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Bottomonium hyperfine splittings from lattice nonrelativistic QCD including radiative and relativistic corrections

R. J. Dowdall,[1,*] C. T. H. Davies,[2] T. Hammant,[1] R. R. Horgan[1]
(HPQCD Collaboration)

[1]*DAMTP, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, United Kingdom*
[2]*SUPA, School of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, United Kingdom*
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We present a calculation of the hyperfine splittings in bottomonium using lattice nonrelativistic QCD. The calculation includes spin-dependent relativistic corrections through $\mathcal{O}(v^6)$, radiative corrections to the leading spin-magnetic coupling and, for the first time, nonperturbative effects of four-quark operators which enter at $\alpha_s^2 v^3$. We also include the effect of u, d, s and c quark vacuum polarization. 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 $(M_{\Upsilon}(2S) - M_{\eta_b}(2S))/(M_{\Upsilon}(1S) - M_{\eta_b}(1S)) = 0.425(25)$.

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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 Υ radiative decays in 2008 by *BABAR* [1], and subsequent results have led to a fairly wide error being placed on the Particle Data Group (PDG) average [2–5]. The $2S$ state has recently been observed by two groups, Belle [5] and Dobbs *et al.* [6] using CLEO data, but the results differ significantly. Belle finds a $2S$ hyperfine splitting of $24.3^{+4.0}_{-4.5}$ MeV and Dobbs *et al*. have 48.7 ± 3.1 MeV. These difficulties are in contrast to the vector particle Υ 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 [9–14], with systematic errors that are hard to quantify. Next-to-leading-order continuum perturbation theory gives 41(14) MeV [15]. 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 $\mathcal{O}(v^4)$ 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 discretization errors appear instead. It is now becoming possible to handle b quarks relativistically with the highly improved staggered quark (HISQ) 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 $\mathcal{O}(v^4)$ spin-magentic 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. HPQCD calculated these corrections to one-loop in Refs. [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. Reference [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). Reference [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 $\mathcal{O}(\alpha_s^2 v^3)$. By power counting these terms could have a similar impact to the

*R.J.Dowdall@Damtp.cam.ac.uk

$\alpha_s v^4$ 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 Sec. II, before our results in Sec. III and a discussion in Sec. IV.

II. LATTICE CALCULATION

We use a lattice NRQCD action correct through $\mathcal{O}(v^4)$ that includes discretization corrections, spin-dependent terms through $\mathcal{O}(v^6)$ and four-quark contact interactions that enter at $\mathcal{O}(\alpha_s^2 v^3)$ [24,25]. As described in Ref. [24], the b-quark velocity in bottomonium is of order $v^2 \sim 0.1$. For power-counting estimates, we assume $\alpha \sim 0.3$. The $\mathcal{O}(v^4)$ action, with radiative corrections discussed below, has already been used to study S-, P- and D-wave splittings in Refs. [21,26] and B-meson mass splittings in Refs. [27,28]. The Hamiltonian is

$$\begin{aligned}
aH &= aH_0 + a\delta H_{v^4} + a\delta H_{v^6} + a\delta H_{4q}, \\
aH_0 &= -\frac{\Delta^{(2)}}{2am_b}, \\
a\delta H_{v^4} &= -c_1 \frac{(\Delta^{(2)})^2}{8(am_b)^3} + c_2 \frac{i}{8(am_b)^2}(\nabla\cdot\tilde{\mathbf{E}} - \tilde{\mathbf{E}}\cdot\nabla) \\
&\quad - c_3 \frac{1}{8(am_b)^2}\sigma\cdot(\tilde{\nabla}\times\tilde{\mathbf{E}} - \tilde{\mathbf{E}}\times\tilde{\nabla}) \\
&\quad - c_4 \frac{1}{2am_b}\sigma\cdot\tilde{\mathbf{B}} + c_5 \frac{\Delta^{(4)}}{24am_b} - c_6 \frac{(\Delta^{(2)})^2}{16n(am_b)^2}, \\
a\delta H_{v^6} &= -c_7 \frac{1}{8(am_b)^3}\{\Delta^{(2)}, \sigma\cdot\tilde{\mathbf{B}}\} \\
&\quad - c_8 \frac{3i}{64(am_b)^4}\{\Delta^{(2)}, \sigma\cdot(\tilde{\nabla}\times\tilde{\mathbf{E}} - \tilde{\mathbf{E}}\times\tilde{\nabla})\} \\
&\quad + c_9 \frac{1}{8(am_b)^3}\sigma\cdot\tilde{\mathbf{E}}\times\tilde{\mathbf{E}}.
\end{aligned} \tag{1}$$

