Numerical Methods Endterm Project Report:

Heavy Quarkonium Systems-Cornell Model

Submitted by - SEEMA (seema.s@icts.res.in)

May 12, 2024

1 Introduction

Heavy quarkonium is the bound state of $b\bar{b}$ and $c\bar{c}$ (quark-antiquark)and is one of the most playgrounds for our understanding of strong interactions of quarks and gluons. Quantum chromodynamics (QCD) is thought to be the true theory of these strong interactions. QCD is non-abelian local gauge field theory with the symmetry group SU(3).In principle, one should be able to calculate hadronic properties such mass spectrum and transitions by using QCD principles. The QCD Lagrangian is given by-

$$L_{QCD} = \bar{\psi}_i(i\gamma^\mu(D_\mu)_{ij} - m\delta_{ij})\psi_j - \frac{1}{4}G^a_{\mu\nu}G^{\mu\nu}_a \tag{1}$$

where $\psi_i(x)$ is the quark field,γ^μ are the gamma matrices, D_μ is the gauge covariant derivative. No one has yet succeeded in calculating the effective form of the interquark forces from quantum chromodynamics, even in non-relativistic limit. This theory is faithful but at low energies or large distances, the strong coupling constant becomes large, and perturbative calculations based on the QCD Lagrangian become unreliable. This non-perturbative regime is where phenomena such as quark confinement and the formation of bound states like quarkonium occur.
The potential models like the Cornell potential are introduced as phenomenological descriptions of the effective interaction between the quark and antiquark in these bound states. They are motivated by the general features expected from QCD, such as the short-range Coulomb-like behavior and the long-range confinement(long-range at hadronic scale), but their specific functional forms are not derived directly from the QCD Lagrangian.
Our aim in this project is to get the wave function form for the quarkonium system, because we know almost all the properties of the quantum system can be calculated using the wave function.

2 Cornell Potential

Assumptions in this model- (i) The basic interaction between quarks is assumed to have a color-SU(3) gauge symmetry, which leads to forces that are so strong at large distances that quarks are permanently confined in color-neutral bound states- mesons and baryons. (ii) The large masses of the bound states allows us to treat them non-relativistically. The form of the Cornell potential is given by:

$$V(r) = C_0 - \frac{\kappa}{r} + \frac{r}{a^2} \tag{2}$$

where, V(r)(Figure 1) is the interquark potential as a function of the quark-antiquark separation distance r, κ is the strength of the Coulomb-like term $(1/r)$ whose behaviour is in accordance with asymptotic freedom at short distance, a is related to the string tension parameter, which describes the linearly rising term responsible for quark confinement at large distances. This term ensures that the potential energy increases linearly with the separation distance, making it increasingly difficult to separate the quark and antiquark as they move apart. C_0 is a constant term, often chosen to ensure that the potential is zero at the origin (r = 0).

3 The Schrodinger equation- General consequences

The Schrodinger equation is applicable for this non-relativistic system of two bodies which can be reduced to single body problem. The time-independent Schrodinger equation in three dimensions is written in the form

$$-\hbar^2/2\mu\boldsymbol{\nabla}^2\psi(r) + [V(r) - E]\psi(r) = 0 \tag{3}$$

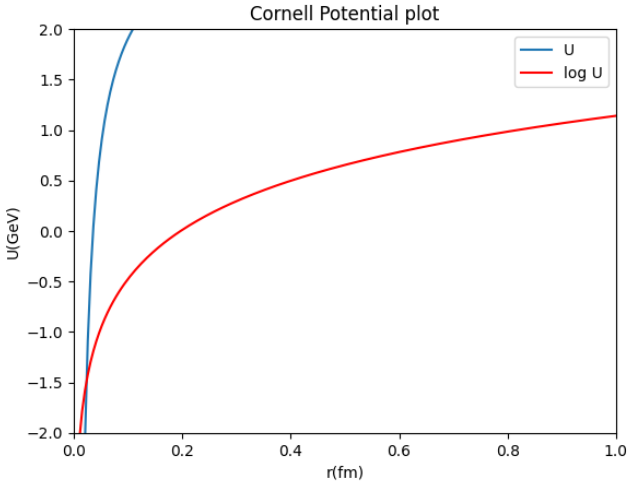

Figure 1: A graph of the potential $V(r)$ versus the relative co-ordinate r

where μ is the reduced mass of the two-body system, r is the relative coordinates. For the central potential, it is convenient to write

