

Numerical Solutions to Charmonium Wavefunctions

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Physics Problem Solving Computing Project

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Introduction

Quarks are fundamental particles of the Standard Model of particle physics, most well-known for being the constituent particles of the proton and neutron. They **cannot exist as free particles**, and so must be studied as part of bound systems. They can form quark-antiquark states called quarkonium - these can be studied similarly to the Hydrogen atom. The charm-anticharm state is known as Charmonium, and this will be the focus of this study.

Theory

The Charmonium wavefunction comes through solving the 3D Schrodinger equation [1],

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

$$V(r) = -\frac{4\alpha_s}{3r} + \beta r. \quad (2)$$

Through separation of variables, $\psi = R_{nl}Y_l^m$, the radial wavefunction, $u_{nl} = rR_{nl}$, for each energy eigenvalue can be solved from a set of ODEs:

$$\frac{du_{nl}}{dr} = v_{nl} \quad (3)$$

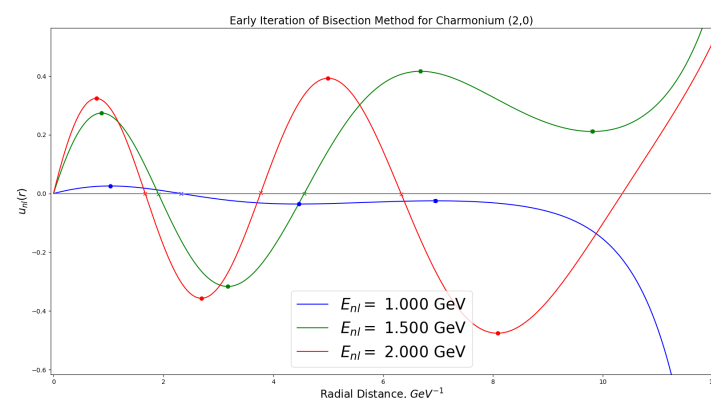
$$\frac{dv_{nl}}{dr} = \frac{l(l+1)}{r^2}u_{nl} - 2\mu[E_{nl} - V(r)]u_{nl} \quad (4)$$

Boundary conditions must be set as $r \rightarrow 0$. We set $u_{nl}(0) = 0$, and $\frac{du_{nl}}{dr} = 1$, ignoring normalisation until later. The program must start a small step away from the origin to compute non-zero solutions. The radial wavefunction must be normalised, such that

$$\int_0^\infty r^2 |R_{nl}|^2 dr = \int_0^\infty |u_{nl}|^2 dr = 1. \quad (5)$$

The Bisection Method

This method guess three energies, E_1, E_3 , and $E_2 = \frac{E_1 + E_3}{2}$ to find u_{nl} . Using `scipy.integrate.odeint`, (3) and (4) are solved for these energies and normalised using Simpson's method. Count the nodes and turning points for each function - if these differ between two solutions, E_{nl} lies somewhere between those energies.



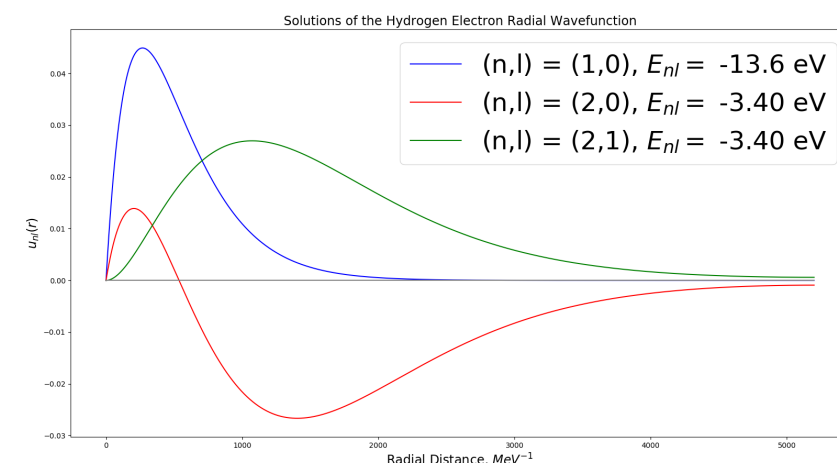
E_1 and E_3 are set to the two energies over the difference, and E_2 calculated again. We repeat this process until we find a correct u_{nl} , which has $(n-1)$ nodes and n turning points. The energy of this solution will be E_{nl} .

