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Mass of the B_c Meson in Three-Flavor Lattice QCD

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We use lattice QCD to predict the mass of the B_c meson. We use the MILC Collaboration's publicly available ensembles of lattice gauge fields, which have a quark sea with two flavors (up and down) much lighter than a third (strange). Our final result is $m_{B_c} = 6304 \pm 12^{+18}_{-10}$ MeV. The first error bar is a sum in quadrature of statistical and systematic uncertainties, and the second is an estimate of heavy-quark discretization effects.

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Recently there has been a significant breakthrough in numerical lattice calculations of QCD [1]. With new, improved techniques for incorporating light sea quarks, lattice QCD agrees with experiment at the few percent level for a wide variety of quantities. They include mass splittings in quarkonium (bound states of heavy quarks and anti-quarks), masses of heavy-light mesons (bound states of a heavy quark and a light anti-quark), and masses and decay properties of light hadrons. This progress suggests that lattice QCD could play a big role in particle physics, especially as an aid to understanding the flavor sector of the Standard Model [2].

In flavor physics, the central aim is to search for evidence of new phenomena. Before applying results from numerical lattice QCD for such purposes, it is helpful to have as many tests as possible. Although lattice gauge theory has a solid mathematical foundation, numerical simulations are not simple. The impressive results of Ref. [1] have been achieved only with the fastest method for simulating light quarks. The price for speed is an unproven assumption (discussed below), which clearly warrants further scrutiny. In addition, the cut-off effects of heavy quarks are controlled using effective field theories. Although most heavy-quark phenomenology relies on this framework, it is important to find out how well it describes discretization errors in lattice calculations.

The ideal way to test a theoretical technique is to predict a mass or decay rate that is not well-measured experimentally, but will be measured precisely soon. Several examples are available in leptonic and semileptonic decays of charmed mesons, which are being measured in the CLEO-*c* experiment. They are sensitive to both the light-quark *and* heavy-quark methods, and are under investigation [3, 4].

Another example, pursued here, is the mass of the pseudo-scalar B_c meson, the lowest-lying bound state of a bottom anti-quark (\bar{b}) and a charmed quark (c). The B_c mass principally tests the heavy-quark methods of lattice QCD. Based on experience with $\bar{b}b$ [5] and $\bar{c}c$ [6] mass splittings, we expect only mild sensitivity to the light quark mass (of the sea quarks) once the mass is small enough to allow uninhibited creation and annihilation of virtual light quark pairs. Preliminary versions of this work have been given at conferences [7].

Until now, B_c has been observed only in the semileptonic decay $B_c^+ \rightarrow J/\psi l^+ \nu_l$, and the undetected neutrino leads to a mass resolution of around 400 MeV [8, 9]. During Run 2 of the Tevatron, B_c is expected to be observed in non-leptonic decays, with a mass resolution estimated to be 20–50 MeV [10]. Our total uncertainty is much smaller than the current experimental accuracy, and comparable to the projections, so we may claim to be predicting the mass of the B_c meson.

Heavy-quark discretization effects are a challenge, because feasible lattice spacings a are about the same as the Compton wavelength of the bottom and charmed quarks. The distances are both shorter than the typical distance of QCD, about 1 fm. The obvious strategy is to use effective field theories to separate long- and short-distance scales. This reasoning has led to the development of non-relativistic QCD (NRQCD) for quarkonium [11] and heavy-quark effective theory (HQET) for heavy-light mesons [12]. In lattice gauge theory, this reasoning has led to two systematic methods for discretizing the heavy-quark Lagrangian: lattice NRQCD [11, 13] and the Fermilab heavy-quark method [14, 15]. A strength of both is that the free parameters of the lattice Lagrangian can be fixed with quarkonium. Then, with no free parameters, one obtains results for heavy-light systems (such as D and B mesons). The same procedure applies here: we obtain m_{B_c} with the same bare quark masses that reproduce the bottomonium [5] and charmonium [6] spectra.

