

## QQ-onia package: a numerical solution to the Schrödinger radial equation for heavy quarkonium

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This paper presents the basics of the *QQ-onia* package, a software based upon the Numerov  $\theta(h^6)$  method which can be used to solve the Schrödinger radial equation using a suitable potential  $V(r)$  for the heavy quarkonium system. This package also allows the analysis of relevant properties of those resonances such as the square of the wave functions at the origin, their corresponding derivatives for  $l \neq 0$  states, typical heavy-quark velocities, and mean square radii. Besides, it includes a tool to analyze the spin dependent contributions to the heavy quarkonia spectrum, providing the splitting of  $n^3S_1 - n^1S_0$ , as well as the  $n^3P_J - n^1P_1$  energy levels. Finally a simple software implemented in *QQ-onia* to compute E1 transition rates is presented.

### PROGRAM SUMMARY

Program title: QQ-ONIA PACKAGE<sup>3</sup>.

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Programming language: PAW (Physics Analysis Workstation).

Operating system(s) for which the program has been designed: Windows-XX and Unix (Linux).

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Nature of the problem: Software to solve the Schrödinger radial equation using a suitable potential  $V(r)$  for the heavy quarkonium system, allowing to perform spectroscopy. It also allows the analysis of relevant quantities of those resonances such as the square of the wave functions at the origin, their corresponding derivatives for  $l \neq 0$  states, typical heavy-quark velocities, and mean square radii. The package is a (user-friendly) multipurpose tool for dealing with different heavy quarkonium systems, providing a way to study the influence of a given potential on a series of relevant physical quantities, by either varying parameterized values of a well-known potential form, or by including new terms.

Solution method: Based upon the Numerov  $O(h^6)$  Method, we perform a matching procedure to the reduced wave function at the cut point. We also perform a normalization technique for these wave functions taking into account the different domains when we use a Numerov backward-forward technique. In the case of  $l \geq 2$  we present a way to find the corresponding derivatives at the origin by only calculating the reduced radial wave function and first derivative. When estimating the heavy quark velocity, we introduce an additional way to compute this quantity from the virial theorem. The calculated reduced wave functions and radial wave functions at the origin are later used to obtain the heavy quarkonia  $nL$  splitting and  $E1$  transition rates.

Additional comments: Using Windows, to optimize the edition of the files, please, open it with MFC-WORDPAD.

Running time: It depends on the choice of the  $r$  range, and the number of energy steps.

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## 1. Introduction

Since the discovery of the charmonium and bottomonium families, much efforts have been spent over 30 years trying to understand the nature of heavy quarkonium, (as a summary see for example [1]); in the meantime various numerical tools have been created in an almost “ad hoc” fashion with the aim of extracting important information about their properties, such as their masses and partial widths.

This package was developed with the aim of providing a multipurpose (user-friendly) tool for dealing with different heavy quarkonium systems, providing a way to study the influence of a given potential on a series of relevant physical quantities, by either varying parameterized values of a well-known potential form, or by including new terms.

The *QQ-onia* package handles the heavy quarkonium system within a non relativistic framework, solving the Schrödinger radial equation (*SRE*) with an appropriate potential for heavy quarks/antiquarks. The basic reason for this choice derives from the Quark Potential Model [2], which establishes a low value for the expected square velocity of the quark for these heavy resonances ( $v^2 \sim 0.1$  for bottomonia and  $v^2 \sim 0.3$  for charmonia). Besides, there is also another reason from a dual ultra-relativistic picture to provide a non relativistic treatment for heavy quarkonium [3]. These low velocities  $v^2 \ll 1$  were also responsible for the success of the Non Relativistic QCD (NRQCD) ([4], [5]), a rigorous effective theory for strong interactions deriving from first principles.

The paper is organized as follows: the first section explains the basics of the heavy quarkonium Non Relativistic potential and its spin-dependent part, according with the Breit-Fermi Hamiltonian. Later we explain the underlying foundations to our way of solving the Schrödinger equation. Although the arguments presented are already well-known, we consider this introduction necessary to facilitate the understanding of the rest of the article. We then look into the specific details about the calculation of the wave functions of heavy quarkonia in our code.

We initially focus on a procedure for matching the reduced wave function at the cut point and its normalization when we use a Numerov backward-forward technique. We also explain how to extract useful quantities in order to analyze the heavy quarkonium system such as mean square radius, and heavy quark velocity (introducing an additional way to calculate this quantity from the virial theorem). For  $l = 0$  states we also focus on square of the wave functions at the origin, and, for  $l \neq 0$  states, we examine their corresponding derivatives; in the case of  $l \geq 2$  we present a way to find these values by only calculating their corresponding reduced radial wave function and first derivative. It follows an explanation on the spin-dependent terms in the bottomonia case and, finally, we focus on the calculation of the E1 transition rates.

The software will be explained in more detail in the second part of the paper, where we also present several results obtained using the programme to illustrate the procedure and foreseen precision.

Several potentials for the heavy quarkonium system are given as examples. Our first (main) choice is the well-known funnel or Cornell potential, i.e. a Coulomb plus Lineal static potential (CpL) [6],

$$V(r) = \sigma r - \frac{C_F \alpha_s \hbar}{r}$$

with string tension  $\sigma$  and strong coupling constant  $\alpha_s$ ;  $C_F$  is a colour factor.

Nevertheless, other static and non-static potentials will also be used in this paper in order to illustrate some results. Note that we will focus on the equal masses. Thus one can write for bottomonium  $m_Q = m_{\bar{Q}} = m_b \equiv m$  with reduced mass  $\mu = m_Q/2$ .

## 2. Physical Bases of the package

### 2.1. Heavy quarkonium potential and spin-dependent terms

If  $V_{NR}$  stands for the Non Relativistic potential, one can split it in two terms consisting of a vector ( $V$ ) and a scalar ( $S$ ) contribution [7,8]

$$V_{NR}(r) = V_V(r) + V_S(r) \quad (1)$$

In our example with a funnel type potential (being  $k \equiv C_F \alpha_s \hbar$ )

$$V_V(r) = -k/r ; V_S(r) = \sigma r$$

In accordance with literature (e.g. [7]), additional terms have been included in the potential  $V_{NR}$  to take into the account the spin orbital and the spin-spin interactions, causing the splitting of the different mass levels. The additional potential reads [8]

$$V(r)_{spin-dependent} = V_{LS} + V_{SS} + V_T \quad (2)$$

where  $V_{LS}$ ,  $V_{SS}$ , and  $V_T$  are the spin-orbit, the spin-spin, and the tensor terms, respectively. The spin-orbit term, in the equal quark masses case, is

$$V_{LS}(r) = \frac{(\mathbf{L} \cdot \mathbf{S})}{2 m^2 r} \left[ 3 \frac{d}{dr} V_V(r) - \frac{d}{dr} V_S(r) \right] \quad (3)$$

where  $\mathbf{L}$  is the relative angular momentum of the constituents (1 and 2), and  $\mathbf{S}$  is the total spin of the bound state,  $\mathbf{S} \equiv \mathbf{S}_1 + \mathbf{S}_2$  ( with  $\mathbf{J} \equiv \mathbf{L} + \mathbf{S}$  );  $\langle (\mathbf{L} \cdot \mathbf{S}) \rangle$  for different  $j$  and  $l$  values is shown in Table 1.

Table 1

$\langle (\mathbf{L} \cdot \mathbf{S}) \rangle$  coefficients ( $\langle (\mathbf{L} \cdot \mathbf{S}) \rangle = 0$  if  $l = 0$  or  $S = 0$ ).

$j$ value	$(l + 1)$	$l$	$(l - 1)$
$\langle \mathbf{L} \cdot \mathbf{S} \rangle$	$l$	$-1$	$-(l + 1)$

The spin-spin term can be written as

$$V_{SS}(r) = \frac{2 (\mathbf{S}_1 \cdot \mathbf{S}_2)}{3 m^2 r} \left[ \Delta( V_V(r) ) \right] \quad (4)$$

where the  $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$  coefficients take the values:

( $-3/4$ ) for the spin-singlet case ( $S = 0$ ), and ( $+1/4$ ) for the spin-triplet case ( $S = 1$ ).

The tensor term can be written as

$$V_T(r) = \frac{1}{12 m^2} (S_{12}) \left[ \frac{1}{r} \frac{d}{dr} V_V(r) - \frac{d^2}{dr^2} V_V(r) \right] \quad (5)$$

where  $(S_{12})$  is the spin-dependent factor (for  $l \neq 0$  and  $S = 1$ ), shown in Table 2 for different  $j$  and  $l$  values.

