Mass of the *Bc* **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 ensembles of lattice gauge fields, which have a quark sea with two flavors much lighter than a third. Our final result is $m_{B_c} = 6304 \pm 12^{+18}_{-0}$ 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. 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 cutoff 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. Some examples are 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* heavyquark methods, and are under investigation [3,4].

Another example, pursued here, is the mass of the pseudoscalar *Bc* meson, the lowest-lying bound state of a bottom antiquark (*b*) and a charmed quark (*c*). The B_c mass principally tests the heavy-quark methods of lattice QCD. Based on experience with *bb* [5] and *cc* [6] mass splittings, we expect only mild sensitivity to the lightquark 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 $B_c^+ \rightarrow J/\psi l^+ \nu_l$, with a mass resolution of around 400 MeV [8,9]. During run 2 of the Fermilab Tevatron, B_c is expected be observed in nonleptonic 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, which is 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 nonrelativistic 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 heavy quarks in lattice gauge theory [16]. The couplings of the Lagrangian are adjusted so that [15]

$$
\mathcal{L}_{lat} \doteq \mathcal{L}_{QCD} + \delta m(\bar{h}^+h^+ + \bar{h}^-h^-) + \sum_{n} a^{s_n} f_n(m_Q a) \mathcal{O}_n, \tag{1}
$$

where $\dot{=}$ can be read "has the same mass spectrum as." The δm term is an unimportant overall shift in the mass spectrum; h^+ (h^-) is a effective field for quarks (antiquarks); the \mathcal{O}_n are the effective operators of the heavyquark expansion, of dimension dim $\mathcal{O}_n = 4 + s_n$, $s_n \ge 1$; and *a* is the lattice spacing. The coefficients f_n arise from the short-distance mismatch 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, one must vary *a* and also estimate 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 heavyquark 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 $m_l = 0.1 m_s$, $m_l = 0.2m_s$, and $m_l = 0.4m_s$. The gluon and sea-quark Lagrangians are improved to reduce discretization effects. We use three lattice spacings, $a \approx \frac{1}{11}$, $\frac{1}{8}$, $\frac{2}{11}$ fm. 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 (nontrivial) 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,

$$
\Delta_{\psi\Upsilon} = m_{B_c} - (\bar{m}_{\psi} + m_{\Upsilon})/2, \tag{2}
$$

$$
\Delta_{D_{s}B_{s}} = m_{B_{c}} - (\bar{m}_{D_{s}} + \bar{m}_{B_{s}}), \tag{3}
$$

where $\bar{m}_{\psi} = (m_{\eta_c} + 3m_{J/\psi})/4$, $\bar{m}_{D_s} = (m_{D_s} + 3m_{D_s^*})/4$, and $\bar{m}_{B_s} = (m_{B_s} + 3m_{B_s})/4$ are spin-averaged masses. We refer to $(\bar{m}_{\psi} + m_{\Upsilon})/2$ 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 $a\Delta_{\psi Y}$ and $a\Delta_{D,B_s}$ (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 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 the hyperfine operator $\bar{h}^{\pm} i \Sigma \cdot Bh^{\pm}$. (We do not spin-average Y 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 light quarks. (Hence we use D_s and B_s , not D and B_s .)

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. The statistical precision on $\Delta_{\psi Y}$ is about 4% and on Δ_{D, B_s} about 1.5%. But since $\Delta_{\psi Y} \approx 40 \text{ MeV}$ and $\Delta_{D, B_s} \approx$ -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 lightquark mass m_l for the ensembles with $a \approx \frac{1}{8}$ fm. 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.

The bare masses of the heavy quarks are chosen as follows. Since the overall mass is shifted $\lceil by \delta m \rceil$ in Eq. (1)], we compute the kinetic energy of *bb* and $\bar{c}c$ mesons of (small) momentum *p* and choose the bare *b* and *c* quark masses so that it is $p^2/2m$, where *m* is the physical *QQ* 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 Δ_{D,B_s} from this source.

FIG. 1. Sea-quark mass dependence of $\Delta_{\psi\Upsilon}$ and $\Delta_{D_sB_s}$.

Figure 2 shows how $\Delta_{\psi Y}$ depends on lattice spacing *a*. 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_ca [of the coefficients in Eq. (1)] does not provide a simple Ansatz for extrapolation.