am_b is the bare b-quark mass, $\tilde{\mathbf{E}}$, $\tilde{\mathbf{B}}$ are improved field strengths and $\Delta^{(2)}$, $\Delta^{(4)}$, ∇, $\tilde{\nabla}$ are lattice derivatives that are described in Ref. [20]. The c_i are the Wilson coefficients of the effective action; the terms are normalized so that they have the expansion $c_i = 1 + \alpha_s c_i^{(1)}$. The matching coefficients for the kinetic terms c_1, c_5, c_6 and the spin-magnetic coupling c_4 are given for the $\mathcal{O}(v^4)$ action in Ref. [21]. The matching of the Darwin, c_2, and spin-magnetic terms are described in detail for both the $\mathcal{O}(v^4)$ and $\mathcal{O}(v^6)$ actions in Ref. [22]. In principle the $\mathcal{O}(v^6)$ terms will have an effect on the renormalization of the kinetic terms but since these have a negligible effect on the hyperfine splittings (compare with Refs. [20,21]) we neglect this small effect. These terms also affect the error on the tuning of the b-quark mass and the determination of the lattice spacing. We estimated their effect in Ref. [21] and this error is included in our error budget. In practice we find that the coefficient of the $\sigma\cdot\mathbf{B}$ term also changed very little when adding the $\mathcal{O}(v^6)$ terms. The parameters used for the NRQCD valence quarks are given in Table I.

The four-quark interactions relevant for the hyperfine splitting are

$$\mathcal{L}_{4q} = \frac{d_1\alpha_s^2}{(am_b)^2}\psi^\dagger\chi^*\chi^T\psi + \frac{d_2\alpha_s^2}{(am_b)^2}\psi^\dagger\sigma^i\chi^*\chi^T\sigma^i\psi, \tag{2}$$

where ψ, χ 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 η with two color and two spin indices using the following Lagrangian:

$$\mathcal{L}_{4q} = z\psi^\dagger\eta\psi + z^*\chi^T\eta^\dagger\chi^*, \qquad z = -\frac{d_1^{\frac{1}{2}}\alpha_s}{am_b}, \tag{3}$$

TABLE I. Parameters used for the valence quarks. am_b is the bare b-quark mass in lattice units, and u_{0L} is the Landau link. The c_i, d_i are coefficients of terms in the NRQCD action [see Eq. (1)]. c_4, d_1 and d_2 use α_s in the V-scheme at the scale π/a. The other coefficients use different scales as discussed in Ref. [21].

Set	am_b	u_{0L}	c_1, c_6	c_5	c_4	$d_1\alpha_s^2$	$d_2\alpha_s^2$	$\alpha_s(\pi/a)$
1	3.31	0.8195	1.36	1.21	1.23	−0.1469	0.0455	0.275
2	2.73	0.834	1.31	1.16	1.19	−0.096	0.029	0.255
3	1.95	0.8525	1.21	1.12	1.18	−0.056	0.016	0.225

TABLE II. Parameters of the gauge configurations used. β is the Yang-Mills coupling, a_Υ is the lattice scale in fm determined using the $\Upsilon(2S-2S)$ splitting. am_q are the sea-quark masses, L, T are the spatial and temporal extents of the lattice and n_{cfg} is the size of the ensemble.

