

# Reliability of Fourier grid Hamiltonian method to study bottomonium states in non-relativistic model

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**Abstract**—Many techniques were used to study eigenvalues and eigenvectors of Schrödinger equation. One of them is the three-dimensional Fourier grid Hamiltonian. This method will be developed and tested for calculating theoretical spectra of bottomonium meson. Non-relativistic quark potential model is used in our work. A high accuracy results which are in a good agreement with recently published experimental masses for the ground and the radially excited states are obtained for S-wave mesons states.

**Index Terms**—Fourier grid Hamiltonian, quantum chromo-dynamics, bottomonium, Schrödinger equation, potential model.

## 1 INTRODUCTION

QUARKONIUM is the name given to a subatomic system composed of two heavy quarks. While the system containing a bottom and anti-bottom ( $b\bar{b}$ ) quark pair is known as bottomonium. The S-wave ( $L = 0$ ) vector ( $S = 1$ )  $J^{PC} = 1^{--}$  states  $\Upsilon$ , are very well studied [1], [2] since they could be produced in  $e^+ e^-$  annihilation and can thus decay to the experiment clean  $e^+ e^-$  and  $\mu^+ \mu^-$  final states. Following the discovery of the  $\Upsilon(1S)$  state, many other quarkonium states were discovered. The theoretical studies of the heavy quarkonium system [3] and its applications to bottomonium [4] are one of the special interest because of its relies entirely on the first principles of quantum chromo-dynamics.

The results may be helpful in understanding the nature of current and future experimentally observed bottomonium states. In this work, we are introducing and testing the reliability of Fourier grid Hamiltonian (FGH) method in investigate the mass spectra of a bottomonium system in the non-relativistic quark model. In section 2, we review the main formalism of FGH method [5], [6] used in our analysis and the used model. The non-relativistic potential model for quarks is introduced in section 2.3. After that, numerical results and discussion are given. Finally, in the last section, we summarize our main results and conclusions.

## 2 THEORETICAL BASIS

### 2.1 Three-Dimensional FGH Method

The theory behind the method is based on relating the potential energy at the  $N$  grid points with the kinetic energy in the momentum space via forward and reverse Fourier transforms between the coordinate and the momentum space [7], [8], [9]. The  $N \times N$  symmetric matrix  $H$ , obtained by discretization has elements in the form of cosine sums. The task of calculating the bound state eigenvalue and eigenfunctions is thereby transformed to the task of finding eigenvalues and eigenvectors of the matrix  $H$ .

The Hamiltonian could be written as the sum of the kinetic energy  $\hat{T}$  and a potential energy operator  $\hat{V}$ . The eigenvalue equation for a stationary state is given by

$$[\hat{T} + \hat{V}]|\psi\rangle = E|\psi\rangle \quad (1)$$

Where  $\hat{T}$  depends only on the square of the relative momentum  $\vec{P}$  between the particles,  $\hat{V}$  is a local interaction which depends on the relative distance, and  $E$  is the eigenenergy of the stationary state. This equation is a nonrelativistic Schrodinger equation if

$$\hat{T} = m_1 + m_2 + (\vec{P}^2 / 2\mu) \quad (2)$$

Where  $m_1$  and  $m_2$  are the masses of the particles and  $\mu$  is the reduced mass of the system in configuration space, (1) is written

$$\int [ \langle \mathbf{r} | \hat{T} | \mathbf{r}' \rangle + \langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle ] \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' = E \langle \mathbf{r}' | \psi \rangle \quad (3)$$

In the following, we only consider the case of a local central potential

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$$\langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle = V(r) \delta(\mathbf{r} - \mathbf{r}') \quad \text{with } r = |\mathbf{r}| \quad (4)$$

Consequently, the wave function has the form

$$\langle \mathbf{r} | \psi \rangle = R_l(r) Y_{lm}(\hat{r}) \quad \text{with } r = \mathbf{r} / r \quad (5)$$

Using the method developed in [7], (3) can be rewritten

$$(2 / \pi) r \int_0^\infty dr' r' u_l(r') \int_0^\infty dk (k^2) T(k^2) \quad (6)$$

$$j_l(kr) j_l(kr') + V(r) u_l(r) = E u_l(r)$$

Where  $u_l(r) = r R_l(r)$  is the regularized radial function and the functions  $j_l(kr)$  are spherical Bessel functions, This equation is the basis of the three-dimensional Fourier grid Hamiltonian method.