We shall treat discretization errors with Eq. (1), using calculations of the short-distance mismatch and estimates of the \mathcal{O}_n . This approach is itself uncertain, but it is preferable to ignoring the issue. The results of such an analysis are given in Table I, and 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 *Ds* and B_s mesons, HQET). Table I lists those of order v^4 in NRQCD; in HQET they are of order $1/m_Q^n$, $n = 1, 2, 3, 3$. The spin-orbit interaction $\bar{h}^{\pm} i\Sigma \cdot (D \times \tilde{E}) h^{\pm}$ is omitted, because its matrix elements vanish in the *S*-wave states considered here.

The contribution of the hyperfine interaction $\bar{h}^{\pm} i \Sigma$. $\mathbf{B}h^{\pm}$ 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 in the coefficient. The hyperfine entries for m_Y and m_{B_c} are obtained by combin-

FIG. 2. Lattice-spacing dependence of $\Delta_{\psi Y}$.

ing the coefficient mismatch with the computed hyperfine splittings.

For m_{B_c} , $\frac{1}{2}\overline{m}_{\psi}$, and $\frac{1}{2}m_Y$, the matrix elements of the Darwin term \bar{h}^{\pm} $\mathbf{D} \cdot \mathbf{E} \bar{h}^{\pm}$ and the relativistic corrections \overline{h}^{\pm} $(D^2)^2 h^{\pm}$ and $\sum_{i=1}^{3} \overline{h}^{\pm} D_i^4 h^{\pm}$ are obtained from potential models. For \bar{m}_{D_s} and \bar{m}_{B_s} we use HQET dimensional analysis: $\langle \mathbf{D} \cdot \mathbf{E} \rangle \sim \bar{\Lambda}^3$, $\langle D^4 \rangle \sim \bar{\Lambda}^4$, with $\bar{\Lambda} = 700$ MeV. Next we multiply the estimated matrix elements $\langle \mathcal{O}_n \rangle$ with the mismatch coefficients $f_n(m_0a)$. We have explicit treelevel 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 but their sign is definite.

The entries in Table I for $(D^2)^2$ 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 $m_{h_c} - \bar{m}_{\psi}$ of about -10 MeV, consistent with the computed discrepancy [1,6]. Thus the charmonium spectrum suggests that they are reasonable.

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. We could apply 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. Repeating this analysis at other lattice spacings yields consistent error estimates.

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

$$
\Delta_{\psi\Upsilon} = 39.8 \pm 3.8 \pm 11.2^{+18}_{-0} \text{ MeV}, \tag{4}
$$

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

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 results for $\Delta_{\psi Y}$ at $a = \frac{1}{11}, \frac{2}{11}$ fm are completely consistent. For the *Bc* mass we find

TABLE I. Estimated shifts (in MeV) of masses and splittings Δ_{ψ} and $\Delta_{D_sB_s}$ at $a=\frac{1}{8}$ fm. Entries show what should be added to the masses and splittings to compensate for discretization errors. Dots (\cdots) imply the entry is negligible.

Operator			m_{B_c} $\frac{1}{2}\bar{m}_{\psi}$ $\frac{1}{2}m_{\Upsilon}$ $\Delta_{\psi\Upsilon}$ \bar{m}_{D_c} \bar{m}_{B_c}				Δ_{D,B_s}
$\Sigma \cdot B$	-14	Ω		$+3$ -17	0		-14
Darwin		$-3 -3$	∓ 1 +1		-4	\cdots	$+1$
$(D^2)^2$	$+34$	$+10$	\pm 3	$+24$	\cdots	\cdots	$+34$
D_i^4		$+16 +5$	$+2$	$+11$	\cdots	\cdots	$+16$
Total				$+18$			$+37$

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

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

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

restoring, respectively, the quarkonium and heavy-quark baselines. We have carried out more checks on the quarkonium baseline, so we take Eq. (6) as our main result. Given the rough nature of the last error bar, we consider the agreement of the two results to be reasonable. Further work with more highly improved Lagrangians and at finer lattice spacing should reduce this error.

