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Numerical Solutions of a Three-Dimensional Schrödinger Equation for a Non–Relativistic Quark Model

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Abstract: An accurate bound state eigenvalues are evaluated and plotted utilizing the non–relativistic quark model by using three different methods. The methods are employed perfectly within the three-dimensional time–independent Schrödinger equation. Therefore, developing an effective technique to manipulate this well–known equation is the main reason for publishing this study. In this regard, an extensive comparison of the calculated numerical approaches with experimental data was conducted. In most cases, the three considered methods reflected optimal results for heavy mesonic family members by satisfying the minimization condition of χ^2 values for each.

Keywords: Non–relativistic quark model, numerical methods, Schrödinge equation, heavy mesons

1 Introduction

In many scientific fields, including physics and chemistry, the solution of Schrödinger equation (SE) is considered as a significant challenge due to the mysterious nature of the wavefunction. By using Hamiltonian, SE could be solved to determine the eigenvalues that characterize the relative motion of quarks and antiquarks in the framework of the quark model. In physics and quantum mechanics, numerical methods play an important role, where is often no empirical solution to the SE. In physical problems, the exact solution of SE is important because it provides a deep understanding of the problem of physics[1,2,3,4] and, in most cases, it is the only method to obtain a usable solution. In the perturbation methods, relative to the Hamiltonian of the system, the disturbed potential should be minimal. The need to solve a set of complex integrals is one of the problems with perturbation methods. Since there is no particular limit to the form of this technique, the numerical solution of SE is on the spot point of researchers.

On the hypothetical side, the heavy quarkonia analysis provides data for certain hadronic scales associated with Quantum Chromodynamic (QCD) and verifies the validity of perturbative QCD; possible models even lattice QCD calculations[5]. Theoretically, heavy quarkonia, for example bottomonium states $b\overline{b}$ have rich spectroscopy with several narrow states below those b-b processing thresholds. Large numbers of such states have not been experimentally confirmed or understood[5,6,7,8]. The study of the characteristics of heavy quark and antiquark mesons offers a very valuable insight into heavy quark dynamics and a deeper understanding of the constituent quark masses. There are many papers investigating the spectroscopy of heavy mesons over the years, as seen in Refs.[9]-[17]. The non–relativistic model is one of the most popular models used. The implementation of this model helps to measure the spectrum on the basis of the non-relativistic Schr?dinger equation. The goal for this research is, first, to extract Eigenvalues E and Eigenvectors ψ numerically in a defined potential model for the Schr?dinger Wave Equation using three different methods. Second, to analyze the reliability of those numerical methods for calculating masses of some heavy mesons by comparing the experimental data with the calculated results. Finally, the most effective numerical

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method is picked. These three different methods were applied to calculate the masses of $b\overline{b}$ states.

This paper is organized as follows: The non–relativistic quark model is used to calculate the mass spectrum as outlined in Section 2. A brief description of the numerical techniques that was used in this work as described in Section 3. The mass predictions are given with numerical agreement between the results obtained and useful experimental evidence that offers a very non–trivial proof of the precision and internal consistency of our calculations in Section 4. And finally a concluding remarks are given in Sec.6.

2 Non–relativistic quark model

This section is devoted to summarize the model of heavy–heavy bound state systems ($b\overline{b}$) by using SE as per below

$$[\frac{-\hbar^2}{2\mu}\nabla^2 + V(r)]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

where $V(r)$ is the quark–antiquark potential, and $-\hbar^2/2\mu$ represents the kinetic energy operator. The sum of these two terms is of course the non–relativistic Hamiltonian given by [18]-[22]

$$H = M + \frac{p^2}{2\mu} + V(r) \tag{2}$$

$$M = M_Q + M_{\overline{Q}} \tag{3}$$

$$\mu = \frac{M_Q M_{\overline{Q}}}{M_Q + M_{\overline{Q}}} \tag{4}$$

where $M_Q/M_{\overline{Q}}$ are the quark/antiquark mass parameters. The relative momentum of each quark is referred to as p. Solving this equation for radius–centered potentials in recent years has attracted many researchers. Non–relativistically, A bound state of interacting quarks and antiquarks is commonly roughly described as the meson. This interaction potential composed to as mentioned in Ref.[22].