Table 2

Spin-dependent  $S_{12}$  factor. ( $\langle S_{12} \rangle = 0$  if  $l = 0$  or  $S = 0$ )

$j$ value	$(l + 1)$	$l$	$(l - 1)$
$\langle S_{12} \rangle$	$- 2 l / (2l + 3)$	2	$- 2 (l + 1) / (2l - 1)$

## 2.2. Schrödinger radial equation

Basically, our code has to solve the well known Schrödinger radial equation (*SRE*):

$$\frac{d^2}{dr^2} u_l(r) + \frac{2\mu}{\hbar^2} \left[ [E - V(r)] - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] u_l(r) = 0 \quad (6)$$

where  $\Psi(r, \theta, \phi) = R_{nl}(r) Y_{lm_l}(\theta, \phi)$  is the complete wave function,  $r$  stands for the *relative* radial coordinate, and  $u_l(r) \equiv r R_{nl}(r)$  is the reduced radial wave function.

With respect to the boundary conditions, a regular solution near the origin for  $u_l(r)$  could be [9]

$$u(r \rightarrow 0) \rightarrow r^{l+1} \quad (7)$$

Since asymptotically  $u(r \rightarrow \infty) \rightarrow 0$  we can take:

$$u(r \rightarrow \infty) \rightarrow \exp \left[ -\frac{\sqrt{2\mu|E|}}{\hbar} r \right] \quad (8)$$

where  $|E|$ , as later will be seen, is an educated guess about the energy eigenvalue.

The normalization condition reads

$$\int_0^\infty dr |u_l(r)|^2 = \int_0^\infty dr |R_l(r)|^2 r^2 = 1 \quad (9)$$

### 3. Numerical solution of *SRE*

The *SRE* can be written as

$$\frac{d^2u(r)}{dr^2} + k(r) u(r) = s(r) \quad (10)$$

Here (setting  $l = 0$ ),  $k(r) \equiv \frac{2\mu}{\hbar^2} [E - V(r)]$  is the kernel of the equation, and  $s(r) \equiv 0$ .

We can integrate these equations by means of the Numerov Algorithm [10] as follows:

First we split the  $r$  range into  $N$  points according to  $r_n = r_{n-1} + h$  (where  $h$  is the step); then we write the wave function  $u_n \equiv u(r_n) = u(r_{n-1} + h)$ , and  $k_n \equiv k(r_n) = k(r_{n-1} + h)$ .

Expanding  $u(r)$  around  $r_n$ :

$$u_{n+1} \equiv u(r_n + h) = u(r_n) + hu'(r_n) + \frac{h^2}{2}u''(r_n) + \frac{h^3}{6}u'''(r_n) + \frac{h^4}{24}u^{(iv)}(r_n) + o(h^5) \quad (11)$$

$$u_{n-1} \equiv u(r_n - h) = u(r_n) - hu'(r_n) + \frac{h^2}{2}u''(r_n) - \frac{h^3}{6}u'''(r_n) + \frac{h^4}{24}u^{(iv)}(r_n) + o(h^5) \quad (12)$$

Then approximating the second derivative by the three-point difference formula, and using it within the second-order differential equation we get the following recursive formulas, with a local error  $o(h^6)$ :

a) Forward recursive relation

$$u_n = \frac{2(1 - \frac{5h^2}{12}k_{n-1}) u_{n-1} - (1 + \frac{h^2}{12}k_{n-2}) u_{n-2}}{(1 + \frac{h^2}{12}k_n)} \quad (13)$$

b) Backward recursive relation

$$u_{n-1} = \frac{2(1 - \frac{5h^2}{12}k_n) u_n - (1 + \frac{h^2}{12}k_{n+1}) u_{n+1}}{(1 + \frac{h^2}{12}k_{n-1})} \quad (14)$$

Therefore, when we calculate our wave function using the backward-forward technique, we should note that the recursive formulas imply having knowledge of two initial values for each direction.

It is also necessary to know the first derivative at the appropriate order. Following the above expansions, we then get:

$$u'_n = \frac{1}{2h} \left[ (1 + \frac{h^2}{6}k_{n+1}) u_{n+1} - (1 + \frac{h^2}{6}k_{n-1}) u_{n-1} \right] + o(h^4) \quad (15)$$

#### 4. Wave function and normalization

For the sake of simplicity, let us first focus on  $l = 0$  states. The *SRE* reduces to

$$\frac{d^2 u(r)}{dr^2} + \frac{2\mu}{\hbar^2} [E - V(r)] u(r) = 0 \quad (16)$$

To illustrate this point we choose an harmonic oscillator potential  $V(r) \equiv \beta r^2$ , with  $\beta$  a constant. We then start, for instance, by using a forward calculation (with an appropriate energy eigenvalue).

Since we are dealing with bound states, we find eigenfunctions at the classically allowed region with  $E > V(r)$  and classically forbidden region where  $E < V(r)$ , they are separated at a turning point,  $r_c$ , which can be estimated from the equality  $E = V(r_c)$ . If we perform a forward calculation, its asymptotic solution at the forbidden region may behave either as  $\sim e^{\pm\alpha r^2}$ , where the positive value is non-physical. Thus, we have an admixture of those solutions and then, with successive iterations, the integration would be numerically unstable due to the dominance of the exponentially growing solution. As a general rule [10], integration *into* a classical forbidden region tends to be inaccurate.

Hence, for a given energy eigenvalue, we consider a calculation using both forward and backward solutions: from the allowed towards the forbidden region, with  $u_{out}(r)$  (outwards) eigenfunctions and from the forbidden towards the allowed region with  $u_{in}(r)$  (inwards) eigenfunctions .

Let us note here that, to avoid numerical overflows in the forward calculation, we do not usually start with  $u(r = 0)$ : once included the centrifugal barrier term, the  $1/r^2$  piece would originate an overflow at  $r = 0$ .

##### 4.1. Bound state energy

Since both  $u_{out}(r)$  and  $u_{in}(r)$  satisfy an homogeneous equation, their normalization can always be chosen so that they are set to be equal at the  $r_c$  point. An energy eigenvalue is then signaled by the equality of derivatives at this point [10]. At the matching point the eigenfunctions  $u_{out}(r)$  and  $u_{in}(r)$  and first derivatives  $u'_{out}(r)$  and  $u'_{in}(r)$  must all satisfy the continuity conditions:

$$\left( u_{out} \right)_{r_c} = \left( u_{in} \right)_{r_c} \quad \left( u'_{out} \right)_{r_c} = \left( u'_{in} \right)_{r_c} \quad (17)$$

thus, we can write the corresponding condition for the logarithmic derivative at  $r_c$  as

$$\left[ \frac{u'_{out}}{u_{out}} \right]_{r_c} = \left[ \frac{u'_{in}}{u_{in}} \right]_{r_c} \quad (18)$$

and then we can define a  $G(E)$  function at  $r_c$  whose zeros correspond to the energy eigenvalues as

$$G(E) \equiv \left[ \frac{u'_{out}}{u_{out}} \right]_{r_c} - \left[ \frac{u'_{in}}{u_{in}} \right]_{r_c} \quad (19)$$



Therefore we proceed numerically in the following way: we set a trial energy range splitting this  $E$  range into  $N$  points, according to  $E_n = E_{n-1} + \Delta_E$ , where  $\Delta_E$  is the energy step. For each  $E_n$  we calculate their eigenfunctions  $u_{out}$  and  $u_{in}$  at the  $r_c$  point; and we build the  $G(E)$  function here, looking for a *change of sign* in it (which implies a zero cross). Once we find it, we perform a fine tuning closing the energy range until the required tolerance.

## 4.2. Matching eigenfunctions at the $r_c$ point

When we find the energy eigenvalue, the calculated inwards and outwards eigenfunctions will tend not to match at the  $r_c$  point. However we can look for a strategy to solve this problem:

Denoting the outwards and inwards functions *directly* obtained from the recursive formulas as  $\Phi(r)$  and  $I(r)$ , respectively, the physical  $u_{out}(r)$  and  $u_{in}(r)$  eigenfunctions can be rewritten as

$$u_{out}(r) = A\Phi(r) \qquad u_{in}(r) = BI(r) \qquad (20)$$

$A$  and  $B$  are constants. Their respective derivatives are

$$u'_{out}(r) = A\Phi'(r) \qquad u'_{in}(r) = BI'(r) \qquad (21)$$

By substituting eqs. (20) and (21) into eq.(17):

$$\left(A\Phi\right)_{r_c} = \left(BI\right)_{r_c} \qquad \left(A\Phi'\right)_{r_c} = \left(BI'\right)_{r_c} \qquad (22)$$

and performing the difference, we get

$$A = \left[\frac{I - I'}{\Phi - \Phi'}\right]_{r_c} B \equiv f_c B \qquad (23)$$

where  $f_c$  will be a scaling factor to be applied to  $u_{out}(r)$ . Therefore

$$u_{out}(r) = B f_c \Phi(r) \qquad u_{in}(r) = B I(r) \qquad (24)$$

and  $B$  is a global factor that must be taken into account in the normalization process.