It is beyond the scope of this Letter to review the details of the heavy quarks in lattice gauge theory [16]. An accurate summary is that the couplings of the lattice Lagrangian are adjusted so that [15]

$$\begin{aligned} \mathcal{L}_{\text{lat}} &\doteq \mathcal{L}_{\text{QCD}} + \delta m(\bar{h}^+ h^+ + \bar{h}^- h^-) + \\ &\sum_n a^{s_n} f_n(m_Q a) \mathcal{O}_n \end{aligned} \quad (1)$$

where \doteq can be read “has the same mass spectrum as.” The δm term is an unimportant overall shift in the mass spectrum; h^+ (h^-) is an effective field for quarks (anti-quarks); the \mathcal{O}_n are the effective operators of the heavy-quark expansion, of dimension $\dim \mathcal{O}_n = 4 + s_n$, $s_n \geq 1$; and a is the lattice spacing. The coefficients f_n arise from the short-distance mis-

match between lattice gauge theory and continuum QCD. By choosing an *improved* lattice Lagrangian \mathcal{L}_{lat} , the f_n can be reduced. In practice, however, it is necessary to monitor their effect, by varying a and by estimating the effects of the leading \mathcal{O}_n on the mass spectrum.

Our calculation employs an idea from a quenched calculation [17] (omitting sea quarks), namely to use lattice NRQCD for the b quark and the Fermilab method for the c quark. The lattice NRQCD Lagrangian [13] has a better treatment of interactions of order v^4 , where v is the heavy-quark velocity. The Fermilab Lagrangian [14] has a better treatment of higher relativistic corrections, which is helpful since the velocity of the c quark in B_c is not especially small, $v_c^2 \approx 0.5$. Thus, we expect this combination to control discretization effects well. This choice also means that our calculation directly tests the heavy-quark Lagrangians used in Ref. [1].

We work with ensembles of lattice gauge fields from the MILC Collaboration [18]. Each ensemble contains several hundred lattice gauge fields, so statistical errors are a few per cent. The gluon fields interact with a sea of “2 + 1” quarks: one with mass m_s tuned close to that of the strange quark, and the other two as light as possible. In this work we use ensembles with light mass $m_l = 0.2m_s$ and $m_l = 0.4m_s$. The gluon and sea-quark Lagrangians are improved to reduce discretization effects. We use two lattice spacings, $a \sim \frac{1}{8}, \frac{1}{11}$ fm. (These are handy estimates; a depends slightly on m_l .) Further details are in the MILC Collaboration’s papers [18].

A drawback of the MILC ensembles is that the sea quarks are incorporated with “staggered” quarks. A single staggered quark field leads to four species, or “tastes,” in the continuum limit. Sea quarks are represented (as usual) by the determinant of the staggered discretization of the Dirac operator. To simulate 2 tastes (1 taste), the square root (fourth root) of the 4-taste determinant is taken. The validity of this procedure is not yet proven for lattice QCD, although a proof does go through in at least one (non-trivial) context [19]. Moreover, one finds that interacting improved staggered fields split into quartets [20], as is necessary. Since our prediction of the B_c mass tests this ingredient of the calculation (albeit indirectly), we do not assign a numerical error bar to this issue.

As in Ref. [17], we calculate mass splittings, namely

$$\Delta_{\psi\Upsilon} = m_{B_c} - \frac{1}{2}(\bar{m}_\psi + m_\Upsilon), \quad (2)$$

$$\Delta_{D_s B_s} = m_{B_c} - (\bar{m}_{D_s} + \bar{m}_{B_s}), \quad (3)$$

where $\bar{m}_\psi = \frac{1}{4}m_{\eta_c} + \frac{3}{4}m_{J/\psi}$, $\bar{m}_{D_s} = \frac{1}{4}m_{D_s} + \frac{3}{4}m_{D_s^*}$, and $\bar{m}_{B_s} = \frac{1}{4}m_{B_s} + \frac{3}{4}m_{B_s^*}$ are spin-averaged masses. We refer to $\frac{1}{2}(\bar{m}_\psi + m_\Upsilon)$ and $(\bar{m}_{D_s} + \bar{m}_{B_s})$ as the “quarkonium” and “heavy-light” baselines, respectively. Our result for m_{B_c} comes from our calculated $a\Delta_{\psi\Upsilon}$ and $a\Delta_{D_s B_s}$ (in lattice units), combined with the lattice spacing a and the experimental measurements of the baselines. We use the 2S–1S splitting of bottomonium to define a , but on the MILC ensembles several other observables would serve equally well [1].

