Bottomonium hyperfine splittings from lattice NRQCD including radiative and relativistic corrections

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(Dated: May 22, 2014)

We present a calculation of the hyperfine splittings in bottomonium using lattice Nonrelativistic QCD. The calculation includes spin-dependent relativistic corrections through $\mathcal{O}(v^5)$, radiative corrections to the leading spin-magnetic coupling and, for the first time, non-perturbative 4-quark interactions which enter at $\alpha_s^2 v^4$. We also include the effect of $u, d, s$ and $c$ quark vacuum polarisation. Our result for the $1S$ hyperfine splitting is $M_\Upsilon(1S) - M_{\eta_b}(1S) = 62.8(6.7)$ MeV. We find the ratio of $2S$ to $1S$ hyperfine splittings $(M_\Upsilon(2S) - M_{\eta_b}(2S))/ (M_\Upsilon(1S) - M_{\eta_b}(1S)) = 0.425(25)$.

I. INTRODUCTION

The energy splittings between the vector and pseudoscalar bottomonium states have, until recently, proved difficult for both experimentalists and theorists. Experimentally, the $\eta_b(1S)$ was only discovered in $\Upsilon$ radiative decays in 2008 by Babar [1], and subsequent results have led to a fairly wide error being placed on the PDG average [2,3]. The $2S$ state has recently been observed by two groups, Belle [4] and Dobbs et al. [5] using CLEO data, but the results differ significantly. Belle finds a $2S$ hyperfine splitting of $24.3^{+4.6}_{-4.5}$ MeV and Dobbs et al. have $48.7 \pm 3.1$ MeV. These difficulties are in contrast to the vector particle $\Upsilon$ which was found in 1977 [7] and whose mass is now known to sub-MeV precision.

On the theory side, predictions of the hyperfine splittings generally suffer from large systematic errors. Potential model estimates quoted in the Quarkonium Working Group review [8] range from 46-87 MeV for the $1S$ splitting [9,10], with systematic errors that are hard to quantify. Next-to-leading order continuum perturbation theory gives $41(14)$ MeV [11]. First principle lattice QCD calculations offer the prospect of much more accurate results but there too control of systematic errors (as opposed to statistical errors) is the key issue. The most successful approaches to date have used an effective field theory for the $b$ quark such as nonrelativistic QCD (NRQCD). The hyperfine splitting is generated by an operator in the Lagrangian that appears first at $\mathcal{O}(v^3)$ in a power-counting in terms of the velocity of the $b$-quark. Including only the leading term, as was done in the first calculations, gives the penalty of a large systematic error from missing radiative corrections to the leading term and missing higher order terms. These systematic errors would be avoided by treating the $b$ quark as a relativistic quark but in that case significant discretisation errors appear instead. It is now becoming possible to handle $b$ quarks relativistically with the Highly Improved Stag-}

\[ \text{gated Quark action on very fine lattices [16,17] but results for the bottomonium hyperfine splitting are still in the future. A middle ground between nonrelativistic and relativistic approaches is the Fermilab approach to heavy quarks which interpolates between heavy and light regimes. Early work yielded rather inaccurate results [18] but improvements currently underway for charmonium splittings [19] will be applied to bottomonium in future.}

Motivated by the experimental discrepancies, we revisit the hyperfine splittings with NRQCD and make the necessary improvements to the action to eliminate the dominant systematic errors. In NRQCD the hyperfine splitting arises from the $\mathcal{O}(v^3)$ spin-magnetic coupling term $\sigma \cdot \mathbf{B}/2m_b$, whose coefficient we denote $c_4$. At tree level this action gave a hyperfine splitting of $61(14)$ MeV [20] where the large systematic error comes from unknown radiative corrections to $c_4$. HPCD calculated these corrections to one-loop in [21,22]. Including the corrections gave a hyperfine splitting of $70(9)$ MeV, where the error is now dominated by missing $\mathcal{O}(v^6)$ relativistic corrections. Ref [21] also included a calculation of the ratio of the $2S$ to $1S$ hyperfines, which is very insensitive to $c_4$, finding $0.499(42)$. Ref [23] included spin-dependent $\mathcal{O}(v^6)$ corrections with $c_4$ tuned from experimental results for P-wave splittings in the Upsilon system. The results were a $1S$ hyperfine splitting of $60.3(7.7)$ and a $2S$ to $1S$ hyperfine ratio of $0.403(59)$.