## 4.3. Normalization

Once the energy eigenvalue has been determined, we first insert it into the kernel,  $k(r)$ , thereby generating their corresponding  $\Phi(r)$  and  $I(r)$  functions; subsequently we calculate the  $f_c$  factor. To find the remaining  $B$  factor, and therefore find the  $u_{out}$  and  $u_{in}$  eigenfunctions, we use the normalization condition

$$\int_0^{r_{max}} dr |u_l(r)|^2 = 1 \qquad (25)$$

where, following the asymptotic requirement  $u(r \rightarrow \infty) \rightarrow 0$ , taking  $r_{max}$  as a cutoff value.

By separating the  $u_{out}(r)$  and  $u_{in}(r)$  domains in the above integral, we can write

$$\int_0^{r_{max}} dr |u_l(r)|^2 = \int_0^{r_c} dr |u_{out}(r)|^2 + \int_{r_c}^{r_{max}} dr |u_{in}(r)|^2 = 1 \quad (26)$$

Using the equations (24)

$$\int_0^{r_{max}} dr |u_l(r)|^2 = (Bf_c)^2 \int_0^{r_c} dr |\Phi(r)|^2 + B^2 \int_{r_c}^{r_{max}} dr |I(r)|^2 \quad (27)$$

the normalization condition then reads

$$B^2 \left[ (f_c)^2 \int_0^{r_c} dr |\Phi(r)|^2 + \int_{r_c}^{r_{max}} dr |I(r)|^2 \right] = 1 \quad (28)$$

Denoting the result of the above integrals within brackets as  $N$ , we can write  $B = \frac{1}{\sqrt{N}}$ , thereby deriving the normalized eigenfunctions

$$u_{out}(r) = \frac{1}{\sqrt{N}} f_c \Phi(r) \quad (29)$$

$$u_{in}(r) = \frac{1}{\sqrt{N}} I(r) \quad (30)$$

## 5. Integration and expectation values

When performing the integration with the *QQ-onia* package, we use the following procedure: If we name

$$T_N \equiv \int_{r_0}^{r_N} dr f(r) ; f_n \equiv f(r_n)$$

from the Euler-McLaurin summation formula [11] with a given step  $h$

$$T_N = h \left[ \frac{f_0}{2} + f_1 + f_2 + \dots + f_{N-1} + \frac{f_N}{2} \right] - \frac{B_2 h^2}{2!} (f'_N - f'_0) - \frac{B_{2k} h^{2k}}{(2k)!} (f_N^{(2k-1)} - f_0^{(2k-1)})$$

where  $B_{2k}$  are Bernoulli numbers. The first term of the r.h.s. in the above equality corresponds to the *extended trapezoidal rule*.

If we set a number of steps to a *multiple of 4*, and apply the above formula for steps  $h$ ,  $2h$ , and  $4h$  we obtain

$$T_h \approx h \left[ \frac{f_0}{2} + f_1 + f_2 + f_3 + \dots + \frac{f_N}{2} \right] - \frac{h^2}{12} (f'_N - f'_0) - \frac{h^4}{4!30} (f_N''' - f_0''') + o(h^6)$$

$$T_{2h} \approx 2h \left[ \frac{f_0}{2} + f_2 + f_4 + \dots + f_{N-2} + \frac{f_N}{2} \right] - \frac{(2h)^2}{12} (f'_N - f'_0) - \frac{(2h)^4}{4!30} (f_N''' - f_0''') + o(h^6)$$

$$T_{4h} \approx 4h \left[ \frac{f_0}{2} + f_4 + f_8 + \dots + f_{N-4} + \frac{f_N}{2} \right] - \frac{(4h)^2}{12} (f'_N - f'_0) - \frac{(4h)^4}{4!30} (f'''_N - f'''_0) + o(h^6)$$

where  $T_N = T_h = T_{2h} = T_{4h}$ . If we solve this system to eliminate derivatives up to  $o(h^6)$  we arrive at the final formula of

$$\int_{r_0}^{r_N} dr f(r) \approx \frac{64T_h - 20T_{2h} + T_{4h}}{45} + o(h^6) \quad (31)$$

that is used in our calculations.

Several expectation values are needed to be computed in our method. Once the eigenfunctions have been normalized, one can calculate the expectation value of a given operator  $O$  according to the definition

$$\langle O \rangle = \int_0^{r_{max}} dr u_l^*(r) O u_l(r) \quad (32)$$

by using the above  $o(h^6)$  integration.  $O$  can be  $r^2$  (if we want to obtain the mean square radius of the state  $\sqrt{\langle r^2 \rangle}$ ), the potential or the derivative of the potential, etc.

### 5.1. Square of the radial wave function at the origin

We need to distinguish between the calculation of the square radial wave function at the origin ( $WFO$ ) for  $l = 0$  states,  $|R_n(0)|^2$ , and the calculation of the squared derivatives of the radial wave function at the origin for  $l \neq 0$  states,  $|R_n^{(l)}(0)|^2$ , with  $l = 1, 2, 3$  respectively corresponding to the  $P, D$  and  $F$  states.

#### 5.1.1. $l = 0$ states

From the well known calculation [3] derived from the Schrödinger equation we obtain

$$|\Psi_{nlm_l}(0)|^2 = \frac{\mu}{2\pi} \langle V'(r) \rangle \quad (33)$$

where  $\langle V'(r) \rangle$  is the expectation value of the derivative of the potential, and  $\mu$  stands for the reduced mass. If we are dealing with  $b\bar{b}$  or  $c\bar{c}$  systems:  $\mu = m_Q/2$  where  $m_Q$  is the heavy quark mass.

For  $l = 0$  states the wave function is:  $\Psi_{n00}(r) = \frac{1}{\sqrt{4\pi}} R_{n0}(r)$ , then

$$|R_n(0)|^2 = m_Q \langle V'(r) \rangle \quad (34)$$

Therefore, since the corresponding eigenfunctions have been already obtained, the evaluation of the radial  $WFO$  reduces to a calculation that gives the expectation value of the derivative of the potential  $\langle V'(r) \rangle$ .

Another method that can be used to evaluate the  $WFO$  is to extrapolate directly from the normalized eigenfunctions, taking values of the square  $|R_n(r)|^2 = [ |u(r)|^2 / r^2 ]$  from the region near to  $r = 0$  using an appropriate interpolating function. Even so, the previously stated technique yields a more accurate result, if the  $\langle V'(r) \rangle$  calculation is reliable. Nevertheless both procedures can be employed together as a check.

### 5.1.2. $l \neq 0$ states

Here we consider the *SRE*, eq.(6), containing the centrifugal barrier term. If we rename the potential:

$$W(r) \equiv V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

the kernel of the *SRE* (see eq.(10)) now becomes:  $k(r) \equiv \frac{2\mu}{\hbar^2} [E - W(r)]$ .

**$l=1$  CASE:** The main goal here is to evaluate the square first derivative at  $r = 0$ ,  $|R'_n(0)|^2$ . Since we have a tool for directly calculating the derivatives  $u'(r)$ , according to eq. (15), once we have the normalized eigenfunctions  $u(r)$ , then using

$$R'_{nl}(r) = \left[ \frac{u(r)}{r} \right]' = \frac{u'(r) - R(r)}{r} \quad (35)$$

we can extrapolate the square of the derivative, taking those values from the region near to  $r = 0$  with an appropriate interpolation function.

**$l=2$  CASE:** We will obtain the second derivative at  $r = 0$ ,  $|R''_n(0)|^2$  but *only* in terms of its radial wave function and first derivative. To do this we proceed as follows: from *SRE*

$$u''(r) = -k(r) u(r) \quad (36)$$

If we calculate the second derivative using the above identity

$$R''_{nl}(r) = \left[ \frac{u(r)}{r} \right]'' = -k(r) R(r) - \frac{2 R'(r)}{r} \quad (37)$$

we can again extrapolate the  $|R''_n(0)|^2$  function. The main advantage of this procedure is that there is no need for any additional derivatives, and since  $u(r)$  and  $u'(r)$  have already been calculated at the suitable order, the result holds with the foreseen precision.