Many uncertainties cancel in mass splittings. Lattice calculations integrate the QCD functional integral with a Monte

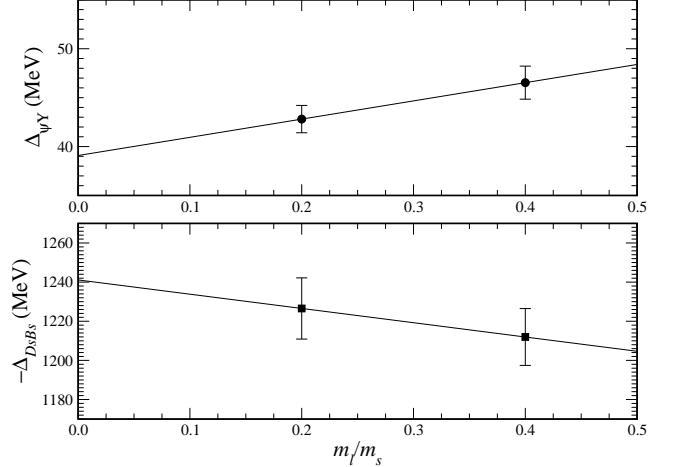


FIG. 1: Dependence of $\Delta_{\psi\Upsilon}$ and $\Delta_{D_s B_s}$ on the light sea quark mass.

Carlo method, and the ensuing statistical error largely cancels when forming a difference. The mass shifts δm in Eq. (1) drop out. The spin-averaging cancels the contribution of a leading uncertainty from the hyperfine operator $\mathcal{O} = \bar{h}^\pm i\boldsymbol{\Sigma} \cdot \mathbf{B} h^\pm$. (We do not spin-average Υ with η_b , because the latter remains unobserved.) The discretization errors from further terms in Eq. (1) cancel to some extent, especially with the quarkonium baseline. Most crucially, all masses in Eqs. (2) and (3) are “gold-plated” [1], in the sense that the hadrons are stable and not especially sensitive to the light quark sea. (Hence we use D_s and B_s , not D and B .)

We turn now to a discussion of our numerical work. First we discuss briefly how to compute the meson masses. Then we consider systematic effects that can be addressed directly by varying the bare quark masses (light and heavy). Finally, we consider the remaining discretization effects, by changing the lattice spacing and by studying the corrections in Eq. (1).

In lattice QCD, each meson mass is extracted from a two-point correlation function, which contains contributions from the desired state and its radial excitations. We use constrained curve fitting [21], usually including 5 states, but checking the results with 2–8 states in the fit. We find that the extraction of the raw masses is straightforward on every ensemble.

Statistical errors are obtained with the bootstrap method, allowing us to incorporate the correlated fluctuations when combining the masses as in Eqs. (2) and (3). The statistical precision on $\Delta_{\psi\Upsilon}$ is about 4% and on $\Delta_{D_s B_s}$ about 1.5%. But since $\Delta_{\psi\Upsilon} \approx 40$ MeV and $\Delta_{D_s B_s} \approx -1200$ MeV, the statistical error on m_{B_c} ends up being much larger with the heavy-light baseline.

Figure 1 shows how the splittings depend on the light quark mass m_l , for the ensembles with $a \approx \frac{1}{8}$ fm. One sees that the dependence on m_l is hardly significant. We extrapolate linearly in m_l/m_s , down to the value that reproduces the pion mass [2]. The mild dependence on m_l also suggests that the uncertainty from the known (but small) mistuning of the strange quark sea is completely negligible.

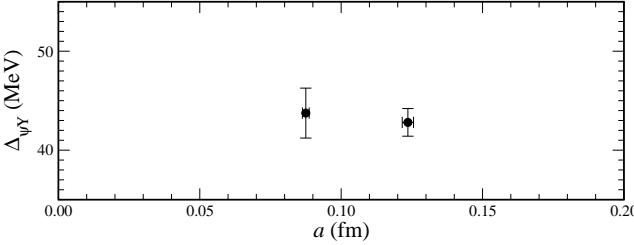


FIG. 2: Dependence of $\Delta_{\psi Y}$ on the lattice spacing at $m_l = 0.2m_s$.

The bare masses of the heavy quarks are chosen as follows. Since the overall mass is shifted [by δm in Eq. (1)], we compute the kinetic energy of $\bar{b}b$ and $\bar{c}c$ mesons of (small) momentum \mathbf{p} , and choose the bare b and c quark masses so that it is $\mathbf{p}^2/2m$, where m is the physical $\bar{Q}Q$ mass. The statistical and systematic uncertainties of the kinetic energy imply a range of bare quark masses. We compute the effect on B_c for different bare b and c masses and derive an error of 10 MeV (5 MeV) in $\Delta_{\psi Y}$ and $\Delta_{D_s B_s}$ from this source.