Set	β	a_Υ (fm)	am_l	am_s	am_c	$L\times T$	n_{cfg}
1	5.8	0.1474(5)(14)(2)	0.013	0.065	0.838	16×48	1020
2	6.0	0.1219(2)(9)(2)	0.0102	0.0509	0.635	24×64	1052
3	6.3	0.0884(3)(5)(1)	0.0074	0.037	0.440	32×96	1008

with η normalized 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 antiquark. 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 four-quark operators was determined in Refs. [22,29] and d_1 includes a contribution $-2\alpha_s^2(2-\ln 2)/9$ from $\bar{b}b$ annihilation. We use α_V at $q = \pi/a$. The coefficients used on each ensemble are given in Table I.

We employ three ensembles of gluon configurations at different lattice spacings but with the same light-quark masses, see Table II. We demonstrated in Ref. [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 Ref. [21] did not change within errors when the $\mathcal{O}(v^6)$ terms were added. We use the retuned values which are slightly different to those in Ref. [21]. To reduce statistical errors we used U(1) random wall sources on 36 time slices and used five smearing combinations as described in Ref. [21]. All correlators on the same configuration are binned. Correlators are fit using a simultaneous multi-exponential Bayesian fit [30]; however, the vector and pseudoscalar 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 $\Delta_{\rm hyp}(1S) = M_\Upsilon(1S) - M_{\eta_b}(1S)$ and the ratio of hyperfine splittings $R_H = \Delta_{\rm hyp}(2S)/\Delta_{\rm hyp}(1S)$. The ratio can be calculated much more accurately than the separate splittings since the dominant NRQCD systematics cancel. We find that the effect of the four-quark operators on the hyperfine splitting is within 2 MeV (or 4%) of the expected shift calculated in perturbation theory. This is given by $6\alpha_V^2(\pi/a)(d_1-d_2)|\psi(0)|^2/m_b^2$, where $\psi(0)$ is the wave function at the origin obtained from the spin-averaged amplitude of the ground state at each lattice spacing.

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

$$f(a^2, am_b) = f_{\rm phys}\left[1 + \sum_{j=1,2} k_j (a\Lambda)^{2j}(1 + k_{jb}\delta x_m + k_{jbb}(\delta x_m)^2)\right]. \tag{4}$$

The lattice-spacing dependence is set by a scale $\Lambda = 500$ MeV, and $\delta x_m = (am_b - 2.7)/1.5$ allows for mild dependence on the effective theory cutoff am_b. We take Gaussian priors of mean 0 and width 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.

TABLE III. Fit results in lattice units for the $1S$ and $2S$ energies of the Υ and η_b for the $\mathcal{O}(v^6)$ action with and without four-quark interactions.

Set	$aE_\Upsilon(1S)$	$aE_\Upsilon(2S)$	$aE_{\eta_b}(1S)$	$aE_{\eta_b}(2S)$
$\mathcal{O}(v^6)$ action				
1	0.27547(6)	0.6917(14)	0.22950(5)	0.6748(12)
2	0.28786(3)	0.6332(9)	0.25148(3)	0.6180(6)
3	0.30269(3)	0.5573(10)	0.27484(2)	0.5461(9)
$\mathcal{O}(v^6)$ action + four-quark interactions				
1	0.27776(6)	0.6992(14)	0.22247(5)	0.6745(13)
2	0.28910(3)	0.6325(9)	0.24734(3)	0.6143(7)
3	0.30304(2)	0.5562(6)	0.27267(2)	0.5437(5)