**$l=3$  CASE:** In the same way, using eq. (36), we can obtain the third derivative to extrapolate

$$R'''_{nl}(r) = \left[ \frac{u(r)}{r} \right]''' = \left( \frac{2 k(r)}{r} - k'(r) \right) R(r) + \left( \frac{6}{r^2} - k(r) \right) R'(r) \quad (38)$$

where  $k'(r)$  stands for the derivative of the kernel,  $k'(r) = -\frac{2\mu}{\hbar^2} W'(r)$ .

## 5.2. Calculating the heavy-quark velocity

To obtain the  $\langle v^2 \rangle$  value we perform a double calculation as a check: the first is from the Hamiltonian definition and the second uses the virial theorem.

- i) If  $\vec{r} = \vec{r}_1 - \vec{r}_2$  is the relative radial coordinate between the quarks 1 and 2, with velocities  $|\vec{v}_1| = |\vec{v}_2| \equiv |\vec{v}_q|$ , its relative velocity  $\vec{v}$  at the center of mass frame is  $\vec{v} = 2\vec{v}_1 = -2\vec{v}_2$ . Then, we can obtain the quark velocity using the Hamiltonian,  $E = \langle T \rangle + \langle V(r) \rangle$ , (where  $T$  represents the relative kinetic energy  $T = \frac{1}{2}\mu(\vec{v})^2$ )

$$\langle (\vec{v}_q)^2 \rangle = \frac{1}{2\mu} \left[ E - \langle V(r) \rangle \right] \quad (39)$$

- ii) Taking relative spherical coordinates, the virial theorem implies

$$\langle T \rangle = \frac{1}{2} \langle r V'(r) \rangle$$

Then, we derive the quark velocity from the expectation value of the product  $rV'(r)$  according to:

$$\langle (\vec{v}_q)^2 \rangle = \frac{1}{4\mu} \langle r V'(r) \rangle \quad (40)$$

in both calculations for  $b\bar{b}$  or  $c\bar{c}$  systems where  $2\mu = m_Q$ .

Table 3  
 $A_J$  and  $B_J$  coefficients.

$j$ value	$A_J$	$B_J$
${}^3P_0$	$-(16/3)$	$+1$
${}^3P_1$	$-(4/3)$	$+(1/2)$
${}^3P_2$	$+(28/15)$	$-(1/2)$

## 6. Bottomonia mass level splittings

In this section we address different splittings of the mass levels of bottomonia in accordance with the expressions shown in section 2.1:

$n^3S_1 - n^1S_0$  **splitting:** In this case the only term that gives a non vanishing contribution is the spin-spin term. Since from *QQ-onia* package we can previously calculate the  $nS$  state WFO, instead of eq.(4) we choose to use its final and well-known form [12]

$$\Delta \left[ M({}^3S_1) - M({}^1S_0) \right] = \alpha_s(\mu^2) \frac{8}{9m^2} |R_{n0}(0)|^2 \quad (41)$$

where we will evolve the  $\alpha_s(Q^2)$  to the appropriate scale [13]

$$Q^2 = \langle \mathbf{P}^2 \rangle = 2 \langle T \rangle \mu = m_b \langle v^2 \rangle$$

where we know the quark-velocity  $\langle v^2 \rangle$  for each  $nS$  state from *QQ-onia*.

$n^3P_J$  **and**  $n^1P_1$  **splitting:** We have to take into account altogether the spin-orbit and tensor terms, i.e. eqs. (3) and (5). Using a funnel potential, the explicit expressions to be computed read

$$\Delta \left[ M({}^3P_J) - M(\text{centroid}) \right] = \frac{1}{m^2} \left[ A_J \alpha_s \hbar^3 \left\langle \frac{1}{r^3} \right\rangle + B_J \sigma \hbar^2 \left\langle \frac{1}{r} \right\rangle \right] \quad (42)$$

where  $A_J$  and  $B_J$  are the corresponding coefficients for each case, as can be seen in Table 3;  $\alpha_s$  denotes again the evolved value up to the quarkonium scale. The expectation values are calculated using the wave function  $\forall r$  corresponding to the  $nP$  centroid from a previous calculation, as we will see later. Once the  ${}^3P_J$  masses are calculated, the  ${}^1P_1$  value will be obtained according to [12], as

$$M({}^1P_1) = \left[ 5 M({}^3P_2) + 3 M({}^3P_1) + M({}^3P_0) \right] \quad (43)$$

## 7. Electric Dipole Transitions

*QQ-onia* package allows us to calculate the wave functions of different states. Therefore one can calculate, e.g., the  $E1$  transition rate  $initial (i) \rightarrow final (f) + \gamma$  through the well-known expression [12]

$$\Gamma_{E1}(i \rightarrow f + \gamma) = \frac{4 \alpha \langle e_Q \rangle^2}{27} k^3 (2J_f + 1) S_{if} |\langle f | r | i \rangle|^2 \quad (44)$$

where  $\alpha = 1/137$ , and  $\langle e_Q \rangle$  is the mean charge [  $(-1/3)$  in the bottomonia case ]. In the *QQ-onia* file-example we will focus on  ${}^3S_1 \rightarrow {}^3P_J$  radiative transitions with  $S_{if} = 1$ . The photon energy,  $k$  is directly calculated from energy-momentum conservation law. If  $m_f$  and  $m_i$  stands for the experimental [14] masses of the final resonance ( $nP_J$ ) and the initial one ( $nS$ ), respectively, one has

$$k = \frac{m_i^2 - m_f^2}{2 m_i} \quad (45)$$

$\langle f | r | i \rangle$  (in  $\text{GeV}^{-1}$ ) is the matrix element connecting final and initial state; we will evaluate it according to

$$\langle f | r | i \rangle = \int_0^{r_{max}} dr u_f^*(r) r u_i(r) \quad (46)$$

extracting the reduced wave functions of the  $nP$  and  $nS$  states from a previous calculation with *QQ-onia*.

## 8. The *QQ-onia* package

The *QQ-onia package* is written with *PAW* software (*Physics Analysis Workstation*), which can be obtained for free from the *CERN* web site [15] for several operative systems. This software contains a FORTRAN interface, called *SIGMA*. The *QQ-onia* package provides a version of this software named *PAW-NT* for *WINDOWS*. The package also runs with *UNIX-LINUX*, pasting the *bbnia-nl.kum* files directly into any *UNIX* text editor.

The package contains the files prepared to work with each of the previously mentioned cases. To illustrate how the machinery runs, and as a potential reference, we choose a standard static potential for heavy quarkonium: the Coulomb plus linear potential [6], and also as a further reference, we take a known set of parameters from [6], [16] with which to perform spectroscopy (for a comparison of the Cornell model with other approaches of the heavy quarkonium potential in the static limit, see [17]).

The files solve the *SRE* for:  $l = 0$  states  $\Upsilon(nS)(n = 1, 2, 3, 4)$ , and their file names are *bbnia-ns.kum*; the  $l = 1$ ,  $\chi(nP)(n = 1, 2)$  states, (*bbnia-np.kum*); and the  $l = 2$ ,  $\Upsilon(nD)$  ones, (*bbnia-1d.kum*). The package also contains a file called *bbnia-4f.kum* which is prepared for working with theoretical  $l = 3$  ( $nF$ ) states. The differences between these files is related to the centrifugal barrier and the calculation of either square of the radial wave functions or square of the derivatives at the origin. Since there are parts that are common

to both we will begin by explaining them.

It must be pointed out here that in some parts of the software it is necessary to type in some analytic expressions (such as the derivative of the potential and the product  $rV'(r)$ ). Although this procedure can be shortened, this is a good way to ensure control over the different variables, useful to analyze partial results.

## 9. Getting ready to calculate energy levels: general settings

First we open the file section SETTINGS in which we can read (to insert) the characteristic items:

v/cr igma(1) r 0.9255 creates and defines the string tension (in  $GeV/fm$ ).

v/cr mq(1) r 5.18 creates and defines the b-quark mass.

v/cr alf(1) r 0.39 creates and defines the strong coupling constant.

v/cr hb(1) r 0.19732858 is the  $\hbar c$  constant (in  $GeV fm$  units).

ni sets the number of total steps; h=0.001 ( $fm$ ) is the step.

x0 sets the minimum  $r$  value,  $r_{min}$ : the h value is the default.

xm=[x0]+([ni]-1)\*[h] sets the maximum  $r$  value,  $r_{max}$

xc sets the cut  $r$  value  $r_{cut}$  according to  $B_{est} = V(r_{cut})$ , where we use  $B_{est}$  as an estimated binding energy  $B_{est} = M_{exp} - 2m_b$ , and  $M_{exp}$  stands for the experimental mass of the resonance. Sometimes, if needed, we can also set  $r_{cut}$  as the point at which the inwards integration has its first maximum.

v/cr ele(1) r ''value'' (with ele= 1, 2, 3) *only* appears in  $l \neq 0$  files, where it creates and defines the eigenvalue of the angular momentum that needs to be inserted into the centrifugal barrier term.

