Bottomonium Hyperfine Splitting on the Lattice and in the Continuum.

M. Baker,1 A.A. Penin,1,2 D. Scidel,3 and N. Zerf1

1Department of Physics, University of Alberta, Edmonton, Alberta T6G 2J1, Canada
2Institut für Theoretische Teilchenphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany
3Theoretische Physik 1, Universität Siegen, 57068 Siegen, Germany

We revise the analysis of the bottomonium hyperfine splitting within the lattice nonrelativistic QCD. The Wilson coefficients of the radiatively improved lattice action are evaluated by a semianalytic approach based on the asymptotic expansion about the continuum limit. The nonrelativistic renormalization group is used to estimate the higher-order radiative corrections. Our result for the 1S hyperfine splitting is $M_{(1S)} - M_{(1S)} = 52.9 \pm 5.5$ MeV. It reconciles the predictions of the continuum and lattice QCD and is in very good agreement with the most accurate experimental measurement by Belle collaboration.

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The bottomonium hyperfine splitting defined by the mass difference $E_{\text{bs}} = M_{(1S)} - M_{(1S)}$ has been a subject of much controversy since the first observation of the spin-singlet $\eta_b$ state in radiative decays of the $\Upsilon(3S)$ mesons by the Babar collaboration [1]. The measured value of the hyperfine splitting overshoot the predictions of perturbative QCD [2] by almost a factor of two, well beyond the experimental and theoretical uncertainty bands, see Table I. Further experimental studies [3–5] were consistent with the initial measurement, while the Belle collaboration reported a significantly lower value of the splitting with higher experimental precision [6]. On the theory side the most accurate estimates of the hyperfine splitting are obtained from lattice simulations within the effective theory of nonrelativistic QCD (NRQCD). This method is entirely based on first principles, allows for simultaneous treatment of dynamical heavy and light quarks and gives a systematic account of the long-distance nonperturbative effects of the strong interaction. The first analysis [7] with fully incorporated one-loop radiative corrections [8] favored the larger value of the splitting [1]. The most recent analysis [9] includes the leading relativistic corrections and gives a lower value, which is close to the PDG average [10] but nevertheless not consistent with Ref. [2]. This might indicate a serious failure of perturbative QCD in the description of the bottomonium ground state in clear conflict with general concept of the heavy quark dynamics. Thus the current experimental and theoretical status of the bottomonium hyperfine splitting remains ambiguous and sets up one of the most interesting open problems in the QCD theory of hadrons, which yet inspired a discussion about possible signal of physics beyond the standard model [11].

In this Letter we revise the analysis of the radiative corrections to the lattice NRQCD action. We develop a semianalytical approach based on the asymptotic expansion about the continuum limit [12], which provides a very powerful tool for the radiative improvement of lattice NRQCD. Our result for the one-loop Wilson coefficient of the effective spin-dependent four-quark interaction significantly differs from the result of the previous calculation [8] used in the subsequent analyses [7, 9], which leads to a sizable reduction of the lattice NRQCD prediction for the hyperfine splitting. We give an estimate of the higher order radiative corrections by evaluating the two-loop double-logarithmic terms within the nonrelativistic renormalization group approach [13, 14]. The main result of this paper is a new theoretical value for bottomonium hyperfine splitting, Eq. (10).

The idea of the NRQCD approach [13, 16] is to separate the hard modes, which require a fully relativistic analysis, from the nonrelativistic soft modes. The dynamics of the soft modes is governed by the effective nonrelativistic action given by a series in heavy quark velocity $v$, while the contribution of the hard modes is encoded in the corresponding Wilson coefficients. The nonrelativistic action can be applied in a systematic perturbative analysis of the heavy quarkonium spectrum [17–19]. At the same time the action may be used for lattice simulations of the heavy quarkonium states [20, 21]. The latter approach gives full control over nonperturbative long-distance effects and can be used for the description of excited states where perturbative QCD is not applicable.