Here we go beyond previous calculations by including radiative corrections to $c_4$, spin-dependent $\mathcal{O}(v^6)$ terms and four-quark operators which enter at $\mathcal{O}(\alpha_s^2 v^4)$. By power counting these terms could have a similar impact to the $\alpha_s^2 v^4$ terms. These improvements mean a reduction in systematic errors to the level of 6.7 MeV.

We begin by describing the improvements made to the NRQCD action in Section III before our results in Section III and a discussion in Section IV.

II. LATTICE CALCULATION

We use a lattice NRQCD action correct through $\mathcal{O}(v^4)$ that includes discretisation corrections, spin-dependent
The strengths and $\Delta$ amplitudes of the effective action, the terms are normalised such that $\psi, \chi$ are coefficients for the kinetic terms and $\sigma$ is the Landau link. The matching of the Darwin, spin-magnetic terms are described in detail for both the $O(v^4)$ and $O(v^6)$ actions in [22]. In principle the $O(v^6)$ terms will have an effect on the renormalisation of the kinetic terms but since these have a negligible effect on the hyperfine splittings (compare [21]) we neglect this small effect. In practice we find that the coefficient of the $\sigma \cdot B$ term also changed very little when adding the $O(v^6)$ terms. The parameters used for the NRQCD valence quarks are given in table [1].

The 4-quark interactions relevant for the hyperfine splitting are

$$L_{4q} = \frac{d_1}{a m_b} \bar{\psi}^1 \chi^* T \psi + \frac{d_2}{a m_b} \bar{\psi}^1 \sigma^i \chi^* T \sigma^i \psi,$$

(2)

where $\psi, \chi$ are the quark and antiquark respectively. These operators cannot be included directly in the Hamiltonian, since they involve both the quark and antiquark, but they can be implemented stochastically with a Hubbard-Stratonovich transformation [25]. The quarks are propagated in an auxiliary complex Gaussian noise field $\eta$ with two colour and two spin indices using the following Lagrangian

$$L_{4q} = z \bar{\psi}^1 \eta \psi + z^* \bar{\psi}^2 \eta^2 \chi^*, \quad z = -\frac{d_1}{a m_b},$$

(3)

with $\eta$ normalised such that $\langle \eta \eta^\dagger \rangle = 1$. This requires that the quark Hamiltonian includes a term $a \delta H_{4q} = z \eta$, and similarly for the anti-quark. By solving the equations of motion, one can show that this is equivalent to the first term in Eq. [2]. A similar method can be used for the second term.

The spin-dependent contribution to the coefficients of the 4-quark operators was determined in [22] and $d_1$ includes a contribution $-2\alpha_s^2(2 - \ln 2)/9$ from $b \bar{b}$ annihilation. We use $\alpha_s$ at $q = \pi/a$. The coefficients used on each ensemble are given in table [14].

We employ three ensembles of gluon configurations at different lattice spacings but with the same light quark masses. We demonstrated in [21] that the light quark mass dependence of hyperfine splittings is much smaller than our other systematic errors. The bare lattice $b$ quark mass was tuned using the spin averaged kinetic mass. As expected, the tuned values given in [21] did not change within errors when the $O(v^6)$ terms were added. We used the retuned values which are slightly different to those in [21]. To reduce statistical errors we used $U(1)$ random wall sources on 36 time slices and used 5 smearing combinations as described in [21]. All correlators on the same configuration are binned. Correlators are fit using a simultaneous multi-exponential Bayesian fit [30], however the vector and pseudo-scalar states were fit separately. Autocorrelations and finite volume effects are negligible for low lying bottomonium states [21].

III. RESULTS

Our results are: the hyperfine splitting $\Delta_{hyp}(1S) = M_{Y(1S)} - M_{\eta_b}(1S)$ and the ratio of hyperfine splittings $R_H = \Delta_{hyp}(2S)/\Delta_{hyp}(1S)$. The ratio can be calcu-
4-quark operators are also significant, and depend on perturbative expression for the hyperfine splitting and certainty due to scale dependence, we fit results from all the amplitude of the ground state at each lattice spacing.