File section SIGMA APPLICATION BLCK1 calculates the  $r$  range and defines the potential:

x=array([ni],x0#xm) it calls `sigma application (appl sigma)` to establish the  $r$  range.  
The numerical values of ni, x0, xm, must be inserted here.

POTENTIAL DEFINITION for  $l = 0$  files The  $V(r)$  value, (vo variable) is calculated for the full  $r$ -range. In our case vo=(igma\*x)-(kfac1\*(x\*\*(-1))).

POTENTIAL DEFINITION for  $l \neq 0$  files;

vo=(igma\*x)-(kfac1\*(x\*\*(-1)))+(bfac2\*(x\*\*(-2))), which contains the centrifugal barrier term, sets the  $W(r)$  value.



**ENERGY SETTINGS** The programme calls the `sigma` application (`appl sigma`) to establish the energy range (using the variable `e`); here the numerical values of `[ne]`, `E-min`, `E-max` must be inserted as follows:  
`e=array(number of energy steps, minimum energy value# maximum energy value).`

**ENERGY BLCK2** to insert the number of energy steps (`ne`). The programme will calculate the corresponding energy values, `e`, to cover the full energy range.

**BOUNDARY CONDITIONS** this section of the programme runs automatically, the default values are those previously discussed in section **2.2**  $u(r \rightarrow 0) \sim r^{l+1}$  and  $u(r \rightarrow \infty) \sim \exp\left[-\frac{\sqrt{2\mu|B_{est}|}}{\hbar}r\right]$ .

those conditions are inserted into the two first values of  $u_{out}(r)$  (`uo` variable) and  $u_{in}(r)$  (`ui` variable), respectively

**In summary** ,we set `h`, `[ni]`, `x0`, `xm`, `xc`, `[ne]`, `E-min`, `E-max`, the potential, and the corresponding constants.

### 9.1. Starting and determination of the bound state energy level

Once we have inserted the previous settings, we write `exec bbnia-nl.kum` in the *PAW* interface. The programme then automatically searches for bound states within the  $[E_{min}, E_{max}]$  range. If there is any change of sign in the  $G(E)$  function the programme stops, showing the new energy range  $[E'_{min}, E'_{max}]$  in which the bound state can be found, and it asks for the next instruction

(Type `<CR>` to continue or `Q` to quit). We then proceed in an iterative way: to improve the precision of the energy level, we skip the programme (by typing in `q`) and on opening the file, we type in the new energy range in the **ENERGY SETTINGS** file section. We then restart the programme and repeat this process until the energy level has the desired tolerance.

Once the programme stops showing a suitable energy range  $[E_{min}^{last}, E_{max}^{last}]$ , we push the `enter` key. The programme will then ask for the *final* (`ee(1)`) energy eigenvalue, then we type in this value (which could be the mean value of  $[E_{min}^{last}, E_{max}^{last}]$ ), and it will calculate automatically the eigenfunctions  $\forall r$ , showing at the screen the normalization proof.

As a final result we get:

- 1 The normalized reduced radial wave function,  $u(r)$  throughout the full range, stored as a `[ni]`-dimensional vector (`y1`)
- 2 The  $u^*(r) u(r)$  product (*in  $fm^{-1}$  units*) which is also stored as a `[ni]`-dimensional vector (`fc`). These values can be either displayed in a graph, by typing in `v/dr fc`, or obtained numerically (`v/wr fc`).

## 9.2. Mean square radius

File section **\*\*BEGINS SQR(<r2>) CALCULATION\*\***. The software automatically calculates the mean square radius of the state ( $\sqrt{\langle r^2 \rangle}$ ) according to its expectation value. The [ni]-dimensional variable (fi) to integrate is  $\mathbf{fi}=\mathbf{fc}*\mathbf{xx}$ , where  $\mathbf{xx}$  is the  $r^2$  variable. As this is the final result, this value is stored at the **rad** variable (in *fm* units), and displayed.

## 9.3. Computing the heavy-quark velocity using the virial theorem

File section **\*\*1) <v2>/c2 calculation USING VIRIAL THEOREM\*\***

- 1 The first step is to calculate the expectation value of the product of  $X \cdot \nabla V$ , ( $\langle rV'(r) \rangle$ ); to do this, *BEFORE running the programme*, we must *TYPE* in its corresponding expression at the variable **xdpot**. Using our example we must insert:  
 $\mathbf{xdpot}=(\mathbf{igma}*\mathbf{x})+(\mathbf{kfac1}*(\mathbf{x}**(-1)))$
- 2 The programme integrates the variable  $\mathbf{fi}=\mathbf{fc}*\mathbf{xdpot}$  and performs the velocity calculation. The result is displayed and stored at the variable **v2**.

## 9.4. Computing the heavy-quark velocity using the Hamiltonian

File section **\*\*2) <v2>/c2 calculation USING <H>=<T>+<V(r)>\*\***.

- 1 The programme first calculates the expectation value of the potential  $\langle V(r) \rangle$ . The variable to integrate is **ffi**, where  $\mathbf{ffi}=\mathbf{vo}*\mathbf{fc}$ . The result is stored at the variable **vbar**. If desired, it can be read by dropping the comment variable **\*** at line:  
 $*\mathbf{v}/\mathbf{pr} \mathbf{vbar}$ .
- 2 It calculates the velocity value using the variables: **vbar**, the energy eigenvalue, **ee**, and the inverse of the quark mass, **inq**, and displays the final result.

## 10. Computing the radial wave function squared and derivatives at the origin

**Square of the radial WFO** (For  $l = 0$  states: **bbnia-ns.kum** files).

File section **\*\*BEGINS WAVE FUNCTION AT THE ORIGIN CALCULATION\*\***. First the expectation value of the derivative of the potential  $\langle V'(r) \rangle$  is calculated; to do this, *BEFORE the programme runs*, we must type in its corresponding expression at the variable **dpot**. Using our example, we must insert:

$$\mathbf{dpot}=(\mathbf{igma})+(\mathbf{kfac1}*(\mathbf{x}**(-2)))$$

The variable to integrate is **fi**, where  $\mathbf{fi}=\mathbf{dpot}*\mathbf{fc}$ . Later, the final calculation is performed and the result is displayed (in  $\text{GeV}^3$  units) and stored at the **wfo** variable.

**Square of the first derivative of the radial WFO** (For  $l = 1$  states: **bbnia-np.kum** files).

File section **WAVE FUNCTION DERIVATIVE CALCULATION**. General settings are equal than before by changing  $V(r) \rightarrow W(r)$ , then the centrifugal barrier term appears ( $\mathbf{bfac2}*(\mathbf{x}**(-2))$ ). As a result we obtain, according to eq.(35), the squared first

derivative of the radial wave function  $|R'_n(r)|^2$  for all  $r$  value (in  $\text{GeV}^5$  units). The result is stored at the [ni]-dimensional variable `derc`. Then, to obtain its value at the origin, we must export the (`derc`) values in order to extrapolate with an appropriate tool (such as the *PAW* inner routine `vector/fit`). By typing in `v/dr derc`, we can plot these values to select the range before exporting. To do this numerically type in `v/wr derc`.

**Square of the second derivative of the radial *WFO*** (For  $l = 2$  states:

`bbnia-nd.kum` files).

File Section WAVE FUNCTION DERIVATIVE(2) CALCULATION We obtain, by using the eq.(37), the second derivative of the radial wave function (in  $\text{GeV}^7$  units)  $|R''_n(r)|^2$  values for all  $r$ , these values are stored at the [ni]-dimensional variable `sed2`, and ready to be extrapolated.

**Square of the third derivative of the radial *WFO*** (For theoretical  $l = 3$  states:

`bbnia-nf.kum` files)

File section WAVE FUNCTION DERIVATIVE(3) CALCULATION. Before starting the programme, we must *TYPE* in the corresponding derivative  $W'(r)$  expression into the variable `kerd0`. Then the programme will calculate the derivative of the kernel,  $k'(r)$ . As a result, according to eq.(38), we have the [ni]-dimensional variable `thrd2`, which stores the full  $r$ -range of the third derivative of the radial wave function  $|R'''_n(r)|^2$  (in  $\text{GeV}^9$  units).

### 10.1. Wave function plot

When a `bbnia-n1` file stops, a plot of the dimensionless reduced wave function can be obtained (from the same *PAW* screen), by running the routine `graph-n1.kumac`. We obtain the plot of the `u2` variable as output, which is the  $|u(r)|^2$  value multiplied by the Böhr radius of the resonance,  $a_0 = \hbar/(C_F \alpha_s \mu)$ .