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. 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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- [1] HPQCD, UKQCD, MILC and Fermilab Lattice Collaborations, C. T. H. Davies *et al.*, Phys. Rev. Lett. **92**, 022001 (2004).
- [2] HPQCD, MILC, and UKQCD Collaborations, C. Aubin *et al.*, Phys. Rev. D **70**, 031504 (2004); MILC

Collaboration, C. Aubin *et al.*, Phys. Rev. D **70**, 114501 (2004).

- [3] M. Wingate, C. T. H. Davies, A. Gray, G. P. Lepage, and J. Shigemitsu, Phys. Rev. Lett. **92**, 162001 (2004); J. Shigemitsu *et al.*, Nucl. Phys. B, Proc. Suppl. **140**, 464 (2005); A. Gray *et al.*, Nucl. Phys. B, Proc. Suppl. **140**, 446 (2005).
- [4] Fermilab Lattice, MILC, and HPQCD Collaborations, C. Aubin *et al.*, Phys. Rev. Lett. **94**, 011601 (2005); M. Okamoto *et al.*, Nucl. Phys. B, Proc. Suppl. **140**, 461 (2005); J. N. Simone *et al.*, Nucl. Phys. B, Proc. Suppl. **140**, 443 (2005).
- [5] HPQCD Collaboration, A. Gray *et al.*, Nucl. Phys. B, Proc. Suppl. **119**, 592 (2003).
- [6] M. di Pierro *et al.*, Nucl. Phys. B, Proc. Suppl. **129**, 340 (2004).
- [7] HPQCD, Fermilab Lattice, and UKQCD Collaborations, I. F. Allison *et al.*, Nucl. Phys. B, Proc. Suppl. **140**, 440 (2005).
- [8] CDF Collaboration, F. Abe *et al.*, Phys. Rev. Lett. **81**, 2432 (1998).
- [9] D0 Collaboration, D0 Note 4539-CONF, 2004 (unpublished).
- [10] K. Anikeev *et al.*, hep-ph/0201071.
- [11] W. E. Caswell and G. P. Lepage, Phys. Lett. B **167**, 437 (1986); G. P. Lepage and B. A. Thacker, Nucl. Phys. B, Proc. Suppl. **4**, 199 (1988); B. A. Thacker and G. P. Lepage, Phys. Rev. D **43**, 196 (1991).
- [12] E. Eichten, Nucl. Phys. B, Proc. Suppl. **4**, 170 (1988); E. Eichten and B. Hill, Phys. Lett. B **234**, 511 (1990); **243**, 427 (1990).
- [13] G. P. Lepage, L. Magnea, C. Nakhleh, U. Magnea, and K. Hornbostel, Phys. Rev. D **46**, 4052 (1992).
- [14] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997).
- [15] A. S. Kronfeld, Phys. Rev. D **62**, 014505 (2000).
- [16] For a review see, e.g., A. S. Kronfeld, Nucl. Phys. B, Proc. Suppl. **129**, 46 (2004).
- [17] UKQCD Collaboration, H.P. Shanahan, P. Boyle, C.T.H. Davies, and H. Newton, Phys. Lett. B **453**, 289 (1999).
- [18] MILC Collaboration, C. W. Bernard et al., Phys. Rev. D **64**, 054506 (2001); MILC Collaboration, C. Aubin *et al.*, Phys. Rev. D **70**, 094505 (2004).
- [19] D. H. Adams, Phys. Rev. Lett. **92**, 162002 (2004); Nucl. Phys. B, Proc. Suppl. **140**, 148 (2005).
- [20] HPQCD Collaboration, E. Follana, A. Hart, and C.T.H. Davies, Phys. Rev. Lett. 93, 241601 (2004); S. Dürr, C. Hoelbling, and U. Wenger, Phys. Rev. D **70**, 094502 (2004).
- [21] G. P. Lepage *et al.*, Nucl. Phys. B, Proc. Suppl. **106**, 12 (2002).
- [22] W. k. Kwong and J. L. Rosner, Phys. Rev. D **44**, 212 (1991).
- [23] E. J. Eichten and C. Quigg, Phys. Rev. D **49**, 5845 (1994).
- [24] N. Brambilla and A. Vairo, Phys. Rev. D **62**, 094019 (2000).
- [25] N. Brambilla, Y. Sumino, and A. Vairo, Phys. Lett. B **513**, 381 (2001).
- [26] N. Brambilla, Y. Sumino, and A. Vairo, Phys. Rev. D **65**, 034001 (2002).