Mixing Parameters from Unquenched Lattice QCD

Emel Dalgic,1 Alan Gray,1 Elvira Gamiz,2 Christine T. H. Davies,2 G. Peter Lepage,3 Junko Shigemitsu,1 Howard Trottier,4 and Matthew Wingate5

(HPQCD Collaboration)

1Department of Physics, The Ohio State University, Columbus, OH 43210, USA
2Department of Physics & Astronomy, University of Glasgow, Glasgow, G12 8QQ, UK
3Laboratory of Elementary Particle Physics, Cornell University, Ithaca, NY 14853, USA
4Physics Department, Simon Fraser University, Vancouver, British Columbia, Canada
5Institute for Nuclear Theory, University of Washington, Seattle, WA 98195-1550, USA

We determine hadronic matrix elements relevant for the mass and width differences, \( \Delta M_s \) & \( \Delta \Gamma_s \), in the \( B_s^0 - \overline{B_s^0} \) meson system using fully unquenched lattice QCD. We employ the MILC collaboration gauge configurations that include \( u, d \) and \( s \) sea quarks using the improved staggered quark (AsqTad) action and a highly improved gluon action. We implement the valence \( s \) quark also with the AsqTad action and use NonRelativistic QCD for the valence \( b \) quark. For the nonperturbative QCD input into the Standard Model expression for \( \Delta M_s \) we find \( f_{B_s} \sqrt{B_{B_s}} = 0.281(21) \)GeV. Results for four-fermion operator matrix elements entering Standard Model formulas for \( \Delta \Gamma_s \) are also presented.

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INTRODUCTION

Recent developments at the Tevatron Run II have dramatically improved our knowledge of the mass difference \( \Delta M_s \) between the “heavy” and “light” mass eigenstates in the \( B_s^0 - \overline{B_s^0} \) system. The Spring of 2006 witnessed first the two-sided bound on \( \Delta M_s \) by the DØ collaboration \[1\] followed quickly by a precise measurement of this quantity by the CDF collaboration \[2\]. \( B_s \) mixing occurs in the Standard Model through box diagrams with two W-boson exchanges. These diagrams can be reexpressed in terms of an effective Hamiltonian involving four-fermion operators. In order to compare the Tevatron measurements with Standard Model predictions, matrix elements of the four-fermion operators between the \( B_s^0 \) and \( \overline{B_s^0} \) states must be computed. Only then can one test for consistency between experiment and the Standard Model and, in the case that precise agreement fails to be realized, hope to discover hints of new physics. \( B_s^0 - \overline{B_s^0} \) mixing is a \( \Delta B = 2 \) process and sensitive to effects of physics beyond the Standard Model. Hence a large effort is underway to nail down the Standard Model predictions as accurately as possible. In the current article we present a fully unquenched lattice QCD determination of the hadronic matrix elements of several crucial four-fermion operators.

SIMULATION DETAILS

Our simulations use the MILC collaboration \( N_f = 2+1 \) unquenched gauge configurations \[3\]. To date we have completed calculations on two of the MILC coarse ensembles with the light sea quark mass \( m_f \) satisfying \( m_f/m_s = 0.25 \) and \( m_f/m_s = 0.5 \) respectively and with \( m_s \) being the physical strange quark mass. For the strange valence quark we use the improved staggered (AsqTad) quark action. The \( b \)-quark is simulated using the same improved nonrelativistic (NRQCD) action employed in recent studies of the \( \Upsilon \) system \[8\] and for calculations of the \( B \) and \( B_s \) meson decay constants \[6, 7\] and the \( B \to \pi, \tau \) semileptonic form factors \[8\]. As in our previous work using the MILC configurations we use the \( \Upsilon \) 2S-1S splitting to fix the lattice spacing, which in the present case gives \( a^{-1} = 1.596(30) \)GeV and \( a^{-1} = 1.605(29) \)GeV \[5\] for the \( m_f/m_s = 0.25 \) and \( m_f/m_s = 0.5 \) ensembles respectively. The bare \( b \) and \( s \) quark masses have likewise been fixed already in previous simulations of the \( \Upsilon \) \[5\] and kaon \[4\] systems. Some theoretical issues remain having to do with the need to take a fourth root of the AsqTad action determinant while creating the MILC unquenched configurations. This procedure is the focus of intense scrutiny by the lattice community and there has been considerable progress in our understanding of the issues involved during the past year \[10\]. To date no obstacles have been found to invalidate obtaining true QCD in the continuum limit. The MILC configurations and the light and heavy quark actions employed in this article have also been tested by comparing the results of accurate calculations for a large range of hadronic quantities to experimental results \[11, 12, 13, 14, 15\]. The outcome of these tests have been very encouraging. Here we apply the same successful lattice approach to \( B_s^0 - \overline{B_s^0} \) mixing.