## 11. *QQ-onia* package spin-dependent and *E1*

This part of the software is organized within *QQ-onia* package as follows: The file `SSplit-nS.kumac` allows to calculate the  $n^3S_1 - n^1S_0$  splitting for each  $n$  level. The files `Split-nP.kumac` ( $n = 1, 2$ ) calculate as example the  $n^3P_J$  and  $n^1P_1$  splitting. There is also a file `E1-2S1P.kumac`, which analyzes the  $E1 2S \rightarrow 1P$  transitions, which has two subroutines named `ini-2s.kum` and `final-1P.kum` devoted to generate, respectively, the initial and final states for the matrix element calculation.

**SSplit-nS.kumac** This file has mainly three blocks: the first one ask for the values of the quark mass (the `mq` variable), the value of the wave function at the origin (`wfo` variable), and the quark velocity of the  $nS$  state (`v2q` variable), whose values can be previously found with the `bbnia-ns.kum` files. Once these values are entered the programme runs automatically; it calculates the quarkonium scale and the  $\alpha_s$  value (`alf` variable) through the `alpha-s Evolution Block`. Later using the eq.(41) (the `Delta-ss=[M(n3S1)-M(n1S0)]calculation block`) it displays the result of the energy splitting (in  $\text{GeV}$ ) through the variable `deltss`.

**Split-nP.kumac** The first part of the file generates the centroid wave function,(the GENERATION OF THE CENTROID WAVE FUNCTION-BLOCK. This implies to run first the corresponding *bbnia-np.kum* in order to know the energy eigenvalue, the  $r_{max}$  and  $r_c$  values to be inserted here [We *insert* the energy eigenvalue (**ee** variable) when the programme ask for it (**EIGENVALUE?(GeV)**)]. This block can be performed in other cases by pasting from the *bbnia* file the part corresponding to the block labeled ONCE ENERGY LEVEL FOR BOUND STATE IS DETERMINED\*\*\*\*\* WAVEFUNCTION CALCULATION. At the end of this part we have stored the normalized wave function within the **y1** variable. Later the programme will run automatically, it calculates the  $\langle r^{-3} \rangle$  and  $\langle r^{-1} \rangle$  expectation values, evolves the  $\alpha_s$ , and applies the final expression eq.(42). Finally it displays the energy differences and the final  ${}^3P_J$  masses [Also the  ${}^1P_1$  mass using eq.(43)] by means of

$$M({}^3P_J) = \Delta E_J + M_{centroid}$$

where  $\Delta E_J$  is the calculated energy difference of each  $J$  and  $M_{centroid}$  is the centroid mass *previously* calculated from the *bbnia-np.kum* file.

**E1-2S1P.kumac** This file, as a complementary tool, is an example of how to handle *QQ-onia* with the E1 transition rates between  $2S$  and the  ${}^3P_J$  states. First, the programme calls the *ini-2s.kum* subroutine in order to create the initial  $2S$  state, which is performed by inserting the results found using the *bbnia-2S.kum* file: the energy eigenvalue (at the **Enter the energy eigenvalue** line), the  $r_{max}$  and  $r_c$  values; then it generates its corresponding wave function. Later, the software calls the *final-1p.kum* subroutine and, in the same way, it creates the wave function corresponding to the final state. It must be pointed out that, when we want to modify the *common* parameters used generating the final and initial states, we perform it within the *E1-2S1P.kumac* file. The programme then runs automatically: it calculates, using eq.(46), the matrix element  $\langle f|r|i \rangle$  (stored at the **me** variable in  $\text{GeV}^{-1}$ ), the photon energy for each final  $J$  (the **kph0,1,2** variables, in  $\text{GeV}$ ) according to eq.(45), later it computes the final values, in  $\text{keV}$ , by means of the eq.(44), the result is displayed for each  $J = 0, 1, 2$  value through their respective **gma0,1,2** variables. The remaining factors and settings are explained and displayed inside the *E1-2S1P.kumac* file.

## 12. Numerical accuracy

One important issue is determination of the numerical accuracy of the results. Since no complete bottomonium wave function has yet been available, we can make our check using an harmonic oscillator potential, which has a known analytical solution, but it is numerically sensitive (as previously mentioned, this potential exhibits numerical instabilities due to their exponentially growing solutions). It is therefore a good candidate for checking our software.

We test  $V(r) = \frac{1}{2}\mu \omega^2 r^2$  by inserting it in the file block `SIGMA APPLICATION BLCK1`, and by inserting in the `SETTINGS` file section  $\mu = 100 \text{ MeV}/c^2$ ;  $\hbar c = 197.32858 \text{ MeV fm}$ ;  $\omega = 2 \text{ fm}^{-1}c$ . As boundary conditions [9] we use  $u(r \rightarrow 0) \sim r^{l+1}$  and for  $u(r \rightarrow \infty) \sim e^{-\beta r^2}$ , where  $\beta = \frac{\mu \omega}{\hbar c}$ .

The analytical energy levels are  $E(n, l) = \left(2n + l + \frac{3}{2}\right) \hbar \omega$ .

The reduced wave functions expressed in terms of the generalized Laguerre polynomials [9] are:

$$u_{nl}(r) = \left[ \frac{2n! \alpha^3}{\Gamma(n + l + 3/2)} \right]^{1/2} r (\alpha r)^l L_n^{l+1/2}(\alpha^2 r^2) e^{-\alpha^2 r^2/2} \quad (47)$$

We then analyze levels  $1S \equiv (0, 0)$ ;  $2S \equiv (1, 0)$  and  $2D \equiv (1, 2)$ . The results can be found in Table 4.

Table 4

Harmonic oscillator results.

Energy level (MeV)	Analytic	Numeric
$E(0, 0)$	591.986	591.999
$E(1, 0)$	1381.330	1381.315
$E(2, 1)$	2170.614	2170.628

**(0,0)LEVEL** Taking  $r_{cut}$  as the turning point (using  $E(0, 0) = V(r_{cut})$ ), we find that  $r_{cut} = 1.72 \text{ fm}$  with  $r_{max} = 5 \text{ fm}$  and  $r_{min} = h$ , with a step  $h = 0.01 \text{ fm}$ , thus  $[ni] = 500$ . We start searching for the associated energy level through the range  $E(0, 0) \in [400, 800] \text{ MeV}$ , with an energy step of  $\Delta_E = 1 \text{ MeV}$ , i.e.  $[ne] = 401$ .

**(1,0)LEVEL** We repeat the procedure, but now  $r_{cut} = 2.6 \text{ fm}$  with  $r_{max} = 5.6 \text{ fm}$ , thus  $[ni] = 560$ ; starting with an energy range  $E(1, 0) \in [1100, 1500] \text{ MeV}$ , and an energy step of  $\Delta_E = 1 \text{ MeV}$ .

**(1,2)LEVEL** First the centrifugal barrier term  $\frac{\hbar^2 l(l+1)}{2\mu r^2}$  must be added to `SIGMA APPLICATION BLCK1`. We use  $r_{cut} = 1.08 \text{ fm}$ ,  $r_{max} = 6 \text{ fm}$ , with an energy range  $E(1, 2) \in [1900, 2300] \text{ MeV}$ ,  $\Delta_E = 1 \text{ MeV}$ .

Concerning the reduced radial wave functions  $u(r)_{nl}$ , in all cases, we find a deviation of less than 1% with respect to the exact value from eq.(47). Figure 1 shows the result for the  $u(r)_{12}$  case; Figure 2 shows its corresponding  $\Delta|u(r)|_{12}^2/|u(r)|_{12}^2$  relative error (in %).

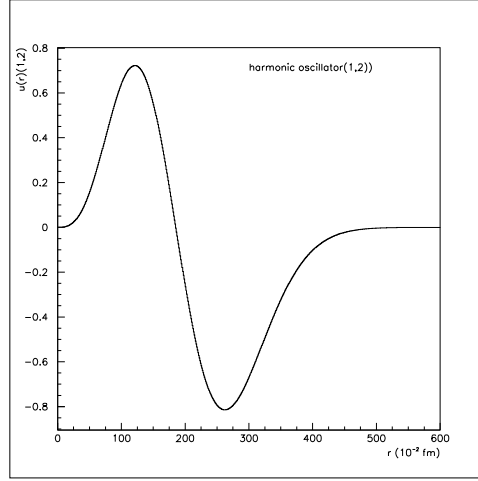


Figure 1. Harmonic oscillator( $n = 1, l = 2$ ) reduced wave function.

