Investigating the Mass Spectra of the B_C Meson

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This program uses the work of Erwin Schrödinger to investigate the mass of the B_{C} meson's bound states. It involves numerically solving the Schrödinger equation using the bisection algorithm. The mass of B_{c} (2S) state was found to be 6.79 \pm 0.09 GeV which is consistent with several literature values including that measured by the Particle Data Group. In addition, multiple other mass states are also predicted using the potential model found. The report explores the errors involved with these calculations and makes suggestions for improvement of the method.

1. Introduction

In the macroscopic world all objects have a defined position, calculable with classical mechanics. As we delve to the atomic scale it is not possible to measure exactly where a particle is and so we must use quantum mechanics. Developed throughout the beginning of the 20th century quantum mechanics became one of the cornerstones of modern physics, this program specifically makes use of the Schrödinger equation which is one of the most important equations in the area. First formulated in 1926 by Erwin Schrödinger the Schrödinger equation expresses the position of a particle as a function of probability using a representative wavefunction.

In a quarkonium system a quark and an anti-quark are bonded together into bound states by the strong force to make a Meson, the strong force was first predicted in 1934 by Yukawa Hideki [1]. As the bottom and charm quarks are heavy in mass compared their binding energy, we can make use of non-relativistic quantum mechanics to investigate their bound states.



Figure 1: Illustrations of the charmonium system (left) and the B_{C} meson (right).

As the quarkonium behaves according to quantum mechanics its wavefunction must obey the Schrödinger equation [1]:

$$\frac{\hbar^2}{2\mu}\nabla^2\psi + V(r)\psi = E_{n,l}\psi \tag{1}$$

Where ψ is the wavefunction, \hbar is the reduced Plancks constant, μ is the reduced mass of the system, V(r) is the potential, r is the separation between the quarks and $E_{n,l}$ is the binding energy according to the principal quantum number, n and angular momentum, l. The reduced mass is given by:

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \tag{2}$$

Where m_1 and m_2 are the masses of the quarks involved.

In order to obtain the energy of the bound states we must first solve the Schrödinger equation by splitting the wavefunction into it's radial and harmonic components, $R_{n,l}(r)$ and $Y_{lm}(\theta,\phi)$ respectively such that:

$$\psi = R_{n,l}(r)Y_{lm}(\theta,\phi) \tag{3}$$

Where m is the spin quantum number. Spin can be considered of interest in quarkonium using hyperfine splitting but for the purpose of this report we will only investigate spin average energies and masses.

If we write, $u_{n,l}(r) = rR_{nl}(r)$ then the Schrödinger equation can be rewritten as the 2^{nd} order differential equation:

$$\frac{d^2 u_{n,l}}{dr^2} - \frac{l(l+1)}{r^2} u_{n,l} + 2\mu \left(E_{n,l} - V(r) \right) u_{n,l} \quad (4)$$

In order to solve equation (4) numerically we first split it into two coupled first order equations and apply several boundary conditions. In addition, all $u_{n,l}$ are normalised to unity such that:

$$\int_0^\infty \left| u_{n,l} \right|^2 = 1 \tag{5}$$

The potential, V(r) describes the quantum chromodynamic behaviour (QCD) between the quarks. Currently there is no mathematical technique which describes QCD perfectly and can predict the bound states of mesons so instead we use a potential as an approximation. The potential used in this program is the Cornell potential [2]:

$$V(r) = \beta r - \frac{4\alpha}{3r} \tag{6}$$

Where the βr term represents a confining potential for the quarks which stops the quarks existing as free particles and the $\frac{\alpha}{r}$ term represents one gluon exchange at short distance.

Predicted by the standard model of particle physics and first observed in 1998 by Collider Detector at Fermilab (CDF) collaboration at the Fermilab Tevatron [3], the $B_{\rm C}$ meson consists of a bottom quark bonded to an anti-charm quark as shown in figure (1). In this program we specifically investigate the masses of the $B_{\rm C}$ meson's states which we will denote mass states for ease of writing. The motivation for doing this is so far only two states, the 1S and 2S have been observed so we wish to build a model to predict further states. We note that 1S and 2S correspond to (n,l), (1,0) and (2,0) respectively.

At this point it is helpful to note that we are working in natural units such that $\hbar = c$ and therefore the mass and energy of the mesons are related to each other by the equation below:

$$M_{n,l} = m_1 + m_2 + E_{n,l} (7)$$

Where $M_{n,l}$ is the mass of the state according to the quantum numbers n and l.