### 2.2 Discretization

We now replace the continuous variable  $r$  by a grid of discrete values  $r_i$  defined by

$$r_i = i \Delta \quad \text{with } i = 0, 1, 2, \dots, N \quad (7)$$

Where,  $\Delta$  is the uniform spacing between the grid points. Regularity at the origin imposes  $u_l(r_0 = 0) = 0$ . For bound states, we have  $\lim_{r \rightarrow \infty} u_l(r) = 0$ . Consequently, we choose to set  $u_l(r_N = N\Delta) = 0$ . Actually, this last condition is not necessary, but it does not spoil the accuracy of solutions. The normalization condition for the radial wave function is

$$\int_0^\infty dr [u_l(r)]^2 = 1 \quad (8)$$

The discretization of this integral on the grid gives

$$\Delta \sum_{i=1}^{N-1} [u_l(r_i)]^2 = 1 \quad (9)$$

As explained in [7], the grid spacing  $\Delta$  in the configuration space determines the grid spacing  $\Delta k$  in the momentum space. Therefore, we have a grid in the configuration space and a corresponding grid in the momentum space

$$k_s = s \Delta k = (s \pi / N \Delta) \quad (10)$$

with  $s = 0, 1, \dots, N$

If we note  $V_i = V(r_i)$ , the discretization procedure replaces the continuous (6) by an eigenvalue matrix problem

$$\sum_{j=1}^{N-1} H_{ij} \phi_j^n = e_n \phi_i^n \quad \text{for } i = 1, 2, \dots, N-1 \quad (11)$$

where

$$H_{ij} = (2\pi^2 / N^3) ij \sum_{s=1}^N S^2 T((\pi s / N \Delta)^2) \quad (12)$$

$$j_l(\pi s i / N) j_l(\pi s j / N) + V_i \delta_{ij}$$

The (N-1) eigenvalues  $e_n$  of (11) correspond approximately to the first (N-1) eigenvalues of (6). In the case of a potential which possesses a continuum spectrum, only eigenvalues below the dissociation energy are relevant. Other eigenvalues, which forma discrete spectrum of positive energies, are spurious and correspond to standing wave solutions satisfying  $u(r) = 0$  at  $r = 0$  and  $r = N\Delta$ . The eigenvector  $\phi_i^n$  gives approximately the values of the radial part of the  $n$ th solution of Eq. (6) at the grid points.

### 2.3 The Non-Relativistic Potential Model

As a minimal model of the bottomonium system we use a non-relativistic potential model, with wave functions determined by the Schrödinger equation with a conventional quarkonium potential which is Coulomb plus linear plus hyperfine interaction model [10], [11], [12].

$$V(r) = -(4\alpha_s / 3r) + br \quad (13)$$

With inter-quark distance  $r$ , here,  $(-4/3)$  is due to the color factor,  $\alpha_s$  is the quark-gluon coupling and  $b$  is the string. In the above equation, the first term is due to one gluon exchange and the second term is the linear confining potential [13]. By including the Gaussian-smearred hyperfine interaction [14] and orbital angular momentum term, the potential of the  $q\bar{q}$  system for the ground state gluonic field has the form.