$$V(r) = \frac{-4\alpha_s}{3r} + br + \frac{32\pi\alpha_s}{9m_Q m_{\overline{Q}}}(\frac{\sigma}{\sqrt{\pi}})^3 e^{-\sigma^2 r^2} S_Q.S_{\overline{Q}} + \frac{l(l+1)}{2\mu r^2} + \frac{1}{m_Q m_{\overline{Q}}}[(\frac{\alpha_s}{r^3} - \frac{b}{2r})\mathbf{L}.\mathbf{S} + \frac{\alpha_s}{r^3}T] \tag{5}$$

(6)

where α_s is the strong running coupling constant, $-4/3r$ is the color factor, b is a potential parameter, and $S_Q.S_{\overline{Q}}$ is the spin–spin contact hyperfine interaction. The spin–orbit operator is considered to be diagonal on the basis of $|J,L,S\rangle$ associated with the following matrix elements

$$\langle \mathbf{L}.\mathbf{S}\rangle = [J(J+1) - L(L+1) - S(S+1)]/2 \tag{7}$$

The tensor operator T has non–vanishing diagonal matrix elements only between $L > 0$ spin–triplet states, as shown in Ref.[22].

The parameters used in this potential for the heavy mesons are tabulated in Table 1. These values were obtained by fitting the masses of twelve known $b\overline{b}$ states based on experimental data. These parameters contribute to a clear definition of the bottomonium masses tabulated in Table 2. Three different techniques will be utilized to numerically determine SE with the potential mentioned above. These methods include the finite difference approach, the Numerov method, and the Fourier grid Hamiltonian method. The numerical approaches utilized in this study will be briefly described in the next section.

3 Numerical methods

The numerical solution of the radial SE in this study results in an eigensystem that can be resolved using a variety of techniques, each of which has some strengths and weaknesses. In most problems of mathematical integration, the traditional integration approach is converted into a matrix problem. In some way, it reduces the estimation of the whole integration into the 'diagonalization' of the said matrix. Our strategy relies on choosing the most optimal numerical technique to examine the static characteristics of heavy mesons. These methods are as follow; Numerov method, the finite difference method, and Fourier grid Hamiltonian method. The numerical approaches utilized in this study will be briefly described in the next subsection.

3.1 Numerov's discretization method

A numerical formula to approximate the solution of the second order differential equation is the Numerov's Discretization Method (NDM). The merits of the Numerov method [23]-[28] have been praised by many authors. Through the use of arbitrary potentials, this method is used to determine various solutions for the radial Schrodinger Equation. Equation **??** can therefore be resolved by using NDM. Numerov method is a specific integration formula for a system of numerical integrating differential equations

$$\psi''(r) = f(r)\psi(r) \tag{8}$$

where, the time–independent $1D$ SE can be written as

$$f(r) = -2m(E - V(r))/\hbar^2 \tag{9}$$

Using a lattice of points uniformly spaced by distance of d to obtain

$$\psi_{i+1} = \frac{\psi_{i-1}(12 - d^2 f_{i-1}) - 2\psi_i(5d^2 f_i + 12)}{d^2 f_{i+1} - 12} \tag{10}$$

$$\psi_{i+1} = \frac{12\psi_{i-1} - \psi_{i-1}d^2 f_{i-1} - 10\psi_i d^2 f_i - 24\psi_i}{d^2 f_{i+1} - 12} \quad (11)$$

By using Eq.8 one can get

$$-\frac{\hbar}{2m}\frac{\psi_{i-1} - 2\psi_i + \psi_{i+1}}{d^2} + \frac{V_{i-1}\psi_{i-1} + 10V_i\psi_i + V_{i+1}\psi_{i+1}}{12} = E\frac{\psi_{i-1} + 10\psi_i + \psi_{i+1}}{12} \quad (12)$$