2. Theory

If the parameters, α and β in the Cornell potential and the binding energy of the state are known, it is easy to solve equation (4) numerically and calculate the wavefunction. However, if the binding energy is slightly incorrect then the wavefunction will exhibit a different number of turning points and nodes as depicted in figure (2).

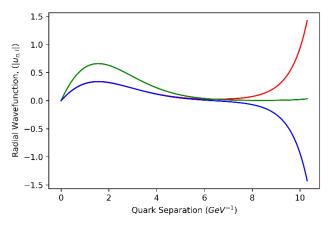


Figure 2: The wavefunction of (1,0) Charmonium state calculated using different binding energies. The red, blue and green lines show the wavefunction for binding energies of 0.387 GeV, 0.389 GeV and 0.388 GeV respectively. The green line shows the correct energy of the (1,0) state.

Examining figure 2 the number of nodes and turning points vary for each energy calculated. When the test energy is too high the number of nodes is too high. When the test energy is too low the number of nodes will either be too low or correct and the number of turning points will be too high. We used this behaviour of the wavefunction to iterate towards a bound solution using the bisection algorithm [4].

To calculate a bound energy state using the bisection algorithm we first take two guess energies in the which we know (or hypothesise) that the solution lies within. We define the lower guess energy as E_1 , the upper guess energy as E_3 and the midpoint of these two guesses as E_2 such that [4]:

$$E_{2} = \frac{1}{2} (E_1 + E_3) \tag{8}$$

We calculate the number of nodes and turning points at each energy E_1 , E_2 and E_3 . If the number of nodes and turning points changes between E_1 and E_2 we redefine E_3

as E_2 and recalculate a new E_2 using equation (7). Similarly, if the number of nodes and turning points changes between E_2 and E_3 we redefine E_1 as E_2 and recalculate a new E_2 .

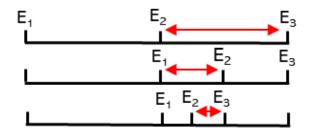


Figure 3: A diagram showing three iterations of the bisection algorithm.

In this program the bisection algorithm was run 100 times, which takes around half a second to compute. Experimenting with the algorithm it was discovered that a reasonable approximation could be achieved in 10 iterations however 100 was chosen to be certain that the highest possible accuracy was chosen.

3. Method

In order to calculate the energy levels of the B_C meson we first formed a potential by calculating both constants α for the B_C meson and β . As the B_C meson is a relatively unseen particle, the strong coupling constant α_B in the B_C meson energy range, (which can vary significantly over different energy ranges) is not well known and instead we calculated its potential using the better documented, Charmonium (charm quark bonded to an anti-charm quark) as an intermediate step.

First, we set α to a value from literature in the Charmonium energy range and call it α_C . Using the ground state mass, $m_{c\bar{c}}$ of the Charmonium obtained from literature we used the bisection algorithm to calculate β , which went into the potential for the B_C meson. Secondly, we fitted the potential to the energy range of the B_C meson. We discarded the literature value of α_C for the Charmonium and used the ground state energy of the B_C meson taken from literature together with the bisection method again to calculate α_B for the B_C meson.

Having calculated α_B and β we then calculated the 1S, 1P, 1D, 2S, 2P and 3S energy states for the B_C meson. Due to its iteration method, the bisection algorithm can only calculate one state at a time over a given energy range. To overcome this issue, we know there are multiple energy levels between approximately 6.1GeV and 7.5GeV so we split this large energy range up into 50 segments and ran the bisection algorithm in each of them, if a bound state was found then it would be reported on, and the probability density function plotted to visually confirm it was indeed a bound energy state.

50 segments were chosen as this balanced the need of computation time being low enough and accuracy being high enough to find all the bound energy states. The bound energy states and probability density functions found were compared with literature values in order to identify which state had most likely been computed. As n and l increase the difference in energy between the states decreases and it becomes more difficult to identify which reported energy state had been calculated. For this reason, only the 1S, 1P, 1D, 2S, 2P and 3S energy states were reported on as these were the only states where it was obvious which one had been calculated. Using equation (8) the energy states were converted to masses as this is the most common format to compare to literature values.