Figure 2 shows how $\Delta_{\psi Y}$ depends on lattice spacing a for $m_l = 0.2m_s$. The change is insignificant. Lattice spacing dependence stems from all parts of the lattice QCD Lagrangian. In our case, the heavy-quark discretization effects, especially for the c quark, are expected to dominate. Unfortunately, the dependence on $m_c a$ [of the coefficients in Eq. (1)] does not provide a simple Ansatz for extrapolation.

Discretization errors could be studied by varying the couplings in the lattice Lagrangian. Indeed, they could be reduced systematically with better matching, but most of the needed short-distance matching calculations are not available. Instead we shall estimate them using potential models and calculations of the short-distance mismatch. This approach is itself uncertain, but it is preferable to ignoring the issue.

The results of our error estimation are in Table I. The following paragraphs explain how the entries are obtained.

As usual, we classify the operators \mathcal{O}_n in Eq. (1) according to the power-counting scheme of NRQCD (or, for D_s and B_s mesons, HQET). The first several operators are listed in Table I, including all terms of order v^4 in NRQCD and $1/m_Q^2$ in HQET. In general, the leading spin-orbit interaction should appear, but we may omit it, because all states considered here are S wave. To compensate the errors, the table entries should be added to our computed masses. The shifts for the splittings are derived directly from the shifts on the masses.

The entries are obtained as follows. Let us start with the hyperfine interaction $\bar{h}^\pm i \Sigma \cdot \mathbf{B} h^\pm$. Its contribution cancels for spin-averaged masses \bar{m} , by construction, but we must still estimate its effect on m_Y and m_{B_c} . In the heavy-quark Lagrangians we are using, the hyperfine coupling is correctly adjusted only at the tree level. Indeed we find discrepancies in the hyperfine splittings $m_{D_s^*} - m_{D_s}$ and $m_{J/\psi} - m_{\eta_c}$ for the c quark and $m_{B_s^*} - m_{B_s}$ for the b quark. The size of the discrepancy agrees with the expectation from the one-loop mismatch. It is then reasonable to derive an empirical estimate of the coefficient mismatch and propagate it to m_Y and m_{B_c} .

TABLE I: Estimated shifts in masses and the splittings $\Delta_{\psi Y}$ and $\Delta_{D_s B_s}$. Entries in MeV. Dashes (—) imply the entry is negligible.

operator	m_{B_c}	$\frac{1}{2}\bar{m}_\psi$	$\frac{1}{2}m_Y$	$\Delta_{\psi Y}$	\bar{m}_{D_s}	\bar{m}_{B_s}	$\Delta_{D_s B_s}$
$a = \frac{1}{8}$ fm							
$\Sigma \cdot \mathbf{B}$	-14	0	+3	-17	0	0	-14
Darwin	-3	-3	∓ 1	± 1	-4	—	+1
$(\mathbf{D}^2)^2$	+34	+10	± 3	+24	—	—	+34
D_i^4	+16	+5	± 2	+11	—	—	+16
total				+18			+37
$a = \frac{1}{11}$ fm							
$\Sigma \cdot \mathbf{B}$	-12	0	+3	-15	0	0	-12
Darwin	-2	-2	∓ 1	± 1	-2	—	—
$(\mathbf{D}^2)^2$	+17	+5	± 3	+12	—	—	+17
D_i^4	+7	+2	± 2	+5	—	—	+7
total				+2			+12

The entries are then obtained by combining this mismatch of the coefficient with the computed hyperfine splittings.

For m_{B_c} , $\frac{1}{2}\bar{m}_\psi$ and $\frac{1}{2}m_Y$, the matrix elements $\langle \mathcal{O}_n \rangle$ for the Darwin term $\bar{h}^\pm \mathbf{D} \cdot \mathbf{E} h^\pm$ and the relativistic corrections $\bar{h}^\pm (\mathbf{D}^2)^2 h^\pm$ and $\sum_{i=1}^3 \bar{h}^\pm D_i^4 h^\pm$ are obtained from potential models. For \bar{m}_{D_s} and \bar{m}_{B_s} we use HQET dimensional analysis, $\bar{\Lambda}^3/8m_Q^2$ with $\bar{\Lambda} = 700$ MeV, to estimate the Darwin term. In HQET power-counting the other two are of order $\bar{\Lambda}^4/8m_Q^3$ and are neglected.