$$\psi(r) = R(r)Y_{lm}(\theta, \phi) \tag{4}$$

where R(r) is the radial wave function and $Y_{lm}(\theta, \phi)$ is a spherical harmonic. With this substitution the Schrodinger equation separates and the radial wave function satisfies

$$\frac{-\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)R(r) - \left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]R(r) = 0 \tag{5}$$

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

$$u(r) \equiv rR(r) \tag{6}$$

which defines the reduced radial wave function. The reduced radial equation is then

$$-\frac{d^2u(r)}{dr^2} = \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]u(r) \tag{7}$$

subject to the conditions on wavefunction - $u(0) = 0$ and $u'(0) = R(0)$ The above eq is identical with the one-dimensional equation for an effective potential given by $V_{eff}(r) + l(l+1)\hbar^2/2\mu r^2$. We will be doing our calculation for S-states(l=0 case). So, now our problem reduces to solving the 1-d Schrodinger equation.

4 Numerical set up of the problem

The time-independent schrodinger equation is given by-

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle \tag{8}$$

here, $\hat{H} = \hat{T} + \hat{V}$ and $\hat{T} = \hat{p}^2/2\mu$. After placing p-operator we have-

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x)\right]|\psi\rangle = E\,|\psi\rangle \tag{9}$$

Step-1: We can discretise the space-coordinates (with spacing l)such that at each point we have a value of the wavefunction, $\psi(x_i)$. We can transform the above differential equation into matrix equation using method of Finite differences, where we can write the double derivative as-

$$\frac{d^2\psi(x_i)}{dx^2} = \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1})}{l^2} \tag{10}$$

Then, the kinetic matrix will become-

$$T = -\frac{\hbar^2}{2\mu}\begin{pmatrix} -2 & 1 & \cdots & 0 \\ 1 & -2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & -2 \end{pmatrix} \tag{11}$$

Similarly, the potential matrix takes the form-

$$V = \begin{pmatrix} V(x_1) & 0 & \cdots & 0 \\ 0 & V(x_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V(x_n) \end{pmatrix} \tag{12}$$

Step-2: We can find eigenvalues and eigenvectors of $\hat{H}$ matrix, using the inbuilt scipy function "linalg.eig".

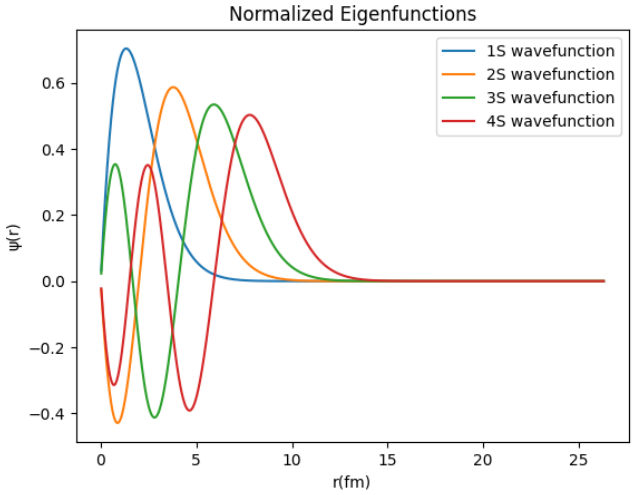

Figure 2: A graph of first four eigenfunctions(l=0 case) versus the relative co-ordinate r

Step-3: Properly normalizing the eigenvectors using normalization condition - $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$. Because of the forms of wavefunctions, we cannot use Trapezoidal or Simpson's method to integrate over spatial coordinate. We need to use Gaussian Quadrature rule.
Step-4: Calculate expectation values of various physical quantities like-radius (rms),Energy, momentum , uncertainity product etc.
Step-5: Take the proposed trial wave functions of the system, we will start with the simple and famous gaussian function and then take some modified versions of it. Using curve fit technique, try to best-fit this wavefunction to the numerically obtained wavefunction data.
Step-6: Compare results obtained using different forms of trial wavefunctions with the numerical result obtained after solving schrodinger equation using FDM.