To achieve a higher speed of computation the number of iterations run initially in the 50 segments was set to 10 instead of 100. Once that had been completed the probability density function of any bound solution found was computed to 100 iterations. Assuming 6 bound solutions were found for a specific 1 this resulted in 1100 total iterations instead of 5000, meaning the program takes approximately 5.5s to complete instead of 30s with little to no loss of accuracy.

Due to the complex nature of the coupled differential equations and the multiple calculations necessary, the associated error for each state was calculated using the functional approach [14].

3. Results

The program successfully calculated the mass of the $B_{\rm C}$ meson states correct to 2 or 3 significant figures with an associated error. The results are displayed in a tabular format as well as an intuitive mass state diagram. The parameters used in the two separate potentials are shown as well as the initial constants used.

| Constant Used | Value (GeV) | |
|-------------------------------------|-----------------------------|--|
| Mass of charm quark, m _c | 1.275 ± 0.025 [5] | |
| Mass of bottom quark, mc | 4.65 ± 0.04 [5] | |
| Mass of B _C meson ground | 6.2749 ± 0.0008 [6] | |
| state, m_{1S} | | |
| Mass of charmonium | 3.096900 ± 0.000006 [6] | |
| ground state, $m_{c\bar{c}}$ | | |

Table 1: All initial constants used in the program.

| α_{c} | 0.174 ± 0.012 [7] | 0.1179 ± 0.010 [8] |
|-----------------------|-----------------------|------------------------|
| α_{B} | 0.25 ± 0.05 | 0.23 ± 0.06 |
| ß | 0.17 ± 0.02 | 0.16 ± 0.02 |

Table 2: The parameters for the Cornell potential of the B_C meson using two different starting $\alpha_C's$. The parameters are dimensionless.

| State | $0.174 \pm 0.012[7]$ | $0.1179 \pm 0.010[8]$ |
|-------|----------------------|-----------------------|
| 1S | 6.27 ± 0.08 | 6.27 ± 0.08 |
| 1P | 6.62 ± 0.08 | 6.59 ± 0.08 |
| 1D | 6.88 ± 0.09 | 6.82 ± 0.09 |
| 2S | 6.79 ± 0.09 | 6.74 ± 0.09 |
| 2P | 7.0 ± 0.1 | 6.96 ± 0.09 |
| 3S | 7.2 ± 0.1 | 7.1 ± 0.1 |

Table 3: Calculated mass states using the Cornell potential for the B_C meson using two different starting $\alpha_C's$. The masses are shown in GeV.

| State | [9] | [6] | [10] | [11] |
|------------|-------|---------------------|-------|-------|
| 1S | 6.327 | 6.2749 ± 0.0008 | 6.305 | 6.274 |
| 1P | 6.651 | | 6.741 | 6.711 |
| 1D | 6.845 | | | |
| 2S | 6.744 | 6.8712 ± 0.001 | 6.871 | 6.872 |
| 2P | 6.933 | | 7.145 | 7.103 |
| 3 S | 7.016 | | 7.261 | 7.179 |

Table 4: A variety of spin-averaged mass state literature values for the $B_{\mathbb{C}}$ meson. The masses are shown in GeV. Take note that [9], [10] and [11] are calculated from computer simulations similar to this program. Where the hyperfine splitting has been used in the literature, we display only the spin average value for that state. Only 1S [6] and 2S [6] have been detected experimentally.

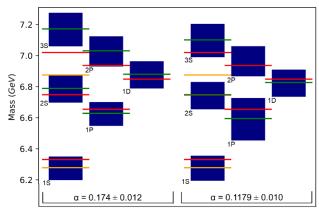


Figure 4: Mass state diagram showing the mass states of the B_C Meson. The energies calculated from the program are shown as a green line with a navy-blue error bar. The masses of [9] and [6] are shown in red and orange respectively without error bars. [10] and [11] are not shown to not overcrowd the diagram. On the left side are energies calculated with $\alpha_C = 0.174 \pm 0.012$ and on the right are energies calculated with $\alpha_C = 0.01179 \pm 0.010$.

In addition to the masses, the program also calculated graphs of the radial probability density function. Only the 1S and 2S states are shown to not overcrowd the graph.

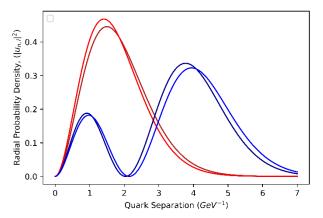


Figure 5: Probability density functions of the 1S and 2S states of both α calculations. The red plots show the 1S state and the blue plots show the 2S state. The darker lines

show the $\alpha_C = 0.174$ model and the lighter lines the $\alpha_C = 0.1179$.