Next we multiply these estimates with the mismatch coefficients $f_n(m_Q a)$. We have explicit tree-level calculations of them for the Fermilab Lagrangian used for the c quark. For the b quark the mismatch starts at order α_s , so we take f_n to be of order α_s with unknown sign. The resulting shifts from the c quark are larger, also because the c quark is less non-relativistic, but their sign is definite.

The entries in Table I for $(\mathbf{D}^2)^2$ and D_i^4 are uncertain. The cancellations across each row are reliable, but the overall magnitude could be larger. The same potential model suggests a shift in our $m_{B_c} - \bar{m}_\psi$, of about -10 MeV, consistent with the computed discrepancy [1, 6]. Thus, although these shifts may be too small, the charmonium spectrum suggests that they are reasonable. The relativistic corrections decrease substantially when a is reduced, so it is clear how to improve on our result in the future.

Table I suggests that our results for m_{B_c} will be too low, and that m_{B_c} will be lower with the heavy-light baseline than with the quarkonium baseline. If our main aim was to guide the search for B_c , we would consider applying the shifts in Table I to our lattice QCD results. Our aim, however, is to test lattice QCD. Therefore, we treat these shifts not as corrections but as uncertainties. Since we claim to know the sign in the important cases, the associated error bars are asymmetric.

After extrapolating the light quark mass and accumulating the other systematic uncertainties we find (at $a = \frac{1}{8}$ fm)

$$\Delta_{\psi Y} = 39.8 \pm 3.8 \pm 11.2^{+18} \text{ MeV}, \quad (4)$$

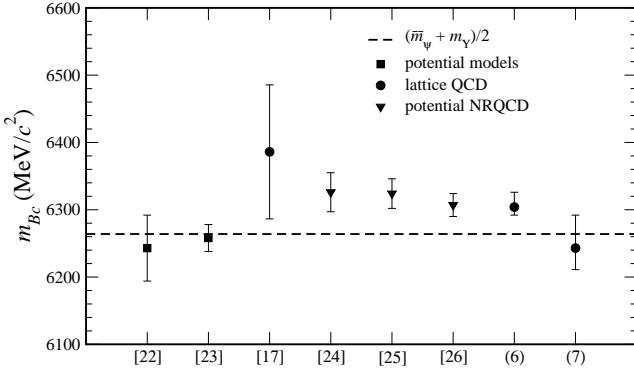


FIG. 3: Comparison of theoretical work, with references in brackets and our equation numbers in parentheses.

$$\Delta_{D_s B_s} = -[1238 \pm 30 \pm 11^{+0}_{-37}] \text{ MeV}, \quad (5)$$

where the uncertainties are, respectively, from statistics (after extrapolating in m_l/m_s), tuning of the heavy-quark masses, and heavy-quark discretization effects. The result for $\Delta_{\psi\Upsilon}$ at $a = \frac{1}{11}$ fm is completely consistent. For the B_c mass we find

$$m_{B_c} = 6304 \pm 4 \pm 11^{+18}_{-0} \text{ MeV}, \quad (6)$$

$$m_{B_c} = 6243 \pm 30 \pm 11^{+37}_{-0} \text{ MeV}, \quad (7)$$

restoring, respectively, the quarkonium and heavy-quark baselines. These two results agree reasonably well. We have carried out more checks on the quarkonium baseline, so we take Eq. (6) as our main result. In both cases the last error bar is itself uncertain, so we have rounded them up, but it is reasonable. It can be reduced at smaller lattice spacing, and with more highly improved Lagrangians for the charmed quark.

Our results are compared to other theoretical predictions in Fig. 3, including potential models [22, 23], quenched lattice QCD [17], and potential NRQCD [24–26]. The quarkonium baseline is shown for reference. The near equality of our result with potential NRQCD is provocative; it seems to say that the truly non-perturbative contributions to the quarkonium masses cancel in the difference $\Delta_{\psi\Upsilon}$.

Our result is so much more accurate than the previous lattice QCD result [17], simply because we have eliminated the quenched approximation. If our prediction, Eqs. (6) and (7), is borne out by measurements, it lends confidence in lattice QCD, not only in MILC’s method for including sea quarks, but also in the control of heavy-quark discretization effects using effective field theory ideas. Moreover, within this framework it is clear how to improve the lattice QCD Lagrangian to reduce the remaining uncertainties.

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