave in three-dimensional (for non-singular central potentials) if we identify S-wave bound states with the odd-parity levels in one dimension, corresponding to odd values of m. therefore the quantization condition (15) then takes the form

$$\int_0^{r_c} dx P(x) = \left[(2n - 1) + \frac{1}{2} \right] \frac{\pi \hbar}{2} \quad (17)$$

Where $n = 1, 2, 3, \dots$ is the principal quantum number in the three dimensions. The equation (17) may be re-written in three-dimensional notation as

$$\int_0^{r_c} dr [2\mu(E - V(r))]^{\frac{1}{2}} = \left(n - \frac{1}{4} \right) \pi \hbar \quad (18)$$

Where r_c is defined by $V(r_c) = E$. For a Power-law potential is general [9]

$$V(r) = \lambda r^\nu \quad (19)$$

With $0 < \nu < \infty$ the integral (18) can be performed exactly, leading to

$$E_n = \lambda^{2/(2+\nu)} (2\mu / \hbar^2)^{-\nu/(2+\nu)} \left[A(\nu) \left(n - \frac{1}{4} \right) \right]^{2\nu/(2+\nu)} \quad (20)$$

Where

$$A(\nu) = \left[2\nu \sqrt{\pi} \Gamma \left(\frac{3}{2} + \frac{1}{\nu} \right) \right] / \Gamma \left(\frac{1}{\nu} \right) \quad \nu > 0 \quad (21)$$

The equation (20) may be generalized to all partial waves by the replacement of $n \rightarrow n + \frac{1}{2}$. In this way we find

$$E_{nl} = \lambda^{2/(2+\nu)} (2\mu / \hbar^2)^{-\nu/(2+\nu)} \left[A(\nu) \left(n + \frac{1}{2} - \frac{1}{4} \right) \right]^{2\nu/(2+\nu)} \quad (22)$$

Here $A(\nu)$ is the same as in (21).

For the Power-law potential of the form

$$V(r) = \lambda r^{0.1} \quad (23)$$

With $\lambda = 6.898$, $m_c = 1.8 \text{ GeV} / c^2$ and $m_b = 5.174 \text{ GeV} / c^2$, we may write

$$w_{nl}(r) = \frac{2\mu}{\hbar^2} [E_{nl} - (6.898)r^{0.1}] - \frac{1(1+1)}{r^2} \quad (24)$$

With E_{nl} given by (22).

For the Power-law potential $V(r) = \lambda r^\nu$ with $\lambda < 0$ and $\nu < 0$, we find

$$|E_{nl}| = |\lambda|^{2/(2+\nu)} (2\mu / \hbar^2)^{-\nu/(2+\nu)} \left\{ \tilde{A}(\nu) \left[n - \frac{1}{2} \left(\frac{1+\nu-2l}{2+\nu} \right) \right] \right\}^{2\nu/(2+\nu)} \quad (25)$$

With

$$\tilde{A}(\nu) = \left[2|\nu| \sqrt{\pi} \Gamma \left(1 - \frac{1}{\nu} \right) \right] / \Gamma \left(-\frac{1}{2} - \frac{1}{\nu} \right) \quad ; -2 < \nu < 0 \quad (26)$$

The appropriate quantization variable in (22) is $n + \frac{1}{2}$ for all values of $\nu > 0$ and we expect this to be true for $\nu = 0$ ($\nu \square \ln r$) by comparing the limits $\nu \rightarrow 0^+$ in (22) and $\nu \rightarrow 0^-$ in (25).

The Logarithmic potential is given as [10]

$$V(r) = C \ln(r / r_0) \quad (27)$$

Although this potential is singular at $r = 0$, there is a certain sense in which it may be regarded as the limit of either a non-singular ($\nu > 0$) or singular ($\nu < 0$) potential. The quantization condition (22) and (25) becomes identical in the limit of $\nu = 0$, indicating that $n + \frac{1}{2} - \frac{1}{4}$ is very likely the optimal variable for this problem. Then we have

$$E_{nl} = C \ln \left[\frac{2\sqrt{\pi} \left(n + \frac{1}{2} - \frac{1}{4} \right)}{(2\mu C / \hbar^2)^{\frac{1}{2}} r_0} \right] \quad (28)$$

With $C = 0.733$, $r_0 = 1$, $m_c = 1.5 \text{ GeV} / c^2$ and $m_b = 4.906 \text{ GeV} / c^2$. Therefore for the Logarithmic potential

$$w_{nl}(r) = \frac{2\mu}{\hbar^2} [E_{nl} - (0.733) \ln(r)] - \frac{1(1+1)}{r^2} \quad (29)$$

With E_{nl} given by (28).

Thus we have specified the energy eigenvalues for quantum numbers n and l which should be replaced in the function W_{nl} for different potentials. Thus functions should be put back in (12) and (14) which at the origin will provide $u'(0) = R(0) = \sqrt{4\pi}\psi(0)$.

V. CONCLUSION

The bound states of our concern here, are quarkonia $\bar{c}c$ and $\bar{b}b$, and the mesonic bound state of $\bar{b}c$. We have used our method to obtain the radial WFO, $|R_{nl}(0)|^2$, for these states benefiting the Power-law and Logarithmic potentials for several quantum numbers. They are tabulated in Table 1. These results are in exact agreement with those obtained in [11]. Of course the contents of Table 1 may easily be extended to any other quantum numbers n and l .

As a concluding remark we add that the need for evaluation of WFO's in high energy physics is growing with application of the method introduced in [2] takes one to the rest frame of the bound state. Therefore as far as the constituents are heavy enough to be treated non-relativistically, a simple, self consistent and efficient method to evaluate the WFO's is in order. The method developed here fulfils such a need.

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TABLE I
RADIAL WFO, $|R_{nl}(0)|^2$, FOR $\bar{c}c$, $\bar{b}b$ AND $\bar{b}c$ STATES WITH POWER-LAW
AND LOGARITHMIC POTENTIALS.

Level state	potential	1 S	2 P	2 S	3 D	3 P	3 S
$\bar{c}c$	Power-law	0.999	0.125	0.559	0.026	0.131	0.410
$\bar{c}c$	Logarithmic	0.815	0.078	0.418	0.012	0.076	0.286
$\bar{b}b$	Power-law	4.591	1.572	2.571	0.892	1.660	1.858
$\bar{b}b$	Logarithmic	4.916	1.535	2.532	0.765	1.513	1.736
$\bar{b}c$	Power-law	1.710	0.327	0.950	0.101	0.352	0.680