4. Discussion

In this section we will evaluate the fit of the two models to literature values, investigate the difference the different values of charmonium α_c have on the result, explore which are the dominant errors and make a judgement as to whether the fit resembles QCD enough such that we can predict higher energy levels. In addition, we will explore improvements to the current method, what other methods could have been used to perform this experiment as well topics for further study. For ease of writing, we will refer to the $\alpha_C = 0.174 \pm 0.012$ model as model 1 and the $\alpha_C = 0.179 \pm 0.010$ model as model 2.

To ascertain how well the potential models follow QCD we must compare the calculated data to the Particle Data Group world average [6]. This data is the average of all observations of the B_C meson using particle detectors and is therefore the most authentic as it is not based on any theoretical models and instead only what has been detected experimentally. One experiment which formed this average was a proton-proton collision; measured with the Compact Muon Solenoid [12] it reconstructed the mass spectrum from the $B_{\mathcal{C}}^+$ decay to J/ψ (charmonium ground state) and π^+ (positive Pion). As both models 1 and 2 are calibrated using the 1S [6] value we can only compare to the 2S [6] state. The 2S value for model 1 of 6.79 ± 0.09 GeV is consistent with the value of $6.8712 \pm$ 0.001 GeV [6] however the model 2 value of 6.74 ± 0.09 GeV is not. The error in model 2 would need to be 0.04 larger to confidently identify consistency.

Both models use the same equations, algorithm and physics. The only difference is the first step of the method where we used two separate values of the strong coupling constant, α_c . Ideally, we would not need this step of the method but unfortunately a value of the strong coupling constant at the B_C meson energy scale was not found in literature. On the contrary the charmonium system has multiple literature values available, the only problem is that the values vary significantly due to the way they are measured or predicted through theory. Model 1's value [7] was measured by 1P-1S splitting in the charmonium system and uses the \overline{MS} , modified minimal subtraction scheme. The negatives of this value are that it is relatively outdated however it is measured at the correct mass scale and produced an accurate result. Model 2 uses the PDG world average value [8], this value was obtained by averaging work on several theoretical QCD lattices and unlike model 1's value is based on theory alone. The negatives of this value are it is measured at the Z-boson mass scale ($\approx 80 \text{ GeV}$) which is significantly larger than that of the B_C meson (1S \approx 6.3 GeV). Calculations were also performed on a value of $\alpha_C = 0.4$ (no associated error) [13] but the results obtained with this were not representative of the B_C meson with some mass states missing and others nowhere near literature values obtained. For this reason, the results were not reported but it is certainly advantageous to know that this value didn't work.

Considering errors, in addition to the error on α_C , errors also arose from the mass of the charm quark, m_c mass of the bottom quark, m_b and the ground mass state of the charmonium, $m_{c\bar{c}}$ and the B_C meson, m_{1S} which were used to calibrate the potential. We say the ground mass state values were used to calibrate the potential because it was from using those states converted to a value of energy that α_B and β were found. The value of α_C was most variable in literature so we repeated the program multiple times with the three different values described in the previous paragraph. Looking at the calculation of B the dominant error came from mc and for both models less than 2% of the error came from the value for α_c . This is most likely due to the way m_c features in the reduced mass equation (2) and therefore the differential equation (4). It could also be because the relative error of m_c is 2.0% instead of 0.85% for the α_C but this would have less of an impact on the result. The ground state mass of the charmonium, $m_{c\bar{c}}$ had a negligible error.

When calculating α_B for the B_C meson potential the dominant errors for both models are similar to calculating B with the mass of the charm quark m_c causing a large error although higher errors were caused by the mass of the bottom quark, m_b , and the value of β calculated in step one. The percentage of error caused by each component in model 1 was 66% for m_b , 18% for m_c , 16% for β . For model 2 the equivalent statistics were 49% for m_b , 15% for m_c , 37% for β . The 1S mass state of the B_C meson, m_{1S} caused a negligible error for both models. These values are interesting as they suggest that a large portion of the error is coming from the masses of the quarks. This is a potential weakness of the method when you can consider how many times the mass of the quarks are used. This is because the functional method [14] is used for calculating errors at each step.