The fitted Υ and ηb energies are given in Table III for the v^6 action with and without the 4-quark operators. To extract a physical result f_{phys}, and determine the uncertainty due to scale dependence, we fit results from all three lattice spacings to the form

\[ f(a^2, \mu_b) = f_{phys} \times \left[ 1 + \sum_{j=1,2} k_j (a \Lambda)^{2j} (1 + k_{j\eta_b} \delta x_m + k_{j\eta_b} (\delta x_m)^2) \right]. \]  

The lattice spacing dependence is set by a scale Λ = 500 MeV, and δx_m = (am_b - 2.7)/1.5 allows for mild dependence on the effective theory cutoff am_b. We take priors of 0(1) on all the coefficients except k_1 which is 0.0(3) since the action includes radiatively improved a^2 lattice spacing corrections. We have tested that our results are not sensitive to the fit form or the priors.

A number of systematic errors must be accounted for in our calculation. Some of these depend on the lattice scale and are included in the fit, others are estimated at the end. The dominant error comes from missing radiative corrections to c_4 since the hyperfine splitting is proportional to c_4^2 at leading order. We multiply the raw result by 1 ± 2(a^2/2.7) with the error correlated between each lattice spacing. This effectively takes the value on the fine lattice as the α^2 v^4 error. We allow for the statistical error in the determination of c_4^{(3)} coming from the Vegas integration by adding an error of \( \delta c_4^{(3)} = (\pi/a)|\psi(0)|^2/m_b^2 \), which comes from the 1-loop perturbative expression for the hyperfine splitting and is a sufficient approximation for estimating this component of the error. Higher order corrections to the 4-quark operators are also significant, and depend on |ψ(0)|^2. We allow a correlated additive error of the form 6a_4^2(\pi/a)|\psi(0)|^2/m_b^2 with a coefficient (±1 ± ln(am_b)). The 4-quark error is applied to both splittings in the ratio R_H but the systematic from c_4 cancels. We allow an additional (small) error from uncertainty in the b-quark mass, using the systematic errors from [21] and assuming the leading order dependence ∝ 1/m_b^2. The error in am_b from scale setting is included by taking twice the lattice spacing error when converting ∆hyp(1S) to GeV.

The dominant uncertainty in the hyperfine splitting are from corrections to the v^4 term c_4 but we also include estimates of the uncertainty from higher order terms in the action since these are now relevant. We take a naive estimate of the radiative corrections to the spin-dependent v^6 terms by allowing a correlated error of ±2 x v^2 α_s(π/a) at each lattice spacing. The v^2 = 0.1 term comes from the fact that this is a radiative correction to a relativistic correction. We verified that this is reasonable by running with a different value of c_7 = 1.25 on the 0.09 fm ensemble. This shifts the hyperfine splitting down by 2 MeV, which is within the error. In Ref. [21] we discussed the fact that the hyperfine splitting calculated from the Υ and ηb kinetic masses was incorrect since relativistic corrections to the σ . B term must be present in the Hamiltonian to feed the hyperfine splitting into the kinetic mass. For the pure v^6 action (with c_7 = 1), we obtained 29(23)_{stat} MeV for the kinetic hyperfine splitting and with c_7 = 1.25 we obtained 52(17)_{stat} MeV. This verifies that shifts to c_7 of the size of radiative corrections are all that is needed to obtain the correct kinetic hyperfine splitting. Finally, we take a multiplicative 1% error on the final answer to allow for missing v^8 terms in the action.

Our final results are

\[ \Delta_{hyp}(1S) = 62.8(6.7) \text{ MeV} \]
\[ \Delta_{hyp}(2S)/\Delta_{hyp}(1S) = 0.425(25). \]  

A full error budget is given in Table IV. The error on Δ_{hyp}(1S) is dominated by the unknown radiative corrections to c_4, reducing this systematic error would require a difficult 2-loop calculation. The α_s^2 corrections to the 4-quark operators are also significant, again improving these further would be difficult. Missing higher order operators are no longer a significant source of error. Statistical errors dominate the uncertainty in the ratio which could in principle be improved. Sea quark mass dependence in the hyperfine splitting was found to be much less than other errors in [21] so we neglect it in Δ_{hyp}(15). For the ratio, we also found no systematic light quark mass dependence in [21], but statistical fluctuations between different ensembles accounted for 3.5% of the error. We apply this additional error to our result for the ratio.

### IV. CONCLUSIONS

The bottomonium spectrum continues to provide a rich environment for increasingly precise tests of QCD in the
low energy regime. Excited states are still being discovered by experiments such as Belle, CLEO and ATLAS [5, 6, 32, 33] and lattice QCD calculations are now able to accurately calculate most of the low-lying states. We have given an improved determination of the hyperfine splittings using nonrelativistic QCD correct through $O(\alpha_s v^4, \alpha_s^2 v^3)$. This is the most accurate calculation to date. Our result for the $1S$ splitting of $63(6) \text{ MeV}$ is consistent with our previous result of $70(9)$ [21], verifying that systematic errors were estimated appropriately. The result agrees with, but is more accurate than other results in full lattice QCD, those of Meinel [23], Fermilab/MILC [18] and RBC/UKQCD [31]. All are consistent with the PDG average.