The hyperfine splitting i.e. the splitting between the spin-singlet and spin-triplet states is generated by the spin-dependent part of the NRQCD Lagrangian. To order $O(v^4)$ it reads (see e.g. [22, 23])

$$\mathcal{L}_\sigma = \frac{c_F}{2m_q} \psi^\dagger B \sigma \psi + (\psi \to \chi_c) + d_\sigma \frac{C_F \alpha_s}{m_q} \psi^\dagger \sigma \chi_c^\dagger \sigma \chi_c,$$  

(1)

where $B$ is the chromomagnetic field, $m_q$ and $\alpha_s$ are the heavy quark mass and the strong coupling constant, the $SU(N_c)$ color group factor is $C_F = (N_c^2 - 1)/(2N_c)$, $\psi$ ($\chi_c$) are the nonrelativistic Pauli spinors of quark (anti-quark) field, and we have projected the four-quark interaction on the color-singlet state. The Wilson coefficients $c_F$ and $d_\sigma$ logarithmically depend on the factorization scale $\mu_f$ which separates the hard and the soft momen-
tum contributions. This dependence can be predicted to all orders of perturbation theory by renormalization group methods. In lattice NRQCD the natural factorization scale is given by the inverse lattice spacing \( a \). The radiative improvement of the action is therefore mandatory for the correct continuum limit.

The coefficient \( c_F \) parameterizes the quark anomalous chromomagnetic moment. It can be determined nonperturbatively by matching the lattice result for particular splittings to the physical bottomonium spectrum \[2,24\]. The perturbative evaluation of the one-loop correction to \( c_F \) \[3\] is in good agreement with the nonperturbative result. The Wilson coefficient of the effective four-quark interaction however can only be obtained perturbatively. It vanishes in the Born approximation and is determined of the coefficient

\[
\delta = \frac{1}{2} \ln (\lambda a)
\]

where the nonlogarithmic nonabelian term \( \delta \) depends on a particular realization of the lattice action. To match Eqs. (2) and (3) we add to the NRQCD Lagrangian the four-quark operator with coefficient

\[
d_s = \alpha_s \left[ \left( \frac{1}{2} L \right) C_A + (\ln 2 - 1) T_F + C_F \right],
\]

where \( L = \ln(m_q a) \). The main problem is therefore in determination of the coefficient \( \delta \). The asymptotic expansion of the lattice loop integrals about the continuum limit \[12\] can in principle be used to get this coefficient in a closed analytic form. Let us consider first a “naive” lattice action with no improvement for gluonic and heavy quark fields (see, e.g., \[25,26\]). The gluonic field tensor of the NRQCD chromomagnetic interaction in the naive action is expressed through the commutator of the left-right symmetrized covariant lattice derivatives. In this case we obtain

\[
\delta^{\text{naive}} = -\frac{7}{3} + 28\pi^2 b_2 - 256\pi^2 b_3 = 0.288972 \ldots
\]

where the irrational constants \( b_2 = 0.02401318 \ldots \), \( b_3 = 0.00158857 \ldots \) parameterize the lattice tadpole integrals and can be computed with arbitrary precision \[12\]. We however need the above coefficient for the improved lattice action which is used in real simulations. Analytic calculation with an improved action is not optimal since

| Experiment | Theory |
|------------|--------|
| Babar, \( \Upsilon(3S) \) decays\[4\] | NRQCD, NLL \[2\] |
| Babar, \( \Upsilon(2S) \) decays | Lattice NRQCD \( \mathcal{O}(v^4) \)[7] |
| Belle, \( b \rightarrow s \) decays \[6\] | Lattice NRQCD \( \mathcal{O}(v^6) \)[9] |
| PDG average \[10\] | Lattice NRQCD \[33\] |
| |

| Result | |
|--------|--------|
| 71.4^{+2.1}_{-3.4} \text{ MeV} | 41 \pm 11 \text{ (th)}^{+0}_{-9} (\delta \alpha_s) |
| 66.1^{+2.0}_{-2.3} \text{ MeV} | 70 \pm 9 |
| 57.9 \pm 2.3 | 62.8 \pm 6.7 |
| 54.0 \pm 12.4^{+1.2}_{-0.8} | 54.0 \pm 12.4^{+1.2}_{-0.8} |
| 52.9 \pm 5.5 | 52.9 \pm 5.5 |

TABLE I. Results of high-precision experimental and theoretical determinations of the bottomonium hyperfine splitting in MeV.