By modifying simply the grid number and the matrix size N, the popular Numerov method can be transformed into a representation of the matrix form on a discrete lattice. To achieve that, a column vector with the symbol will be used $(...\psi_{i-1}, \psi_i, \psi_{i+1}...)$ and define matrices

$$A_{N,N} = \frac{I_{-1} - 2I_0 + I_{+1}}{d^2}, \quad (13)$$

$$B_{N,N} = \frac{I_{-1} + 10I_0 + I_{+1}}{12}, \quad (14)$$

$$V_N = (..,V_{i-1},V_i,V_{i+1},..), \quad (15)$$

where I_{-1}, I_0 and I_{+1} represent sub, main, and up diagonal unit matrices, respectively. The matrix form can be written as per below

$$-\frac{\hbar^2}{2m}A_{N,N}\psi_i + B_{N,N}V_N\psi_i = E_i\, B_{N,N}\psi_i \quad (16)$$

Multiplying both sides by $B_(N,N)^{-1}$, the 3D radial SE can be deduced as

$$-\frac{\hbar^2}{2m}A_{N,N}B^{-1}_{N,N}\psi_i + [V_N(r) + \frac{l(l+1)}{r^2}]\psi_i = E_i\ \psi_i \quad (17)$$

The kinetic energy operator is represented by the Numerov's formula in the first term, while the potential energy operator is represented by the second.

3.2 Matrix method

One of the simplest methods is the matrix schemes which extended to the solution of time–independent SE in spherical symmetric $Q\overline{Q}$ potentials [29]-[32]. Radial SE in wave function form can be rewritten as

$$-\frac{\hbar^2}{2\mu}\nabla^2 U(r) + [E - V(r)]U(r) = 0 \quad (18)$$

where E represents the overall energy of the quark–antiquark system, while r represents the distance between quarks. And hence, Eq.18 can be rewritten as

$$-\frac{\hbar^2}{2\mu}\frac{\delta^2}{\delta r^2}U(r) + [V(r) + \frac{l(l+1)}{2\mu r^2}]U(r) = EU(r) \quad (19)$$

The second derivative form of $U(r$ function will be as

$$-\frac{d^2U(r)}{dr^2} = \frac{U(r_{i+1}) - 2U(r_i) - U(r_{i-1})}{d^2} + O(h^2) \quad (20)$$

where d is the interval between two points

$$d = \frac{R_{max} - R_{min}}{N} \quad (21)$$

where R_{max} and R_{min} are the shortest and the longest distances between the quark–antiquark, respectively. Now, when an arbitrary value of r is defined as

$$r_i = R_{min} + id \quad (22)$$

and $i = 1,2,..,N-1$, and from hens we can rewrite SE as per below

$$EU(r_i) = -\frac{U(r_i + d) - 2U(r_i) + U(r_i - h)}{2\mu d^2} + [V(r) + \frac{l(l+1)}{2\mu r^2}]U(r_i) \quad (23)$$

This equation can be written as

$$e_i U(r_{i+1}) + d_i U_i + e_i U(r_{i-1}) = EU(r_i) \quad (24)$$

$$d_i = \frac{1}{\mu\hbar^2} + V(r) + \frac{l(l+1)}{2\mu r^2} \quad (25)$$

$$e(i) = \frac{-1}{2\mu\hbar^2} \quad (26)$$

Equation 26 could be transformed into a matrix form in which $d(i)(e(i))$ represents the diagonal and non–diagonal elements, respectively.

3.3 Fourier grid Hamiltonian method

A very common way to control boundary–value issues and solve our differential equations is via what is known as Fourier grid Hamiltonian (FGH) method. The key features of the FGH system are reviewed in this subsection. It uses forward and reverse Fourier transformations to correlate potential energy at N grid points with kinetic energy in momentum space[33]-[35].