Our result for the ratio $R_H$ is in excellent agreement with the Belle result but disagrees significantly with the results from Belle and Dobbs et al. [5, 6]. This is the most accurate calculation to date. Our result for the $1S$ splitting of $63(6) \text{ MeV}$ is consistent with our previous result of $70(9)$ [21], verifying that systematic errors were estimated appropriately. The result agrees with, but is more accurate than other results in full lattice QCD, those of Meinel [23], Fermilab/MILC [18] and RBC/UKQCD [31]. All are consistent with the PDG average.

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![Graph](image1.png)

**FIG. 1:** The fit result for the $1S$ hyperfine from the $v^6$ action with spin-dependent 4-quark operators. The two error bars are: statistics and scale setting for the smaller; the larger band includes correlated errors from missing radiative corrections to $c_4, d_3, d_2$ and quark mass tuning errors. The grey band includes all systematic errors. Also shown are the pure $v^6$ results, which are not included in the fit, and the PDG average [2].

![Graph](image2.png)

**FIG. 2:** The fit result for the hyperfine ratio from the $v^6$ action with spin-dependent 4-quark operators. Also shown are the pure $v^6$ results, which are not included in the fit, and the results from Belle and Dobbs et al. [5, 6].

![Graph](image3.png)

**FIG. 3:** Comparison of our result (top) with other lattice calculations [18, 20, 21, 23, 31] and experimental [16] results for the hyperfine splittings. The $2S$ hyperfine splitting is on the left and the $1S$ on the right. The two most recent HPQCD results use the 2013 PDG average to extract the $\Delta_{hyp}(2S)$ from the ratio Meinel quotes two results for $\Delta_{hyp}(2S)$ normalising the result using either the $1S$ hyperfine or the $1P$ tensor splitting. The results are taken as given in Ref. [23].

![Table](table.png)

**TABLE IV:** Full error budget for the $1S$ hyperfine splitting and the $2S$ to $1S$ ratio. All errors are in percent.

| Error %   | $\Delta_{hyp}(1S)$ | $R_H$ |
|-----------|---------------------|-------|
| Stats/fitting | 0.2 | 3.5 |
| Uncertainty in $a$ | 2.2 | 0.0 |
| scale dependence | 1.1 | 2.4 |
| NRQCD $a m_b$ dependence | 3.8 | 0.1 |
| NRQCD radiative $\alpha_s v^6$ | 3.7 | 0.0 |
| NRQCD radiative $\alpha_s^2 v^3$ in $c_4$ | 7.0 | - |
| Statistical error in $c_4^{(3)}$ | 3.1 | 1.3 |
| NRQCD relativistic spin $v^8$ | 1.0 | 0.5 |
| NRQCD radiative 4-quark $\alpha_s^2 v^3$ | 2.9 | 1.5 |
| $m_b$ tuning | 0.7 | - |
| $m_{b,sea}$ dependence | - | 3.5 |
| Total | 10.7 | 5.9 |

Dobbs et al.. For discussion of the discrepancy in the experimental values, see [24]. Using the current PDG average of $62.3(3.2) \text{ MeV}$ for the $1S$ hyperfine gives a $2S$ hyperfine splitting of

$$\Delta_{hyp}(2S) = 26.5(1.6)_{\text{lat}}(1.4)_{\text{exp}},$$

where the error has been divided into components from this lattice calculation and the experimental result. Using our lattice result to normalise the value gives a consistent result. A comparison of the existing lattice and experimental results is shown in Fig. [3] Further im-
provements to lattice calculations of the hyperfine splitting may require relativistic actions. A calculation of the hyperfine splitting using HISQ $b$-quarks is in progress.

Acknowledgements

We are grateful to the MILC collaboration for the use of their gauge configurations. This work was funded by STFC. CTHD is supported by the Royal Society and the Wolfson Foundation. The results described here were obtained using the Darwin Supercomputer of the University of Cambridge High Performance Computing Service as part of the DiRAC facility jointly funded by STFC, the Large Facilities Capital Fund of BIS and the Universities of Cambridge and Glasgow.

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