FIG. 1. One-loop Feynman diagrams contributing to the one-particle irreducible quark-antiquark scattering amplitude in QCD (a-d) and NRQCD (e-f).
the Feynman rules in this case become extremely cumbersome. We bypass this problem by using a semianalytic approach. Indeed the difference between the Wilson coefficients for the improved and naive lattice analytic approach. We therefore neglect this term. We bypass this problem by using a semianalytic approach. Indeed the difference between the Wilson coefficients for the improved and naive lattice analytic approach. We therefore neglect this term.

\[ \delta = 0.1446(28). \]  

Note that since \( d_\sigma = 0 \) in the Born approximation, we do not have to perform the strong coupling constant renormalization not the lattice tadpole improvement. We made a few cross checks of the calculation. For the naive action the numerical evaluation agrees with the gauge-invariant analytic result of the asymptotic expansion for small values of \( \lambda \). The logarithmic part of \( d_\sigma \) is in agreement with the renormalization group analysis. The nonrelativistic renormalization group predicts the all-order dependence of the Wilson coefficients on \( \mu_f \). In the leading logarithmic approximation they read

\[ d_\sigma^{LL} = \frac{C_A}{\beta_0 - 2C_A} (\lambda^{2C_A} - \lambda^{-\beta_0} - 1), \quad c_F^{LL} = \lambda^{C_A}. \]  

where \( \beta_0 = 11C_A/3 - 4T_Fn_l/3 \) is the one-loop QCD \( \beta \) function, \( n_l = 4 \) is the number of light flavors, and \( z = (\alpha_s(\mu_f)/\alpha_s(m_q))^{1/\beta_0} \). In lattice NRQCD the factorization scale should be identified with inverse lattice spacing \( \mu_f \sim 1/a \). By reexpanding the leading logarithmic result we obtain

\[ d_\sigma^{LL} = \frac{\alpha_s}{\pi} \frac{C_A L}{2} \left( \frac{\alpha_s}{\pi} \right)^2 \frac{(\beta_0 + C_A) C_A}{4} L^2 + \ldots, \]
\[ c_F^{LL} = 1 - \frac{\alpha_s}{\pi} \frac{C_A}{2} L + \left( \frac{\alpha_s}{\pi} \right)^2 \frac{(\beta_0 + C_A) C_A}{8} L^2 + \ldots, \]  

in agreement with Eq. (4).

Let us now compare our result with the previous calculation \[8\]. In this paper a different basis of the four-quark operators is used and the Wilson coefficient \( d_{bL}/c_{bL} \) should be identified with the linear combination \( \frac{1}{2}(d_1 - d_2) \). We find that the logarithmic term obtained in Ref. \[8\] has the same absolute value but the opposite sign with respect to Eq. (4) and therefore contradicts the known logarithmic dependence of the one-loop spin-flip effective potential on \( m_q \). \[8\] The difference between the results however is not reduced to the overall sign since the annihilation contribution given in \[8\] in analytic form agrees with Eq. (4).

Now we are in a position to apply our result to the analysis of the hyperfine splitting. The contribution of the four-quark interaction to \( E_{\text{hfs}} \) reads

\[ \Delta E_{\text{hfs}} = -d_\sigma \frac{4C_F\alpha_s}{m_q^2} |\psi(0)|^2, \]  

where \( \psi(0) \) is the wave function of the quarkonium ground state at the origin. Eq. (11) should be added to the result of the lattice simulation with the one-loop Wilson coefficient \( c_F \) and for the \( \mathcal{O}(v^4) \) action \[7\]. For the numerical analysis of Eq. (11) we use the nonperturbative lattice result for \( \psi(0) \) \[7\]. To make our analysis self-consistent we adopt the value of the bottom quark mass \( m_b \) and the value of the strong coupling constant \( \alpha V \) renormalized in the static potential scheme at the scale \( \pi/a \) from Ref. \[7\]. The numerical result for the hyperfine splitting is presented in

|                  | \( \mathcal{O}(v^4) \) action | \( \mathcal{O}(v^6) \) action |
|------------------|---------------------------------|--------------------------------|
| Discretization   | 2.6                             | 3.1                            |
| Relativistic     | 6.0                             | 1.8                            |
| Radiative        | 4.8                             | 4.3                            |
| \( E_{\text{hfs}} \) | 57.5                            | 51.5                           |