The $N \times N$ symmetric matrix H, obtained by discretization, has elements in the form of cosine sums. The task of computing the eigenvalues and eigenfunctions of the bound state is thus transformed into the task of finding eigenvalues and eigenvectors of the matrix H. The equation of eigenvalue for a stationary state is given by

$$[T + V] \mid \Psi >= E \mid \Psi > \quad (27)$$

where T is the particle's kinetic energy which has the following representation

$$\int [< r \mid T \mid r' > + < r \mid V \mid r' >] < r' \mid \Psi > dr' = E < r' \mid \Psi > \quad (28)$$

$$< r \mid V \mid r' >= V(r)\delta(r-r') \tag{29}$$

The wave function can be decomposed into its central and orbital components as

$$< r \mid \psi >= R_l(r)Y_{lm}(r') \tag{30}$$

The basis states $\mid k\lambda\nu >$, which are eigenstates of the operator p^2, are utilized to build the nonlocal representation of the kinetic energy operator. They are identified by the existence of excellent orbital quantum numbers (λ,ν), that obey the relation

$$T(p^2) \mid k\lambda\nu >= T(k^2) \mid k\lambda\nu > \tag{31}$$

And satisfy the orthogonality relation

$$< k'\lambda'\nu' \mid k\lambda\nu >= \delta(k'-k)\delta_{\lambda'\nu}\delta_{\_\nu'\nu} \tag{32}$$

These states are represented by in the configuration space by

$$< r \mid k\lambda\nu >= sqrt(2k^2/\pi)j_\lambda(kr)Y_{\lambda\nu}(r') \tag{33}$$

where the function $j_l(kr)$ is the Bessel radial function in a spherical form. Equation 31, which uses the base state completeness relation $\mid j_l(kr) >$ may be expressed as

$$< r \mid T \mid r' > = \int_0^\infty dk(2k^2/\pi)T(k^2)$$

$$\sum_{\lambda=0}^{\infty}\sum_{\nu=-\lambda}^{\lambda} j_\lambda(kr)j_\lambda(kr')Y_{\lambda\nu}(r)Y^*_{\lambda\nu}(r') \tag{34}$$

By introducing the regularized function $u_l(r) = r\,R_r(r)$, Equation 27 will be introduced as

$$(2r/\pi)\int_0^\infty dr'r'u_l(r')\int_0^\infty dk'(k^2)T(k^2)j_l(kr)j_l(kr')$$
$$+V(r)u_l(r) = Eu_l(r) \tag{35}$$

Equation 35 provides the foundation for the three–dimensional Fourier grid Hamiltonian technique.

3.4 Discretization

Now, the continuous variable will be replaced by a discrete value grid defined by r_i where,

$$r_i = i\Delta \tag{36}$$

where $i = 1,2,..N$, Δ is the constant distance between the grid points and the radial wave function normalization condition is

$$\int_0^\infty dr[u_l(r)]^2 = 1 \tag{37}$$

This integral's discretization on the grid is provided by

$$\Delta\sum_{i=1}^{N=-1}[u_l(r_i)]^2 = 1 \tag{38}$$

In the momentum space, the grid spacing Δk is calculated by the grid spacing Δ. Considered the highest possible value of $r_N = N\Delta$, the wave function acts on a sphere with a diameter of $2r_N$ in the coordinate space. Since this length specifies the longest wavelength λ_max the lowest frequency Δk, that may be seen in k–space is

$$\Delta k = \frac{2\pi}{\lambda_{max}} \tag{39}$$

A grid in coordinate space and an equivalent grid in momentum space are available as

$$k_s = s\Delta k = (s\pi/N\Delta) \tag{40}$$

where $s = 1,2,..,N$. Equation 34 is replaced by an eigenvalue matrix problem during the discretization process as

$$\sum_{j=1}^{N-1} H_{ij}\phi_j^n = e_n\phi_j^n \tag{41}$$

where $s = 1,2,..,N-1$, and

$$H_{ij} = (2\pi^2/N^3)ij\sum_{s=1}^{N} S^2T(\pi S/N\Delta)^2 j_l(\pi Si/N)j_l(\pi Sj/N)$$
$$+V_i\delta_{ij} \tag{42}$$