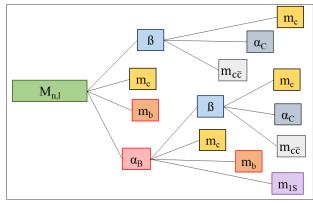


Figure 6: Error propagation diagram: Shows the contribution of errors from each value. The direction of calculation is from right to left.

When we consider the calculation of a given mass state, $M_{n,l}$ some input values are used multiple times. The important ones which are dominant in error analysis are m_c which is used four times and m_b and β which are both used twice. As these values dominate the error at each stage, having them included multiple times could mean the mass error bar is larger than it should be. Looking at the error percentage statistics for the 2S state of B_C meson; for model 1 63% of the error is due to β , 12% due to α_B , 20%

due to m_b and 5% due to m_c . For model 2 the values are of similar magnitudes. With this data and assuming that α_C and all ground mass states are negligible, 73% of the error can be attributed to m_c and 27% of the error to the m_b and hence overall the error on m_c is dominating. This could be because the relative error on m_c of 2.0% is much greater than m_b of 0.65% which makes sense as the ratios between the two are similar. On the contrary it could be caused by the fact m_c was used four times instead of only two for m_b . There is not enough statistical evidence to say either explanation is statistically correct and most likely it is a bit of both ideas which is causing m_c to dominate. We must also remember there is an error associated with converting energy solved by the program to the mass which was included in the functional error analysis.

Due to the way the bisection algorithm works with its iteration the current program only allows one parameter (either α or β) or one energy to be calculated per run. As we have discussed this this means running the program three times to obtain the mass states but consequently this dramatically increases the overall error of the final solution. One simple way to reduce the number of calculations without changing the method would be to measure (or predict) a value α_B in the B_c meson mass range. This would mean only ß would need to be calculated before the mass states. Alternatively, we do not use the bisection algorithm at all and instead use a fitting technique that simultaneously fits the potential's parameters to the B_C mesons 1S and 2S states simultaneously. This could be done by trial and error which may take some time to compute but there will exist a value of α and β which produce the correct values of 1S and 2S to the correct accuracy. Knowing the rough range that both values are in the computer could first attempt all combinations to 1 significant figure, then the best combination would move to 2 significant figures knowing the first significant figure and then 3 significant figures. This would obviously take a little while as many combinations would need to be tried into order to obtain the desired accuracy.

Another way to potentially increase the accuracy and precision of the program would be to use a different potential. The Cornell potential was chosen because it is simple and accurate. There are many more complex potentials available such as the Richardson potential [2] which in addition to the Cornell potential incorporates the asymptotic freedom property for the strong interaction coupling. Better potentials will work to a degree but unfortunately, QCD is more complicated than can be represented by a potential function. Other methods to capture more of QCD's properties include effective field theories or the lattice-gauge theory.

Having deduced that model 1 is consistent with the 2S value from [6] we will now statistically explore how well the result agrees with the work on other potentials. Literature [9] uses the standard Cornell potential to calculate the energy levels of the $B_{\rm C}$ meson. If we calculate the residual of each literature value [9] compared to the model, divide by the individual error (of the model)

and then average it we have a numerical measure that we can use to judge the fit. For model 1 we obtain an average of 0.71 error bars which shows a good fit, there are no outliers and individually all values sit within their respective error bars apart from the 3S state. Considering model 2 this statistic is even lower at 0.46 error bars suggesting an even better fit. This can be visually appreciated by looking at the mass state diagram in figure 4

Unfortunately, if the same error analysis is performed for literature [10] there is far less agreement. Model 1 has an average of exactly 1.0 error bars showing loose agreement. Model 2 shows even less agreement, with an average of 1.4 error bars. This is likely due to the fact the potentials used are different. Literature [10] uses a relativized quark model instead of the Cornell potential. The potential is based on the Cornell potential but due to relativistic effects, the potential is also momentum dependent as well as positionally dependent. This results in the potential being able to approximate many other interactions in addition to those approximated by the Cornell potential, these include colour contact interaction, colour tensor interaction, spin orbit interaction and colour magnetic piece. This is obviously significantly harder to implement into a program however the result is a refined potential more representative of QCD.

Literature [11] uses the Trigonometric Rosen-Morse Potential. It makes use of the generalised fractional derivative of the Schrödinger equation which surprisingly can be solved analytically to obtain an equation for the mass states. Comparing to literature [6] the 1S and 2S mass states agree to a precision of 4 significant figures suggesting the other states predicted are likely to be accurate if they are discovered. Model 1 has good agreement with an average agreement of 0.60 error bars however model 2 does not agree with 1.03 error bars.