THE FOUR-FERMION OPERATORS AND MATCHING

We have studied the following four-fermion operators that enter into calculations of \( \Delta M_s \) and \( \Delta \Gamma_s \) in the Stan-
and V put into this formula is the combination (CKM) matrix elements. The nonperturbative QCD in-

\[ \Delta \text{In continuum QCD in the } MS \text{ scheme, } \langle O \rangle^{MS} = \langle B_s|O|B_s \rangle^{MS} = \frac{8}{3} \rho_{B_s} \langle \mu \rangle M_{B_s}^2. \]  

(4)

The factor \( \frac{8}{3} \) is inserted so that \( B_{B_s} = 1 \) corresponds to the “vacuum saturation” approximation. The four-

fermion operators OS and O3 have similarly each their own bag parameter

\[ \langle OS \rangle^{MS} = \frac{5}{3} \rho_{B_s} \langle \mu \rangle M_{B_s}^2, \]  

(5)

\[ \langle O3 \rangle^{MS} = \frac{1}{3} \rho_{B_s} \langle \mu \rangle M_{B_s}^2. \]  

(6)

with

\[ \frac{1}{R^2} = \left( \frac{M_{B_s}^2}{m_b + m_s} \right)^2. \]  

(7)

The Standard Model expression for the mass difference \( \Delta M_s \) is given by \([10]\),

\[ \Delta M_s = \frac{G_F M_W^2}{16 \pi^2} |V_{ts} V_{td}|^2 \eta_2^B S_{0}(x_t) M_{B_s} f_{B_s}^2 \bar{B}_{B_s}, \]  

(8)

where \( x_t = m_t^2/M_W^2, \eta_2^B \) is a perturbative QCD correction factor, \( S_{0}(x_t) \) the Inami-Lim function and \( V_{ts} \) and \( V_{td} \) the appropriate Cabibbo-Kobayashi-Maskawa (CKM) matrix elements. The nonperturbative QCD input into this formula is the combination \( f_{B_s}^2 \bar{B}_{B_s} \) with \( \bar{B}_{B_s} \) the renormalization group invariant bag parameter.

At two-loops and using \( n_f = 5 \) and \( \alpha_{MS}^{(n_f=5)}(\mu = m_b) = 4.8 \text{GeV} \) one finds \( \bar{B}_{B_s}/B_{B_s} = 1.534 \).

In order to evaluate hadronic matrix elements of the four-fermion operators via lattice QCD methods, one must first relate the operators in continuum QCD to operators written in terms of light quark and heavy quark fields. We carry out this matching between continuum QCD and the lattice theory through \( O(\alpha_s), O(\Sigma_{QCD}^{(3)}), \) and \( O(\Sigma_{QCD}^{(4)}) \). Our lattice theory works with NRQCD b-

quarks. At lowest order in \( 1/M \) the \( b \) fields in \([11-13]\) must be replaced by NRQCD heavy quark or heavy anti-

quark fields. The tree-level relation between NRQCD and full QCD fields is given by the Foldy-Wouthuysen-

Tani transformation. At \( O(\Sigma_{QCD}^{(3)}) \) this brings in dimension seven corrections to the four-fermion operators, which are of the form,

\[ \langle OL_j \rangle = \frac{1}{2M} \left\{ \left[ \langle \bar{V} \gamma \cdot s \rangle |V_{-A} |\bar{V} \gamma \cdot s \rangle \right] |V_{-A} \rangle + \right\}, \]  