### 13. An example: Numerical Results

To illustrate how to the *QQ-onia* package runs, all attached `bbnia-n1.kum` files can be opened; their corresponding settings are listed inside. Here, we will focus on the  $\Upsilon(1S)$  case (`bbnia-1s.kum` file) in order to explain some relevant details.

We look for the lowest state of the  $b\bar{b}$  family. First we estimate its energy eigenvalue,  $B_{est}^{1S}$ , from the experimental data [14], then  $B_{est}^{1S} = M_{exp}^{1S} - 2m_b = -0.8997 \text{ GeV}$ , (with  $M_{exp}^{1S} = 9.4603 \text{ GeV}$  and  $m_b = 5.18 \text{ GeV}$ ). To ensure that we find the lowest state we set a wide energy range below the  $B_{est}^{1S}$ , thus we start typing at **ENERGY SETTINGS** section a trial energy range  $B^{1S} \in [-5., 0.] \text{ GeV}$  with an energy step of  $\Delta_E = 0.5 \text{ GeV}$ , i.e. `[ne]= 11`.

Using  $B_{est}^{1S} = V(r_{cut})$ , we find  $r_c \approx 0.1 \text{ fm}$  (alternatively, instead of  $B_{est} = V(r_{cut})$ , we can take the  $r_c$  point where the inwards integration has its first maximum). To ensure the asymptotic conditions we then take  $r_{max} = 1.0 \text{ fm}$ ; taking  $h = 0.001 \text{ fm}$ , the number of steps is `[ni]= 1000`.

We type in `exec bbnia-1s.kum` at *PAW* screen, then the programme runs until it stops displaying:

```
bound state around
E(10) = -0.5
E(11) = 0
Type <CR> to continue or Q to quit
```

This is the new energy range (in GeV) within which we can find the eigenvalue of the bound state. We then stop the programme (`q`) and insert these new values at the **ENERGY**

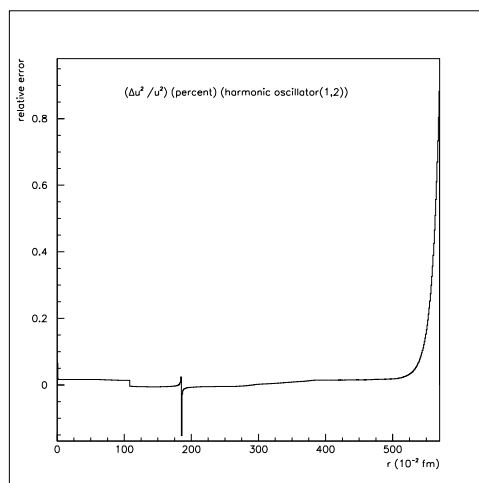


Figure 2. Harmonic oscillator( $n = 1, l = 2$ ) relative error.

SETTINGS section and restart the programme. We repeat the procedure, and after five iterations the screen displays:

```
bound state around
E(10) = -0.170209
E(11) = -0.170208
Type <CR> to continue or Q to quit
```

As there is sufficient precision, when we press the **enter** key, the screen shows:

```
BOUND STATE ENERGY?
EE(1)
```

We then take the mean value of the above quantities  $-0.1702085$  (GeV) as the eigenvalue, and type it in at the screen.

```
EE(1) -0.1702085
```

As the calculated eigenvalue  $B_{calc}^{1S}$  does not match the  $B_{est}^{1S}$  value, we can establish a scale factor ( $F$ ) to be applied to the whole spectrum:

$$F = M_{exp}^{1S} - (2m_b + B_{calc}^{1S})$$

(Alternatively, we can redefine the quark mass according to  $2m'_b \equiv 2m_b + F$ ). The masses of the higher states  $M_{calc}^{nl}$  can therefore be obtained from

$$M_{calc}^{nl} = 2m_b + B_{calc}^{nl} + F$$

where,  $B_{calc}^{nl}$  stands for the calculated energy eigenvalue obtained from the software for each higher state.

In Table 5 the results for the masses of several resonances can be found.

Table 5  
Coulomb plus linear potential: mass results (in GeV units).

$b\bar{b}$ LEVEL	Experimental mass	Mass from [6]	Mass from $QQ$ -onia
$\Upsilon(1S)$	9.4603	9.4603 <sup>a</sup>	9.4603 <sup>a</sup>
$\chi(1P)^b$	9.9001	9.96	9.9584
$\Upsilon(2S)$	10.02326	10.05	10.02772
$\Upsilon(1D)$	10.1622	10.20	10.2080
$\chi(2P)^b$	10.2620	10.31	10.3125
$\Upsilon(3S)$	10.3553	10.40	10.3971
$b\bar{b}(4F)^c$	— — — —	— — — —	10.3995
$\Upsilon(4S)$	10.5794	10.67	10.6739

(a) used to set the ground level in both references

(b)  $\chi_{bJ}(nP)$  centroid (c) Theoretical level

After inserting the energy eigenvalue  $EE(1)$ , the programme will calculate the remaining quantities automatically: it first shows the normalization check and then displays a plot of the  $fc$  value.

```
normalization proof
NNOR(1) = 1
```

```
It continues to show the value of the square of the wave function at the origin
RADIAL WAVEFUNCTION AT THE ORIGIN (in GeV3)
WFO(1) = 14.0927
```

If we run a  $l \neq 0$  file, we do not see this screen but *when the programme finishes* we can export the corresponding  $|R_n^{(l)}(r)|^2(\forall r)$  and extrapolate.

Table 6 summarizes the results for the square of the  $WFO$  (or its derivatives).

```
After the WFO value, the calculation for the mean square radius calculation from the
1S file will show
SQR(<r2>) (in fm)
RAD(1) = 0.201043
```

The results for each resonance can be seen in Table 7.



Table 6

Coulomb plus linear potential:  $|R_n^{(l)}(0)|^2$  values in  $(\text{GeV})^{(3+2l)}$  units.

$b\bar{b}$ LEVEL	$ R_n^{(l)}(0) ^2$ from <i>QQ-onia</i>	$ R_n^{(l)}(0) ^2$ from [16]
$\Upsilon(1S)$	14.09	14.05
$\chi(1P)$	2.062	2.067
$\Upsilon(2S)$	5.947	5.668
$\Upsilon(1D)$	0.835	0.860
$\chi(2P)$	2.440	2.438
$\Upsilon(3S)$	4.276	4.271
$b\bar{b}(4F)^c$	0.551	0.563
$\Upsilon(4S)$	3.675	3.663

Table 7

Coulomb plus linear potential: mean square radius (in *fm*).

$b\bar{b}$ LEVEL	$\sqrt{\langle r^2 \rangle}$ from <i>QQ-onia</i>	$\sqrt{\langle r^2 \rangle}$ from [6]
$\Upsilon(1S)$	0.20	0.20
$\chi(1P)$	0.38	0.39
$\Upsilon(2S)$	0.46	0.48
$\Upsilon(1D)$	0.52	0.53
$\chi(2P)$	0.63	0.64
$\Upsilon(3S)$	0.71	0.72
$b\bar{b}(4F)^c$	0.64	— — —
$\Upsilon(4S)$	0.91	0.92

Finally, the 1S file displays the velocity result obtained applying the two methods

```

(<v^2>/c^2) [virial theorem]
V2(1) = 0.0962335
(<v^2>/c^2) [<H>=<T>+<V>]
V2A(1) = 0.0962476

```

and the corresponding results for each case can be seen in Table 8.

Finally, as an illustrative example, one can observe in Figure 3 the dimensionless  $\Upsilon(1S)$  reduced wave function taken from the *graph-nl.kumac* file.

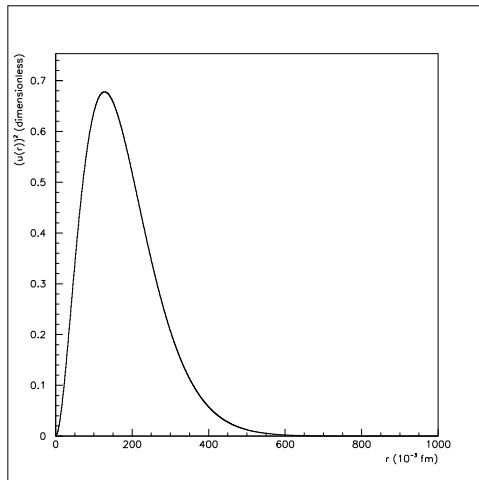


Figure 3.  $\Upsilon(1S)$  reduced wave function.