TABLE II. The central value and the error budget for the lattice NRQCD determination of the bottomonium hyperfine splitting with \( \mathcal{O}(v^4) \) action \[7\] and \( \mathcal{O}(v^6) \) lattice action \[4\] in MeV.
Fig. 2 as function of $a^2$ for three different lattice spacings and two different lattice actions. The error bars of each point include the statistical error and the uncertainty in the value of the lattice spacing from $[7, 9]$ as well as the high-order $a$-dependent radiative corrections which are estimated by the size of the double-logarithmic two-loop terms in Eq. (5). To get the physical result in the continuum limit we use a constrained fit of the data points by a polynomial in $a$ with vanishing linear term. To estimate the coefficients of the higher-order terms in the lattice spacing we represent the result of the fit as $1 + (\Lambda a)^2 + \mathcal{O}(a^3)$, where $\Lambda$ is the mass scale characterizing the approach of the lattice approximation to the continuum limit. The priors for the coefficients of the $a^n$ terms with $n > 2$ in the constrained fit are then given by the intervals $\pm \Lambda^a$. Numerically we get $\Lambda \approx 360$ MeV for the ${\mathcal O}(v^4)$ and $\Lambda \approx 790$ MeV for the ${\mathcal O}(v^6)$ case. Due to a slower approach to the continuum limit the extrapolation error for $\mathcal{O}(v^6)$ action turns out to be larger. This may be related to the fact that the contribution of the operators of higher dimension is more sensitive to the ultraviolet momentum region. Therefore the currently unknown $\mathcal{O}(a \nu^6)$ matching corrections in this approximation can be substantial. The total error budget of our estimate is given in Table II. Besides the discretization errors discussed above it includes the uncertainty due to high-order relativistic and radiative corrections. For a conservative estimate of the radiative corrections we take the value of the double-logarithmic two-loop terms at the soft factorization scale $\mu_f = \alpha_s m_b$ dictated by the bound state dynamics. In Table II this uncertainty is combined with the numerical error in the one-loop coefficient $c_F$.

Our estimate of the relativistic corrections for the $\mathcal{O}(v^6)$ action is based on the difference between the $\mathcal{O}(v^4)$ and $\mathcal{O}(v^6)$ results in the continuum limit. For the $\mathcal{O}(v^6)$ action we multiply this uncertainty by $\alpha_s$ evaluated at the soft renormalization scale to take into account the previously discussed missing matching corrections. The larger discretization uncertainty balances the smaller relativistic corrections in the $\mathcal{O}(v^6)$ case and both actions provide comparable total errors. Since the structure of the relativistic corrections and the behavior of the results at finite lattice spacing are significantly different for the two actions, we consider the corresponding uncertainties as uncorrelated and take the weighted average of the results as the best estimate. At the same time the uncertainty due to the high-order purely radiative corrections is treated as correlated between the two actions. Our final result for the hyperfine splitting reads

$$E_{\text{hfs}} = 52.9 \pm 5.5 \text{ MeV}. \quad (10)$$

We now compare Eq. (10) to the available theoretical and experimental results in Table I. With the new value of the four-quark Wilson coefficient the lattice NRQCD prediction agrees within the error bars with the next-to-leading logarithmic (NLL) perturbative QCD result [2].

Its central value practically coincides with that of the full lattice QCD simulation [3], though the uncertainty of the latter is significantly larger. This may indicate that the matching of the lattice NRQCD to full QCD is now done properly. On the experimental side our result strongly favors the value obtained by Belle collaboration, which has the lowest reported uncertainty.

Thus we have reconciled the theoretical predictions of the lattice and continuum QCD as well as the most accurate experimental data, thereby solving a long-standing puzzle of the bottomonium spectroscopy.

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