The Hydrogen Wavefunction

To check the program is functioning for a simpler model, we apply it to the Hydrogen electron. The solution is found in the same way, with some constant changes:

$$\frac{4\alpha_s}{3} \rightarrow \alpha = \frac{1}{137}, \beta \rightarrow 0, \mu \rightarrow m_e. \quad (6)$$

Due to l -independence of the Hydrogen energies, for $l \neq 0$ the number of nodes and turning points must be counted as $(n-l-1)$ and $(n-l)$ respectively. The program solved for $(n,l) = (1,0), (2,0), (2,1)$, with energies accurate to theory, and was then ready to move on to charmonium.



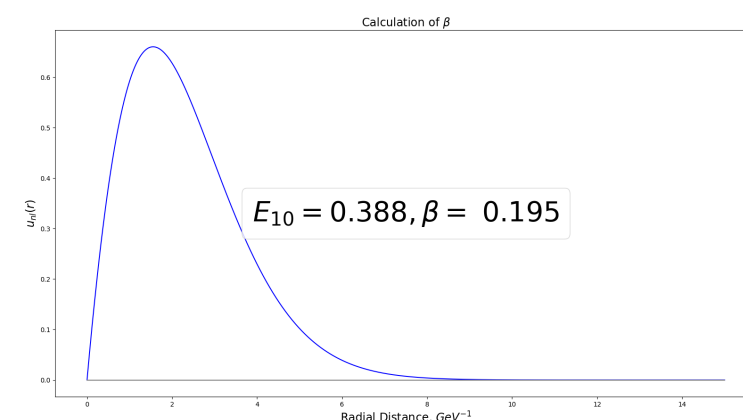
$$E_{10} = -13.6 \text{ eV} \quad E_{20} = -3.40 \text{ eV} \quad E_{21} = -3.40 \text{ eV} \quad (7)$$

Calculating β

To solve the Charmonium wavefunction for any energy level, β must first be known. The ground state energy is known through relation to the bound mass and charm quark mass:

$$M_{nl} = E_{nl} + 2m_c, \quad M_{nl} = 3.068 \text{ GeV}/c^2, \quad m_c = 1.34 \text{ GeV}/c^2 \quad (8)$$

The bisection method is performed over β with ground state energy a constant, and β 's value is found.



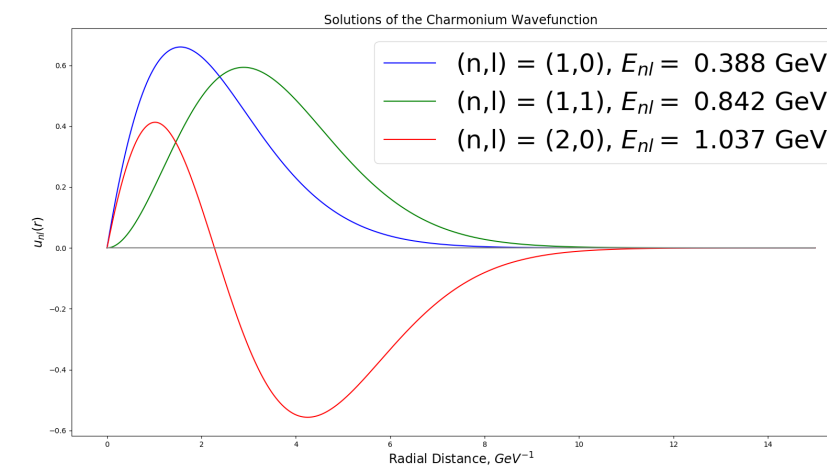
Finding the Charmonium Wavefunctions

With a known value of $\beta = 0.195$, we can proceed to solve the Charmonium wavefunction, with

$$\alpha_s = 0.4. \quad (9)$$

We can check that this value of β yields the correct energy for the ground state of Charmonium, and then apply it to the (1,1) and (2,0) states as well to find their energies. Now using the same method as before, having confirmed the functionality of the program on hydrogen, the solutions of the radial wavefunction are solved.