#### 14. More results using another potential

As a further example, we present results obtained using a Leading Order potential for a heavy quarkonia system

$$V^{\text{LO}} = V^{(0)} + \frac{V^{(1)}}{m_b}$$

which contains a  $V^{(0)}$  static term (which could be a Coulomb plus linear potential), and an additional  $O(1/m)$  piece whose contribution is comparable to the static part. From Lattice analysis [18,19], we set the explicit form of this potential as follows (the so called Cornell-modified potential, see [20] and references therein for a complete description):

$$V_{\text{Cor-mod}}(r) = -\frac{c}{r} - \frac{c'}{r^2} + \sigma r + \mu \quad (48)$$

The values of parameters  $m_b$ ,  $c$ ,  $c'$ ,  $\sigma$  and  $\mu$  were obtained by applying a fitting procedure to the bottomonium spectrum (using  $\Upsilon(1S)$  and  $\Upsilon(2S)$  states), not from Lattice estimates. From the fit we obtained the following values for the parameters of the potential:

$$m_b = 4.7 \text{ GeV}, \quad (\mu = 0)$$

$$\sigma = 0.217 \text{ GeV}^2, \quad c = 0.400, \quad c' = 0.010 \text{ GeV}^{-1}$$

Here, the quark mass redefinition according to  $2m'_b \equiv 2m_b + F$  was used.

The values of the predicted masses, square of the WFOs (or their derivatives), and other parameters of interest for different bottomonium states obtained using this potential are shown in Table 9. It is possible to observe an excellent agreement with experimental mass values.

Table 8  
Coulomb plus liner potential: velocities  $\langle v^2 \rangle$ .

$b\bar{b}$ LEVEL	$\langle v^2 \rangle$ from $QQ\text{-onia}^a$	$\langle v^2 \rangle$ from [6]
$\Upsilon(1S)$	0.096	0.096
$\chi(1P)$	0.065	0.065
$\Upsilon(2S)$	0.078	0.076
$\Upsilon(1D)$	0.067	0.067
$\chi(2P)$	0.075	0.076
$\Upsilon(3S)$	0.085	0.085
$b\bar{b}(4F)^c$	0.073	— — — — —
$\Upsilon(4S)$	0.096	0.097

$a$  : Results doubly checked from Hamiltonian and Virial methods.

Table 9

Values of the predicted and experimental masses (in GeV), square of the WFO (or derivative) in  $\text{GeV}^{3+2l}$ , mean square radius (in fm) and the typical quark velocity for the  $\Upsilon(1S, 2S, 3S, 4S)$ ,  $\chi_b(1P, 2P)$  and  $\Upsilon(1D)$  states for the Cornell-modified potential.

Resonance	Mass	Exp.	$ R_{nl}^l(0) ^2$	$\langle r^2 \rangle^{1/2}$	$\langle v^2 \rangle$
$\Upsilon(1S)$	9.4603	9.4603	12.65	0.23	0.094
$\chi_b(1P)$	9.8929	9.9001	1.409	0.40	0.071
$\Upsilon(2S)$	10.0236	10.0233	6.444	0.51	0.091
$\Upsilon(1D)$	10.1476	10.1622	0.562	0.53	0.078
$\chi_b(2P)$	10.2729	10.2600	1.854	0.63	0.089
$\Upsilon(3S)$	10.3750	10.3552	5.404	0.71	0.103
$\Upsilon(4S)$	10.6477	10.5794	5.194	0.88	0.120

## 15. Spin-dependent splittings and $E1$ width: Numerical Results

In this section we show some results from the above mentioned files. We would like to stress that such results are not exhaustive, but just to illustrate how  $QQ\text{-onia}$  runs.

$n^3S_1 - n^1S_0$  **splitting**: In Table 10 we summarize the results obtained for the  $n^3S_1 - n^1S_0$  splitting running the *SSplit.kumac* file using different potentials. According to section 6, the parameters involved in this calculation are: the heavy-quark mass, its corresponding velocity, and the radial wave function at the origin (rWFO). We present our results from  $QQ\text{-onia}$  using first the set of parameters from the Cornell potential [6]. We also calculate the splitting employing the parameters from the Buchmüller and Tye (B-T) QCD-motivated potential [21]. Lastly, we have reobtained as a final check the hyperfine splitting of a Coulomb plus Linear Potential of Ref.[22] (for the particular case  $\nu = 1$ ) .

Table 10

 $\Delta M = M(^3S_1) - M(^1S_0)$  values (in MeV).

$nS$ level	$\Delta M_{Cornell}$	$\Delta M_{B-T}$	$\Delta M_{CpL-type}$	$\Delta M_{Experimental}$
1S	135	74	66	71.4
2S	57	38	44	— — — —
3S	42	28	33	— — — —

Parameters employed [ $|R_{n0}(0)|^2(\text{GeV}^3)$  and  $m_b(\text{GeV})$  ]:Cornell:  $m_b = 5.18$ ,  $|R_{10}(0)|^2 = 14.06$ ,  $|R_{20}(0)|^2 = 5.668$ ,  $|R_{30}(0)|^2 = 4.271$ B-T:  $m_b = 4.88$ ,  $|R_{10}(0)|^2 = 6.477$ ,  $|R_{20}(0)|^2 = 3.324$ ,  $|R_{30}(0)|^2 = 2.474$ CpL-type:  $m_b = 5.1$ ,  $|R_{10}(0)|^2 = 6.173$ ,  $|R_{20}(0)|^2 = 4.027$ ,  $|R_{30}(0)|^2 = 3.080$ 

A comment is in order here. Recently the BaBar collaboration has claimed the discovery of the long-awaited  $\eta_b(1S)$  state [23]. Its observed mass ( $\simeq 9.389$  GeV) is somewhat lower than expected yielding a somewhat large hyperfine splitting. As can be seen in Table 10, the Cornell potential provides the largest deviation (by excess!), obviously due to the fact that this potential yields the largest value for the rWFO, while the rWFO values from the B-T and CpL-type potential are considerably smaller. In fact, let us note that the Buchmuller-Tye model provides an excellent agreement with the experimental result.

Table 11

 $n(^3P_J)$  and  $n(^1P_1)$  Masses (in GeV); Cornell potential.

$nS$ level	$QQ-onia$	Experimental
$1^3P_0$	9.867	9.860
$1^3P_1$	9.893	9.893
$1^1P_1$	9.900	— — — —
$1^3P_2$	9.911	9.913
$2^3P_0$	10.236	10.232
$2^3P_1$	10.256	10.255
$2^1P_1$	10.262	— — — —
$2^3P_2$	10.271	10.269

$n^3P_J$  and  $n^1P_1$  **splitting:** In Table 11 we summarize the results obtained from the `Split-nP.kumac` files using the Cornell potential, in accordance with eqs.(42, 43), to be compared with the experimental data from [14].

**E1  $2(^3S_1) \rightarrow 1(^3P_J)$  Transitions:** To illustrate this point we show in Table 12 the result obtained from the `E1-2S1P.kumac` file, in accordance with eq.(44). The Cornell

Potential was employed to generate the initial and final state wave functions. A nice agreement with experimental data is found.

Table 12

E1 [ $2(^3S_1) \rightarrow 1(^3P_J)$ ]. From  $QQ$ -*onia*  $\langle f | r | i \rangle = 1.6915 \text{ GeV}^{-1}$ .

Final state	Photon energy (MeV)	Width (keV)	Experiment (keV)
$J = 0$	162.48	1.47	$1.22 \pm 0.16$
$J = 1$	129.63	2.25	$2.21 \pm 0.22$
$J = 2$	110.44	2.32	$2.29 \pm 0.22$

Experimental data obtained from [14].

## 16. Summary

The main goal of this work is to provide a multipurpose (user-friendly) package to obtain the wave functions at the origin and other relevant properties of heavy-quarkonium systems, assuming a basic knowledge of the *PAW* software by the interested reader.

Besides, we would like to stress some special peculiarities of our package, such as providing an easy procedure to normalize the resulting wave functions on account of the the Numerov forward-backward framework. In addition, the calculations of the  $l$ -derivatives at the origin for angular momentum  $l = 2, 3, \dots$  only require a numerical computation of the wave function and first derivative through the analytic expressions given in the main text, thereby keeping the suitable precision for higher derivatives .

In addition, we present an alternative method to estimate the heavy-quark velocity using the well-known virial theorem and a quick 6<sup>th</sup>-order integration, which can be considered as well as a check of the traditional calculation. In fact, this method can also be interpreted as an indirect test of the goodness of the potential-probe together with the (whole range) prior calculated wave function, since it uses the expectation value of  $r$  times the derivative of the potential  $\langle r V'(r) \rangle$ .

Moreover, some worked examples are presented for the bottomonium system using a Cornell-type potential. Finally, an additional machinery has been implemented in the code containing files to analyze the impact of the spin-dependent terms in the potential, as well as a tool dealing with E1 transitions. Another set of worked examples is presented in this regard.

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