Model 1 is the most consistent with the literature models so we can confidently predict the mass states will lie in this range. However we should consider the reason behind this, it is either the value of $\alpha_{\rm c}$ is the most accurate and has produced an accurate model of the mass states or it is that an overestimation of the error bars has made the model look consistent with the literature models. To evaluate this, we shall directly compare the central values of model 1 and 2 to each of the literature models using percentage difference and then compute an average of this for each model. For the purpose of this report a good agreement is anything less than 1%.

For model 1 compared to [9], [6], [10], [11] an average percentage difference of 0.97%, 0.63%, 1.3% and 0.76% was observed respectively. For model 2 a percentage difference of 0.62%, 0.94%, 1.88% and 1.35% was observed respectively. As the average of those numbers is lower for model 1 it again shows that model 1 is more agreeable with the literature values than model 2 further supporting the argument that model 1 is more accurate.

Although model 1 is believed to be more accurate we must recognise that these arguments using percentage

difference and error bar analysis are relatively weak compared to a true statistic such as the χ^2 value or the Durban Watson statistic. Unfortunately, due to the nature of this experiment we not do not have multiple samples to compare because computers do not make random errors. As an area for further study, we could investigate more values of α_c and compute the χ^2 value between multiple models of α_c to evaluate the effectiveness of the Cornell potential compared to another potential such as the Richardson or Martin Power-Law potential.

Finally, we will analyse the graphs of the radial probability density functions. Looking at figure (5) we can visually see the discrepancy between model 1 shown by the darker lines and model 2 shown by the lighter lines. Specifically looking at the 1S state shown by the red lines model 1 appears to have a broader and lower peak compared to model 2. On the contrary looking at the 2S state this trend is the other way around with model 2 having the broader peak and generally lagging model 1. Both models start and end in the same place as would be expected from the boundary conditions. Despite very different numbers for α_C they seem to have relatively little effect on the graphical view of the radial probability density function. In this sense the choice of parameter seems less important, and we conclude the overarching physics is mostly controlled by the physics of the Schrödinger equation. This makes sense as although the α_c values are almost a factor of 1.5 different to each other the energy levels produced by the program are mostly consistent compared to each other to 2 significant figures.

5. Conclusions

In conclusion, model 1 with a value of $\alpha_C = 0.174 \pm 0.012$ was the most accurate at describing the mass states. The value of 6.79 ± 0.09 GeV for the 2S mass state was the most consistent with the literature value of 6.8712 ± 0.001 GeV [6] and agreed with the other literature models [9],[10], and [11] the most. On the contrary model 2's value for the 2S mass state of 6.74 ± 0.09 GeV was not consistent with literature [6] although it was less than half an error bar away from being consistent. The most likely reason model 1 was the most accurate was because the value of α_C used for the charmonium step was measured in the correct energy range of the charmonium. The value of α_C for model 2 was measured in the z-boson energy range which is at an energy significantly higher that of the charmonium. Ultimately though looking at the mass state diagram in figure (4) both mass spectra look very similar and so although the starting constant of α_C is important to set correctly at the beginning it is only a small part of the representative potential. We conclude the overarching physics is controlled mostly by the Schrödinger equation.

Considering the errors in this program, dominant errors came arose from the mass of the quarks with 73% due to m_c and 27% due to m_b . Surprisingly a negligible amount of error was due to the ground energy state of the charmonium and the B_C meson 1S state. The reason the mass of the quarks were dominant was because the program reused their values multiple times due to the

intermediate charmonium step. In addition, the mass of the quarks had a large relative error.

If this program was completed again there are several changes we would make to improve the method. Firstly, we would use a different potential model, one that is more complex and embodies more QCD behaviour such as the Richardson potential. Secondly, we would make use of a numerical trial and error fitting technique to fit any parameters of the new potential model to the known PDG world average values [6] of the 1S and 2S states. This would ensure the potential could be calibrated correctly and would allow avoidance of the intermediate charmonium step which greatly increased the overall error of the program. Thirdly we would set the experiment up in such a way so we can use other statistical techniques such as χ^2 analysis and statistical techniques as purely comparing whether individual values are consistent and using error bar analysis is not as robust.