Without examining the results of computations, it can be seen that the nodes and turning points cannot depend on the value of l as seen in Hydrogen, if the (1,1) state is to have a non-zero wavefunction. So we go back to the original $(n-1)$ nodes and n turning points method original stated for the bisection method.



$$E_{10} = 0.388 \text{ GeV} \quad E_{11} = 0.842 \text{ GeV} \quad E_{20} = 1.037 \text{ GeV} \quad (10)$$

From these results, it is obvious that, unlike the hydrogen atom, the energy of the system depends on both the n and l quantum numbers, instead of just the n .

These energies can then be checked against theory by converting to bound masses through (8) and compared to values for each state given in [2].

The ground state bound mass and charm masses were given values to be used at the beginning of this project, meaning that these differ from the values in [2]. The (1,1) and (2,0) states calculated have energies broadly accurate with the states given in [2] - the difference comes from hyperfine splitting which has not yet been considered, but the average energy of the states roughly agrees with expectations.

References

- [1] J. F. Donoghue and B.R Holsten, E. Golowich. *Dynamics Of The Standard Model*. Cambridge University Press, 2014.
- [2] C. Amsler et al [Particle Data Group]. Review of particle physics 2008. <http://pdg.lbl.gov/>, February 2019.

Outlook

Now with a functioning program, further extensions to be applied to the study are considered. The energies of the states were seen to be somewhat inaccurate to the known measurements, at least partially due to the hyperfine spin-spin interaction causing a splitting in the energy. This splitting is

$$\Delta(n^3S_1 - n_1S_0) = \frac{8\alpha_s}{9m_q^2} |R_{nl}(0)|^2, \quad (11)$$

so the energies calculated in this project will be the average of the two hyperfine energies, and these values can be found using this splitting formula. The splitting depends on the value of the wavefunction at $r = 0$, which is

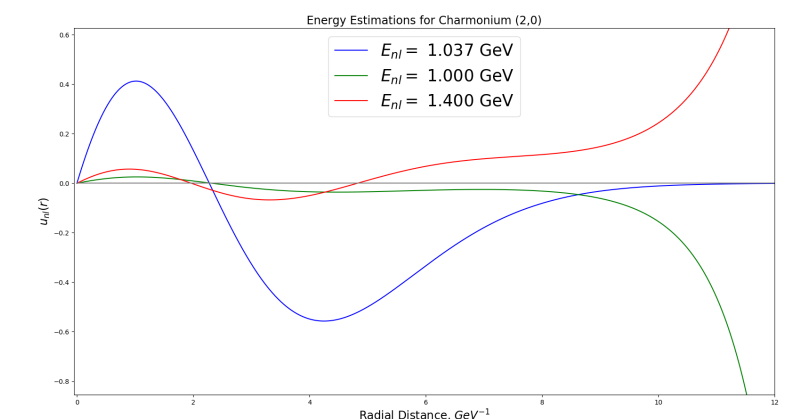
$$\lim_{r \rightarrow 0} R_{nl}(r) = \lim_{r \rightarrow 0} \frac{u_{nl}(r)}{r} = \frac{du_{nl}(0)}{dr}. \quad (12)$$

Further from this, the transition rates between the higher and lower hyperfine energies can be studied.

Faults of the Method

Choice of Energy: If the energy eigenvalue does not lie within the range of the initial guess for energy, then the program will not be able to solve for it, so using this program requires some vague knowledge of where the energy will lie.

Tolerances: The program requires fine tuning of tolerance levels testing for the convergence of the energies. If the tolerance is too high or too low, the energy will be slightly too high or low and the function will diverge to infinity.



Initial Values: The program can only be as accurate as the initial values put in. If the values of mass, and α_s , they will result in different end results for energy. Thus, comparison to known values can only be valid if these parameters are approximately similar.