$$V(r) = -(4\alpha_s / 3r) + br + (32\pi\alpha_s / 9m_c^2)(\sigma / \sqrt{\pi})^3 e^{-\sigma^2 r^2} S_c \cdot S_{\bar{c}} \quad (14)$$

where  $S$  is the total spin quantum number of the meson [15] and

$$S_c \cdot S_{\bar{c}} = (s(s+1) / 2) - (3 / 4) \quad (15)$$

$\mu$  is the reduced mass of the quark and antiquark and  $m_c$  is the mass of the charm quark. So that the potential has the following form for the bottomonium [14]:

$$V(r) = -(4\alpha_s / 3r) + br + (32\pi\alpha_s / 9m_c^2)(\sigma / \sqrt{\pi})^3 e^{-\sigma^2 r^2} S_c \cdot S_{\bar{c}} + (l(l+1) / 2\mu r^2) + (1 / m_c^2)[((\alpha_s / r^3) - (b / 2r)) \vec{L} \cdot \vec{S}] + (\alpha_s / r^3) \vec{T} \quad (16)$$

Where the spin-orbit operator is diagonal in a  $|J, L, S\rangle$  basis, with the matrix elements

$$\langle \vec{L} \cdot \vec{S} \rangle = [J(J+1) - L(L+1) + S(S+1)] / 2 \quad (17)$$

The tensor operator  $\vec{T}$  has non-vanishing diagonal matrix elements only between  $L > 0$  spin-triplet states, which are

$$\vec{T} = \begin{cases} -L / (6(2L + 3)), J = L + 1 \\ 1 / 6, J = L \\ -(L + 1) / (6(2L - 1)), J = L - 1 \end{cases} \quad (18)$$

Now, the potential model (16) will be employed to get the spectra of bottomonium ( $b\bar{b}$ ) bound states, with wave functions determined by the radial Schrödinger equation. Table (1) shows the fitted parameters of the model used.

### 3 NUMERICAL RESULTS

Bottomonium meson spectra have been studied by using FGH method with non-relativistic potential model. We predict the masses of the twelve  $b\bar{b}$  states shown in table 2, where we compared the present theoretical predictions with those from [12]. These new results are fitted by using the experimental spectra [16] to give the most suitable masses with experiments. The  $\chi^2$  relation is used to easily compare among the results obtained by using the non-relativistic potential and this relation is defined as.

$$\chi^2 = (1 / n) \sum_{z=1}^n (mass_z^{Theo.} - mass_z^{Exp.})^2 \quad (19)$$

The summation runs over a selected sample of n mesons, where

$n$  is the number of experimental data.  $Mass_z^{Exp.}$  is the experimental mass of meson labeled k in the sample, while  $Mass_z^{Theo.}$  is the corresponding theoretical mass depending upon the free parameters.

After getting masses of bottomonium mesons we drew the ratio between the obtained theoretical predictions of bottomonium spectra and those from [12] versus experimental data [16] as shown in fig1 and in fig2. It is seen that the ratio converges to one particularly. This means that the yielded results are in a good agreement with recently published predictions.

TABLE 1  
 PARAMETERS USED TO FIT MASSES OF ( $b\bar{b}$ ) STATES IN ACCORDING TO QCD THEORY

Parameters	Theo.(NR) Potential
$m_b = m_{\bar{b}} [GeV]$	4.8097
$\alpha_s$	0.4036
$b [GeV]$	0.1624
$\sigma [GeV]$	2.4948

TABLE 2  
 THE EXPERIMENTAL AND THEORETICAL BOTTOMONIUM MASS SPECTRA WITH THOSE FROM [12]. WE LIST THE WORLD AVERAGE MASSES FROM PDG AS WELL AS THE LATEST OBSERVATIONS.

meson	Mass <sub>theo</sub> [12] (GeV)	Our Mass <sub>theo</sub> (GeV)	Mass <sub>exp</sub> [16] (GeV)	$\chi^2$ (GeV)
$\Upsilon (1^3S_1)$	9.458	9.4584	$9.4603 \pm 0.26$	3.61E-06
$\eta_b (1^3S_0)$	9.393	9.5349	$9.398 \pm 3.2$	1.8742E-02
$\Upsilon (2^3S_1)$	10.017	10.0172	$10.02326 \pm 0.31$	3.67E-05
$\eta_b (2^3S_0)$	9.996	10.0499	$9.999 \pm 3.5^{+2.8}_{-1.9}$	2.591E-03
$\Upsilon (3^3S_1)$	10.345	10.3445	$10.3552 \pm 0.5$	1.14E-04
$\eta_b (3^3S_0)$	10.33	10.3694	-	-
$\Upsilon (4^3S_1)$	10.607	10.6071	$10.5794 \pm 1.2$	7.67E-04
$\eta_b (4^3S_0)$	10.596	10.6285	-	-
$\Upsilon (5^3S_1)$	-	10.8365	10.8899	2.852E-03
$\eta_b (5^3S_0)$	-	10.8559	-	-
$\Upsilon (6^3S_1)$	-	11.0447	$10.9929^{+10.0}_{-3.1}$	2.683E-03
$\eta_b (6^3S_0)$	-	11.0628	-	-

