Prediction of the bottomonium D-wave spectrum from full lattice QCD

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We calculate the full spectrum of D-wave states in the Υ system in lattice QCD for the first time, using an improved version of NonRelativistic QCD on coarse and fine ‘second generation’ gluon field configurations from the MILC collaboration that include the effect of up, down, strange and charm quarks in the sea. Taking the 2S−1S splitting to set the lattice spacing, we determine the 3D2−1S splitting to 2.3%, and find agreement with experiment. Our prediction of the fine structure relative to the 3D2 gives the 3D3 at 10.181(5) GeV and the 3D1 at 10.147(6) GeV. We also discuss the overlap of 3D1 operators with 3S1 states.

Introduction. The spectrum of b¯¯b states has provided a very important testing ground for strong interaction physics because of the number of radial and orbital excitations that are ‘gold-plated’, i.e. well below the threshold for decay to B mesons. The recent discovery of the ηb(1S) [1] and h0(1P) and h0(2P) mesons [2] filled in important gaps in the spin-singlet states. The mass of the ηb meson had previously been predicted by lattice QCD [3] and the h0 meson masses were widely expected, and found, to be very close to the spin-average of their associated spin-triplet states.

The key missing gold-plated mesons are now the Υ(1D) states. These are difficult to find experimentally although the 3D2 has been seen in radiative decay from the Υ(3S) [4]. Masses of the D-wave states have been predicted in potential model calculations (see, for example [5, 6]), but it is hard to quantify the errors in these predictions except by using different forms for the potentials.

In lattice QCD the starting point is QCD itself. The difficulties with the D-wave states then stem from the signal to noise ratio; the signal falls exponentially in lattice time with the D-wave mass but the noise falls with the smaller ground state S-wave mass. Very large samples of meson correlators on full QCD gluon field configurations are then needed to obtain a reliable signal. Here we give the first results from lattice QCD that are able to distinguish the fine structure of D-wave states.

Lattice Calculation. We use ‘second generation’ gluon field configurations recently generated by the MILC collaboration [7]. These have a gluon action fully improved through αsαs^2 [8] and include the effect of u, d, s and c quarks in the sea using the Highly Improved Staggered Quark formalism [9]. The u and d quarks have the same mass, mQ, so the configurations are denoted as n_f = 2 + 1 + 1. We use three ensembles to give two values of the lattice spacing and two values of mQ. The parameters of the ensembles are given in Table I we label them as 3, 4 and 5 from earlier work [10] in which we mapped out the S and P-wave bottomonium spectrum and determined the lattice spacing from the Υ(2S−1S) splitting.

We calculate b quark propagators on these configurations using an improved lattice discretisation of NonRelativistic QCD (NRQCD). NRQCD is an expansion in powers of the heavy quark velocity and therefore good for b quarks since v^2/c^2 ≈ 0.1 inside their bound states. The Hamiltonian includes all terms through O(v^4) [10]:

$$aH = -\frac{\Delta^{(2)}}{2am_b}$$
$$-c_1 \frac{(\Delta^{(2)})^2}{8(am_b)^3} + c_2 \frac{i}{8(am_b)^2} (\nabla \cdot \tilde{E} - \tilde{E} \cdot \nabla)$$
$$-c_3 \frac{1}{8(am_b)^2} \sigma \cdot (\tilde{E} \times \tilde{E} - \tilde{E} \times \tilde{E})$$
$$-c_4 \frac{1}{2am_b} \sigma \cdot \tilde{B} + c_5 \frac{\Delta^{(4)}}{24am_b} - c_6 \frac{(\Delta^{(2)})^2}{64(am_b)^2}.$$ 

Here \(\nabla\) is the symmetric lattice derivative and \(\Delta^{(n)}\) is the lattice discretization of the continuum \(\sum_i D_i^a\). \(\tilde{E}\) and \(\tilde{B}\) are the chromoelectric and chromomagnetic fields. \(am_b\) is the bare b quark mass, which is tuned by determination on the lattice of the spin-average of ground-state Υ and ηb meson masses. This was done in [10] to give the values used here, quoted in Table I.

The v^4 terms in \(\delta H\) have coefficients c_i whose values are fixed from matching lattice NRQCD to full QCD, either perturbatively or nonperturbatively. Here we use coefficients for c_1, c_5 and c_6 that include O(α_s) corrections, as described in [10]. The coefficients c_3 and c_4 of the spin-dependent v^4 terms have been tuned from a study of the fine structure of the χb(1P) states. We find c_3 = 1.0 with an error of 0.1. c_4 is significantly larger. Here we use c_4 = 1.25 on the coarse lattices and 1.10 on the fine lattices. These agree within 0.1 both with the value required to give P-wave fine structure in agreement with experiment and with the O(α_s) improved result [10].

To make meson correlators for D-wave states we use a quark propagator made from either a local or a smeared
source which has appropriate derivatives applied to it to generate a $D^1$-wavefunction'. This propagator is then combined with a local propagator and the same derivatives and smearings applied at the sink to create a $2 \times 2$ matrix of correlators for each $D$-wave state. The complete set of combinations of spin matrices and derivatives needed is given in [11]. Note that the spin-2 and spin-3 representations split into irreducible representations of the lattice rotational group \{A_1, A_2, E, T_1, T_2\}, which must be considered independently since their masses can differ by discretisation errors. Very high statistics is required - we have typically 32,000 correlators for every source operator per ensemble, using multiple time sources per configuration. The time sources are binned over for analysis.
between the fine and coarse sets and between different sea light quark masses for the two coarse sets.