5 Analytic Trial wavefunction Calculations:

We will use Hydrogen atom and Harmonic oscillator wavefunction forms to model the wave functions and generate mass spectrum of the Charmonium S-states for Cornell potential. Other than hydrogen and harmonic oscillator models, a non standard wave function which resembles the blackbody curve is also used in the calculations. All calculations are done for ground state wavefunctions, for excited states we can proceed in the similar way.
We will be using the parameters -

FDM Code Parameters for $c\bar{c}$ Bound states	
Parameter	Parameter value
$r_{min}(GeV^{-1})$	$10^{-6}/0.1972$
$r_{max}(GeV^{-1})$	2.5/0.1972
C_0	2.8375
$\hbar$	1
c	1
N	1001
k	0.52
a (GeV^{-1})	2.34
mass (GeV)	1.84

The energy value for 1S state of $c\bar{c}$ system using numerical methods: 3.0950 GeV

5.1 Trial function 1

The first trial wavefunction is

$$\psi_1(r) = Ar^2 e^{-r/b} \tag{13}$$

where b is a constant and A is found using normalization, $A = \sqrt{\frac{4}{3b^5}}$.

The Hamiltonian obtained is:

$$\langle H \rangle = \frac{1}{6\mu b^2} + C_0 - \frac{k}{2b} + \frac{5b}{2a^2} \tag{14}$$

$b = 0.6869$ obtained from curve fit technique. The Ground state energy value is:$3.1609GeV$.

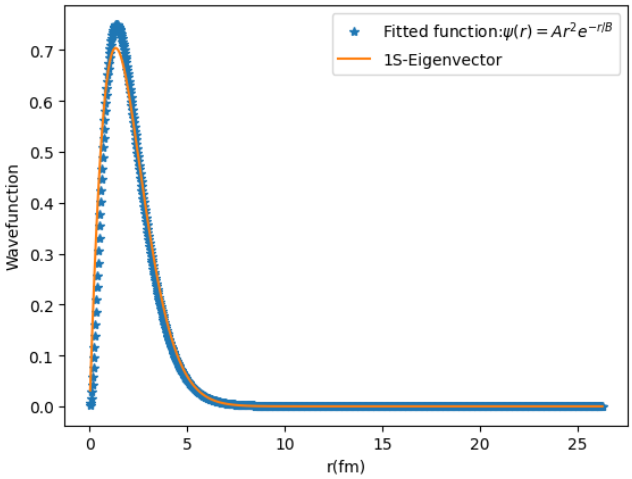

Figure 3: First Trial wavefunction versus the relative co-ordinate r

5.2 Trial function 2

The second trial wavefunction is

$$\psi_2(r) = Are^{-r/b} \tag{15}$$

where b is a constant and A is found using normalization:$A = \sqrt{\frac{4}{b^3}}$
The Hamiltonian obtained is:

$$\langle H \rangle = \frac{1}{2\mu b^2} + C_0 - \frac{k}{b} + \frac{3b}{2a^2} \tag{16}$$

$b = 1.13056$ obtained from curve fit technique. And, The Ground state energy values are:$3.1172GeV$.

5.3 Trial function 3

The third trial wavefunction is

$$\psi_3(r) = Are^{-br^2} \tag{17}$$

where b is a constant and A is found using normalization:$A = \sqrt{\frac{8b\sqrt{2b}}{\sqrt{\pi}}}$. The Hamiltonian obtained is:

$$\langle H \rangle = \frac{3b}{2\mu} + C_0 - \frac{2k\sqrt{2b}}{\sqrt{\pi}} + \frac{\sqrt{2}}{a^2\sqrt{\pi b}} \tag{18}$$

$b = 0.2099$ obtained from curve fit technique. And, The Ground state energy values are:$3.1515GeV$.