In the next part, the obtained results of the heavy meson's masses derived will be explained by using the previously recognized tri–diagonal matrix techniques. This will be done with statistical and numerical investigations to find the preferred numerical scheme appropriate for studying heavy meson spectroscopy

4 Result and Discussion

Based on the obtained numerical results, these results were checked to confirm that the predicted values will not blow up to infinity and that the solutions for the reduced tri–diagonal self-value issues are acceptable. In the current study, optimization via reducing the statistical function is used to show how the computed results and experiments are consistent. The Particle Data Group (PDG)[36,37] review is the source of all experimental masses of several heavy mesons that were chosen for these comparisons. The statistical function was calculated from the following formula

$$\chi^2 = \frac{1}{n}\sum_{k=1}^{n}(M_k^{cal.} - M_k^{exp.})^2 \tag{43}$$

The summation runs over some selective samples of n heavy mesons. $M_k^{exp.}$ is The observed mass of the meson with the symbol k in the sample, whereas $M_k^{cal.}$ is the calculated one. In addition, one of the most important motivations for this work is to draw up a road–strategy to distinguish and decide the best numerical method. However, there are matching between the three

considered methods, there have also such remarked differences. For this purpose, the numerical calculations of the heavy meson masses are repeated for the three considered methods. We noticed that our findings deviate from the published work for S. Godfrey et al.[**?**]. The noticed deviation is a significant in some cases and quite bit for the others. This is primarily due to the chosen potential; in this work the calculations is done via the non–relativistic potential, while S. Godfrey and his research group used the relativistic potential as shown in Table 1. Although we are interested in how the predictions vary against the measured points to verify the reliability of the deduced analytical forms and satisfactorily reflecting the experimental data. Figures 1, 2 and 3 represent, respectively, the calculated masses of the considered bottomonium states for FGH, Numerove and Matrix methos, versus experimental masses.

A numerical comparison between the experimental data and the calculations for some heavy mesons $b\overline{b}$ is given in Table 1. It is remarkable that such high accuracy results can be achieved with a simple program for each method. This examination is based on the minimizing of the χ^2 function, which was done previously, to choose the most strongly experiment–validated approach. The desired optimization was observed utilizing the three methods. Consequently, the optimal minimization of bottomonium states for the FGH, Numerov, and Matrix methods was $0.012, 0.002,$ and 0.002, respectively. However, the study indicated that the Matrix and Numerov approaches are better suited since the results of the experiments and estimated profile were in agreement, and the associated minimization for both was 0.002.

In Fig.1, one can see obviously both the mass trajectories exhibit good behaviors and they are roughly consistent with the experimental data. From Figs.1 and 2, it is clear that the Numerov and Matrix methods are the best choice to evaluate the masses of heavy mesons. Our findings show that the FGH approach can yields results that match with experimental data for lower states but conflict with greater excited levels. The above results can be applied in different fields [38]-[53].

5 Concluding remarks

In this research work, the 3D SE was solved numerically by using three different methods. Probably, there may be some other similar methods which are used popularly in calculating energy and wave functions, but the simplicity of the considered methods in the final analytical forms introduced here make them ideal for the notion of the wave function and eigenvalue problems. Within the non–relativistic potential model, highly accurate numerical methods are employed to estimate the accuracy of the deduced solution. In practice, Mathematica's software packages were used to resolve the eigenvalue problem for a given matrix. Masses spectra for some leading–state flavored mesons are calculated, as an example. To modify the members of the heavy meson family, the observed numerical forms offer an ideal approximation. As a result of a persuaded minimization for χ^2 values, each of them demonstrates an acceptable agreement with experiments. Finally, it could be concluded that the three considered methods yielded highly accurate results against the conducted experiments, and the deviation between them was going to be smaller. The main advantage of the three methods is their ability to achieve high accuracy with minimal programming complexity and a short calculation time.

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