To arrive at a final result for $D$-wave fine structure we study combinations of $^{3}D$ spin-splittings that are sensitive either to an $L \cdot S$ or to a tensor $S_{ij}$ interaction ($S \cdot S$ takes the same value for all $^{3}D$ states). Writing

$$M_{J} = M(3D) + \Delta_{L,S}^{D} \langle L \cdot S \rangle + \Delta_{S_{ij}}^{D} \langle S_{ij} \rangle$$

(4)
gives

$$\Delta_{L,S}^{D} = (14M_{3} - 5M_{2} - 9M_{1})/60$$

$$\Delta_{S_{ij}}^{D} = -7(2M_{3} - 5M_{2} + 3M_{1})/120.$$  (5)

Table II gives our results for these splittings. In Figure 4 we plot ratios to the equivalent $^{3}P$ splitting combinations: $R_{X} = \Delta_{X}^{P} / \Delta_{X}^{D}$ with $\Delta_{L,S}^{P} = (5M_{2} - 3M_{1} - 2M_{0})/12$ and $\Delta_{S_{ij}}^{P} = -5(M_{2} - 3M_{1} + 2M_{0})/72$. Values for $\Delta_{L}^{P}$ for these ensembles are given in [10] (without factors of 1/12 and -5/72). The experimental values are $\Delta_{L,S}^{P} = 13.65(27)$ MeV and $\Delta_{S_{ij}}^{P} = 3.29(9)$ MeV [13].

The advantage of using these combinations is that they depend purely on one of the spin-dependent coefficients of the NRQCD action. On set 5 we did not use exactly the same values for $c_{3}$ and $c_{4}$ in our study of $P$ and $D$ waves. However we can correct for this in Figure 4 since $\Delta_{S_{ij}} \propto c_{4}^{2}$ and $\Delta_{L,S} \propto c_{3}$. Once this slight adjustment is done the dependence on $c_{3,4}$ cancels between $P$ and $D$ states and so errors from the uncertainty in these coefficients are much reduced.

We fit the fine-structure $R$ values to the same form used earlier in eq. 4 to extract physical results:

$$R_{L,S} = 0.49(11); \quad R_{S_{ij}} = 0.26(35).$$  (6)

We have included an additional systematic error of 10% to allow for missing $v^{6}$ terms from our NRQCD action but the lattice statistical error dominates. We then combine the $R$ values with experimental results from $1P$ levels to give the following $^{3}D$ splittings:

$^{3}D_{3} - ^{3}D_{1} = 34(8)$ MeV

$^{3}D_{3} - ^{3}D_{2} = 18(5)$ MeV

$^{3}D_{2} - ^{3}D_{1} = 17(6)$ MeV.  (7)
Our fine structure splittings are somewhat larger than typical results from potential models \cite{5,6}, where the $^3D_3 - ^3D_1$ splitting lies in the range 10-20 MeV. This can be traced to a larger value for $R_{L,S}$ than is obtained, for example, in \cite{4}, based on specific forms for the spin-dependent potentials.

One issue that we have neglected above is that the $^3D_1$ state has $J^{PC} = 1^{--}$ in common with $^3S_1$ states. On the lattice, in principle, any operator with $1^{--}$ quantum numbers will be able to create all $1^{--}$ states. In practice the amplitude for $^3S_1$ states to be created by the operators that we use for the $^3D_1$ is very small and vice versa. We illustrate that in Fig. 5 where we show correlators from set 3 that use a local $^3S_1$ or $^3D_1$ operator at source and sink compared to the cross-correlator that has a local $^3S_1$ operator at the source and $^3D_1$ at sink or vice versa. The cross-correlator is much smaller in magnitude than either of the diagonal correlators at small $t$ values. The exponential fall-off (as seen in the slope of the log plot) of the cross-correlator matches that of the $^3S_1$ correlator at large times, where the $^3D_1$ correlator fall-off is dominated by that of the heavier $^3D_1$ state. If we fit the complete set of $^3S_1$ and $^3D_1$ correlators together, including the local cross-correlators of Fig. 5 we obtain results in agreement with our separate fits for $^3S_1$ (in \cite{10}) and $^3D_1$ masses. We also find, for example, that the amplitude $a(^3D_{1,local}, \Upsilon)$ from eq. \ref{2} is 0.0052(1) times that of $a(^3S_{1,local}, \Upsilon)$.

Conclusions. We give the first full lattice QCD results for the $D$-wave states of bottomonium including the fine structure. We obtain a mass of 10.179(17) GeV for the $^3D_2$ to be compared with 10.1637(14) GeV from experiment \cite{13}. Using the experimental result for the $^1D_2$ mass we predict masses of 10.181(5) GeV for the $^3D_3$, 10.147(6) GeV for the $^1D_3$ and 10.169(10) for the $^1D_2$.

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