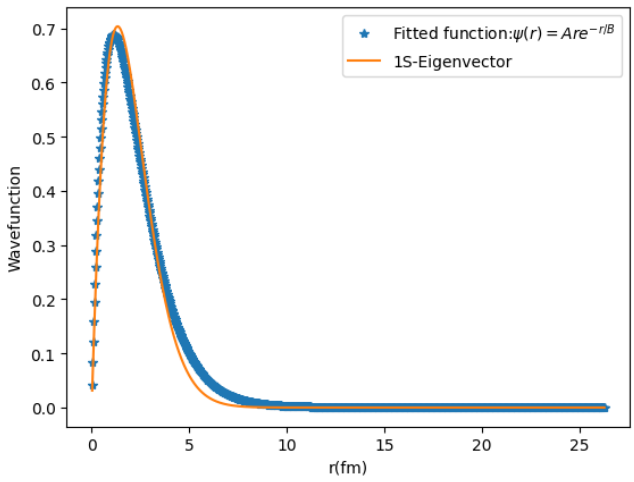

Figure 4: 2nd Trial wavefunction versus the relative co-ordinate r

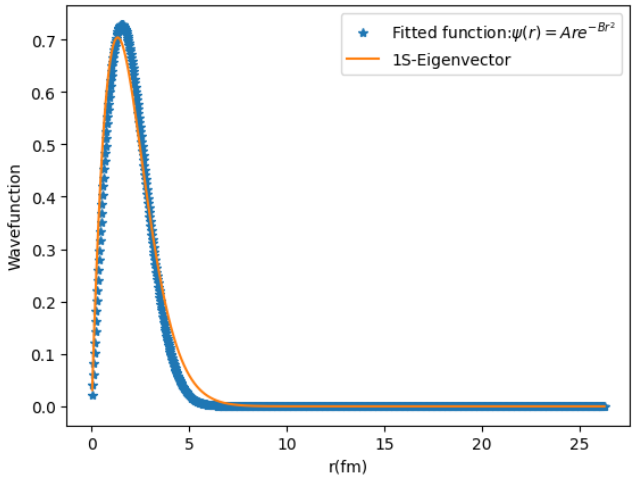

Figure 5: 3rd Trial wavefunction versus the relative co-ordinate r

6 Conclusion

- In similar way, we can estimate wavefunctions for excited states.
- Assumptions made in this calculation- Non-relativistic regime, SU(3) flavoured symmetry being conserved.
- We used simplified model, did not include spin information of quarks.
- Cornell model is just one of many models, we can compare results from different models to get accurate information about these bound states.
- The choice of N(total number of grid points) and grid size should be choosen carefully, because the size of H-matrix increases as $O(N^2)$.
- To check accuracy of our result need to compare the values of other physical quantities. (We also have some experimental data to compare with.)

Energy value (in GeV)comparion for 1S-state					
Physical quantity	Experimental data	From code	From ψ_1	From ψ_2	From ψ_3
Energy	3.095	3.095	3.1609	3.1172	3.1515

[2][1][3]

References

[1] E. Eichten et al. "Charmonium: Comparison with experiment". In: *Phys. Rev. D* 21 (1 Jan. 1980), pp. 203–233. DOI: 10.1103/PhysRevD.21.203. URL: https://link.aps.org/doi/10.1103/PhysRevD.21.203.

[2] E. Eichten et al. "Charmonium: The model". In: *Phys. Rev. D* 17 (11 June 1978), pp. 3090–3117. DOI: 10.1103/PhysRevD.17.3090. URL: https://link.aps.org/doi/10.1103/PhysRevD.17.3090.

[3] M.B. Voloshin. "Charmonium". In: *Progress in Particle and Nuclear Physics* 61.2 (2008), pp. 455–511. ISSN: 0146-6410. DOI: https://doi.org/10.1016/j.ppnp.2008.02.001. URL: https://www.sciencedirect.com/science/article/pii/S0146641008000239.