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, while 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 each raw data point by a Gaussian error with unit mean and width $2\alpha_v^2(\pi/a)$ which assumes an α^2 coefficient of order one. We enforce that this component of the error is correlated between each lattice spacing, i.e. that considering this error in isolation the correlation coefficient between data on two lattice spacings is $\rho = 1$. In practice, this takes the value on the fine lattice as the $\alpha_s^2 v^4$ error. We allow for the statistical error in the determination of $c_4^{(1)}$ [22] coming from the Vegas integration by adding an error of $\delta c_4^{(1)}\alpha_V(\pi/a)|\psi(0)|^2/m_b^2$, which comes from the one-loop perturbative expression for the hyperfine splitting and is a sufficient approximation for estimating this component of the error. Higher-order corrections to the four-quark operators are also significant, and depend on $|\psi(0)|^2$. We allow a correlated additive error of the form $6\alpha_V^3(\pi/a)|\psi(0)|^2/m_b^2$ with a coefficient $(\pm 1 \pm \ln(am_b))$. The four-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 Ref. [21] and assuming the leading-order dependence $\propto 1/m_b^2$. The error in am_b from scale setting is included by taking twice the lattice spacing error when converting $\Delta_{\rm hyp}(1S)$ to GeV.

The dominant uncertainty in the hyperfine splitting is 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. The first is for radiative corrections to c_7 which is the term at order v^6 that contributes to the hyperfine splitting. This uncertainty is

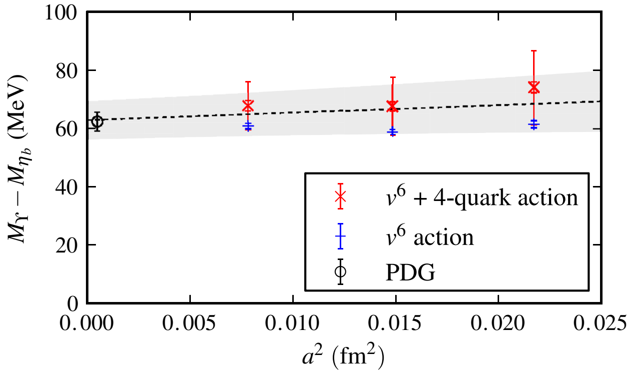

FIG. 1 (color online). The fit result for the $1S$ hyperfine from the v^6 action with spin-dependent four-quark operators. The two error bars are: statistics and scale setting for the smaller; the larger band includes correlated errors from missing radiative corrections to c_4, d_1, d_2 and quark-mass 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].

not as straightforward as for the c_4 term since it is subleading, but we can allow a naive power-counting estimate of the error. The hyperfine splitting is an $\mathcal{O}(v^4)$ effect and these terms are subleading by an additional factor of v^2 so we take an error of $2v^2\alpha_s(\pi/a)$. As above, we make this component of the error correlated between all the lattice spacings. 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. Finally, we take a multiplicative 1% error on the final answer to allow for missing v^8 terms in the action.

As an aside, we verified that corrections to $c_7 = 1$ have the desired effect on the kinetic mass. As discussed in Ref. [21], the hyperfine splitting calculated from the kinetic masses of the Υ and η_b using a v^4 action is incorrect. To get the correct hyperfine splitting from kinetic masses, relativistic corrections to the $\sigma \cdot \mathbf{B}$ term must be present in the Hamiltonian; for a detailed discussion see Ref. [31]. For the pure v^6 action (with $c_7 = 1$), we obtained $29(23)_{\rm stat}$ MeV for the kinetic hyperfine splitting and with $c_7 = 1.25$ we obtained $52(17)_{\rm stat}$ MeV. This verifies that shifts to c_7 of the size of the other radiative corrections are all that is needed to obtain the correct kinetic hyperfine splitting.

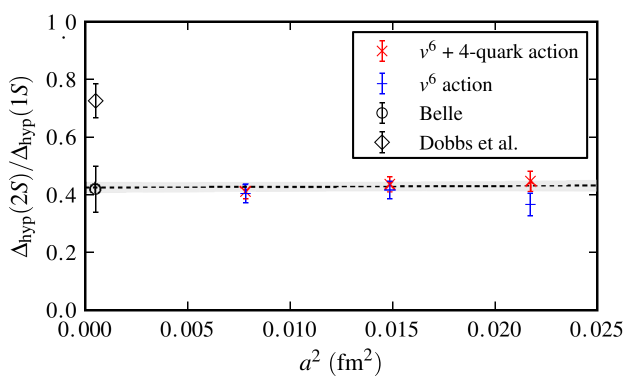

FIG. 2 (color online). The fit result for the hyperfine ratio from the v^6 action with spin-dependent four-quark operators. Also shown are the pure v^6 results, which are not included in the fit, and the results from Belle and Dobbs *et al.* [5,6].