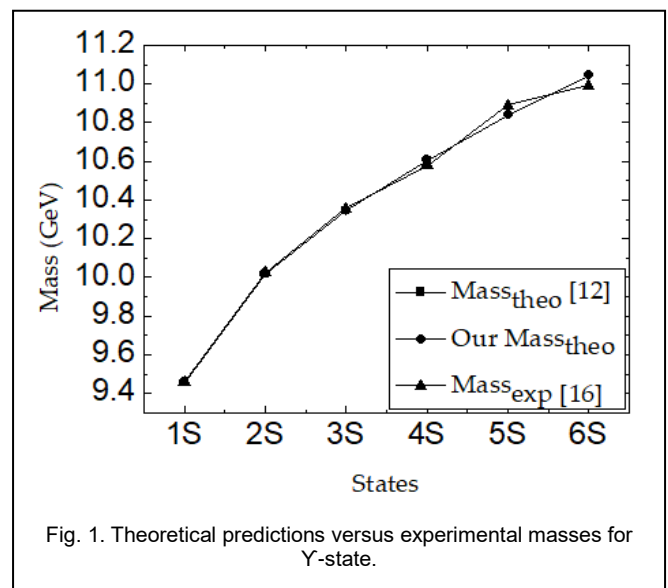
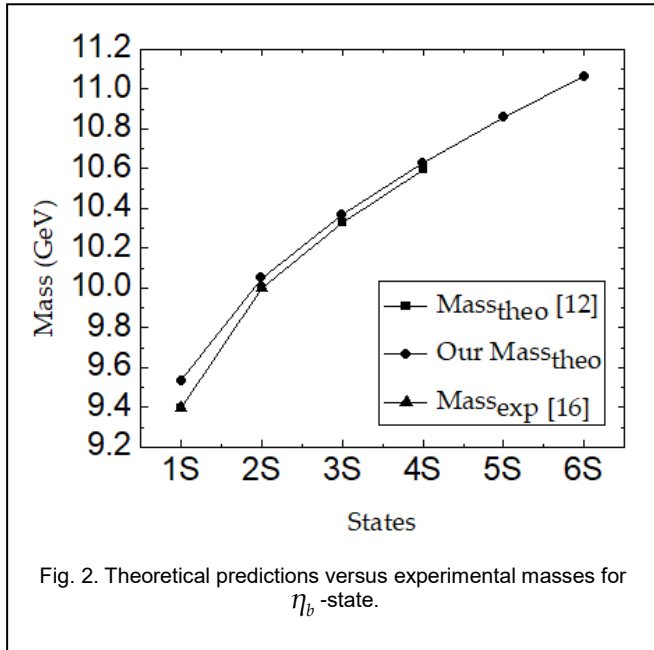


Fig. 1. Theoretical predictions versus experimental masses for Y-state.



#### 4 CONCLUSION

In this work, FGH method discretization has been used for solving Schrödinger equation, by transforming it into a matrix form. Coulomb plus linear plus hyperfine plus tensor term potential model is used. Accurate eigenvalues are obtained for S-wave of bottomonium mesons spectra using few lines of python code. We observed that the method gives high accuracy results which are in a good agreement with experimental results; it gives small values of  $\chi^2$  which shows the validity of the used method. It is recommended to using FGH method for solving radial Schrödinger equation because it is easy to use, saves the time and is very accurate, so we advise using this method to obtain other mesons spectra and properties.

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