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Error Appendix

1. Functional approach to Error Analysis

The functional approach [14] was used to calculate the error of α_B , β and all the mass states, $M_{n,l}$. For each input constant, A with an error, ϵ the functional error is calculated using the following equation:

$$\epsilon = f(\bar{A} + \epsilon) - f(\bar{A}) \tag{9}$$

Where \bar{A} is the mean value of the constant. f(x) represents running the program once with inputs x.

For example: the error on the mass state, $M_{n,l}$ contained error from α_C , β , m_c and m_b so the following calculations were made:

$$\begin{split} \epsilon_{\alpha_c} &= \left| f\left(\overline{M_{n.l}} + \epsilon_{\alpha_c}\right) - f\left(\overline{M_{n.l}}\right) \right| \\ \epsilon_{m_c} &= \left| f\left(\overline{M_{n.l}} + \epsilon_{m_c}\right) - f\left(\overline{M_{n.l}}\right) \right| \\ \epsilon_{m_b} &= \left| f\left(\overline{M_{n.l}} + \epsilon_{m_b}\right) - f\left(\overline{M_{n.l}}\right) \right| \\ \epsilon_{\mathfrak{B}} &= \left| f\left(\overline{M_{n.l}} + \epsilon_{\mathfrak{B}}\right) - f\left(\overline{M_{n.l}}\right) \right| \end{split}$$

The total error $\epsilon_{M_{n,l}}$ for $M_{n,l}$ was then calculated by adding each of the above in quadrature using the following equation:

$$\epsilon_{M_{n,l}} = \sqrt{\epsilon_{\alpha_c}^2 + \epsilon_{m_c}^2 + \epsilon_{m_b}^2 + \epsilon_{\S}^2}$$
 (10)

Similar calculations were performed for the error on α_{B} and ß.

2. Relative Error

Relative error, ϵ_{rel} [14] is calculated using the following equation:

$$\epsilon_{rel} = \frac{\epsilon_x}{x} \tag{11}$$

Where ϵ_x is the absolute error in the variable x. It is sometimes expressed as a percentage in the report.

3. Percentage of Error

Percentage of error κ_x , attributable to a particular variable, x is calculated using the following equation:

$$\kappa_{x} = 100 \left(\frac{\epsilon_{x}^{2}}{\epsilon_{tot}^{2}} \right) \tag{12}$$

Where ϵ_{tot} is the total error attributable to all variables added in quadrature.

If a particular variable is used more than once, then the total error attributable to that variable in the final answer can be calculated by simple multiplication techniques. For example, the percentage of error due to the mass of the bottom quark, κ_{m_b} in B_C 2S state was calculated using the following equation:

$$\kappa_{2S \leftarrow m_h} = \kappa_{2S \leftarrow m_h} + \left(\kappa_{\alpha_R \leftarrow m_h} \kappa_{2S \leftarrow \alpha_R}\right) \tag{13}$$

Where $\kappa_{2S \leftarrow m_b}$ is the percentage of error in $M_{n,l}$ due to m_b , $\kappa_{\alpha_{\mathbb{R}} \leftarrow m_b}$ is the percentage of error in $\alpha_{\mathbb{R}}$ due to the mass of the bottom quark and $\kappa_{2S \leftarrow \alpha_{\mathbb{R}}}$.

4. Error Bar Analysis

The average error bar size, μ is calculated by the following equation:

$$\mu = \frac{1}{N} \sum_{n=1}^{N} \frac{C_n - L_n}{\epsilon_n} \tag{14}$$

Where N is the number of mass states, C_n is the nth calculated value from the model, L_n is the nth literature value and ϵ_n is the nth error bar

Scientific Summary for a General Audience

In the macroscopic world we can measure the force, distance and speed between two objects with ease. When we move to the scale of atoms this is not possible anymore and so we must use the theory of quantum mechanics which describes how particles move and behave at the atomic scale. One of the particles at the atomic scale is the meson, it is made of two even smaller particles called quarks. The quarks are held together by an invisible force called the strong force which is similar to the electromagnetic force but is much stronger and acts only over an atomic distance.

Using an equation called the Schrödinger equation, quantum mechanics describes the likelihood of where a particle may be found at any time. In this program we solve the Schrödinger equation for a meson called the $B_{\rm C}$ meson, which is made of two types of quarks called the bottom and charm quarks. The strong force holds the quarks at certain separations from each other known as bound states. We make use of the calculation power of the computer and a special iteration technique known as the bisection algorithm to solve these states and the energies that hold them together.