Effects from electromagnetism can be estimated from a potential model. The dominant effect of the Coulomb interaction between b and $\bar{b}$ (missing from our calculation) was estimated in Ref. [32] to give an upward shift of 1.6 MeV to both Υ and η_b and therefore with no impact on the hyperfine splitting. Relativistic corrections to this might then be expected to give an effect on the hyperfine splitting of approximately 10% of this, or 0.2 MeV (0.3%).

Our final results are

$$\Delta_{\rm hyp}(1S) = 62.8(6.7)\ \text{MeV},$$
$$\Delta_{\rm hyp}(2S)/\Delta_{\rm hyp}(1S) = 0.425(25). \tag{5}$$

The fit results are plotted in Figs. 1,2 and a full error budget is given in Table IV. The error on $\Delta_{\rm hyp}(1S)$ is dominated by the unknown radiative corrections to c_4; reducing this systematic error would require a difficult two-loop calculation. The α_s^3 corrections to the four-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 Ref. [21] so we neglect it in $\Delta_{\rm hyp}(1S)$. For the ratio, we also found no systematic light-quark mass dependence in Ref. [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.

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

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

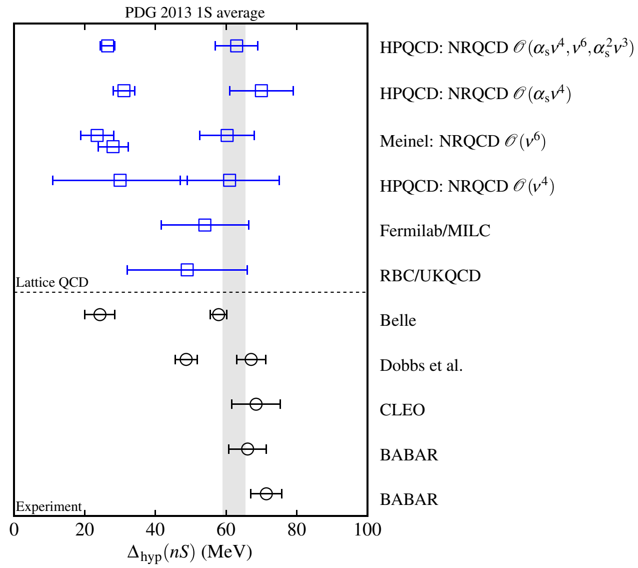

FIG. 3 (color online). Comparison of our result (top) with other lattice calculations [18,20,21,23,35] and experimental [1–6] results for the hyperfine splittings. The $2S$ hyperfine splitting is on the left and the $1S$ on the right. The two most recent HPQCD results use the 2013 PDG average to extract the $\Delta_{\rm hyp}(2S)$ from the ratio. Meinel quotes two results for $\Delta_{\rm hyp}(2S)$ normalizing the result using either the $1S$ hyperfine or the $1P$ tensor splitting. The results are taken as given in Ref. [23].

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 [5,6,33,34] 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 $\mathcal{O}(\alpha_s v^4, v^6, \alpha_s^2 v^3)$. This is the most accurate calculation to date. Our result for the $1S$ splitting of 63(6) 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 [35]. 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 Dobbs *et al.* For discussion of the discrepancy in the experimental values, see Ref. [36]. Using the current PDG average of 62.3(3.2) MeV for the $1S$ hyperfine gives a $2S$ hyperfine splitting of

$$\Delta_{\rm hyp}(2S) = 26.5(1.6)_{\rm latt}(1.4)_{\rm exp}, \tag{6}$$

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

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