(9)

Similar \( 1/M \) corrections OSj1 and O3j1 can be introduced for the four-fermion operators OS and O3. To the order stated above, matching between \( \langle O \rangle^{MS} \) (\( X = L, S \) or 3) and matrix elements in the lattice theory is then given by (we suppress the \( \mu \) dependence),

\[ \frac{a^3}{2M_{B_s}} \langle O \rangle^{MS} = \left[ 1 + \alpha_s \rho_{XX} \langle O \rangle \right] + \alpha_s \rho_{XY} \langle O \rangle \]  

\[ + \left[ \langle O \rangle j1 \rangle - \alpha_s \rho_{XY} \langle O \rangle \right] \left[ \alpha_s \rho_{XX} \langle O \rangle + \rho_{YY} \langle O \rangle \right]. \]  

(10)

\( \langle O \rangle \) without the superscript \( MS \) stands for the matrix element in the lattice theory. Even at lowest order in \( 1/M \) there is mixing between the four-fermion operators. At \( O(\alpha_s) \) the mixing occurs between \( X, Y = L \) and \( S \) for \( \langle OL \rangle \) and \( \langle OS \rangle \) and between \( X, Y \) equal to 3 and \( L \) for \( \langle O3 \rangle \). This mixing takes place already in continuum QCD when one carries out an expansion in \( 1/M \) \([17,18]\). Due to the good chiral properties of AsqTad light quarks, which we use for the valence \( s \) quark in our simulations, no additional operator mixing arises upon going from the continuum to the lattice theory. We have multiplied \( \langle O \rangle^{MS} \) in \([10]\) by a factor of \( a^{-3} \) \( \langle \Sigma_{QCD}^{(3)} \rangle \) in order to take into account the different normalization of states in QCD and the lattice theory and also to render the lattice matrix elements \( \langle O \rangle \) dimensionless. Details of calculations of the one-loop coefficients \( \rho_{XY} \) and \( \rho_{XX} \) will be presented in a separate paper. The methodology is similar to that of \([19,20]\). As in those matching calculations for heavy-light currents, the \( \alpha_s \rho_{XX} \) and \( \alpha_s \rho_{YY} \) terms in \([10]\) are necessary to subtract \( O(\Sigma_{QCD}^{(4)}) \) power law contributions from the matrix elements \( \langle O \rangle j1 \).
TABLE I: Matrix elements in the lattice theory for fixed $b$ and $s$ valence masses and two values of the light $u$, $d$ sea quark mass. Errors are statistical plus fitting errors.

|               | $m_t/m_s = 0.25$ | $m_t/m_s = 0.50$ |
|---------------|------------------|------------------|
| $\langle OL \rangle$ | 0.1036(83)       | 0.1069(92)       |
| $\langle OS \rangle$ | -0.0680(54)      | -0.0687(61)      |
| $\langle O3 \rangle$ | 0.0143(12)        | 0.0142(13)       |
| $\langle O1j1 \rangle$ | -0.0227(18)      | -0.0229(18)      |
| $\langle OSj1 \rangle$ | -0.0130(10)      | -0.0130(11)      |
| $\langle O3j1 \rangle$ | 0.0021(3)         | 0.0026(3)        |
| $\langle O1j1 \rangle_{(sub)}$ | -0.0138(20)      | -0.0140(20)      |
| $\langle OSj1 \rangle_{(sub)}$ | -0.0072(11)      | -0.0081(12)      |
| $\langle O3j1 \rangle_{(sub)}$ | 0.0008(3)         | 0.0012(4)        |

\[
N_{\text{exp}}-1 \sum_{j,k=0}^{N_{\text{exp}}-1} A_{jk} \left( -1 \right)^j t_1 \left( -1 \right)^k t_2 e^{-E^3_{t_1}}(t_1-1) e^{-E^3_{t_2}}(t_2-1),
\]

(12)

\[
C^B(t) = \sum_{j=0}^{N_{\text{exp}}-1} \xi_j \left( -1 \right)^j t e^{-E^3_{t_j}}(t-1).
\]

(13)

Results for $\hat{O}$ are summarized in Table I for our two dynamical ensembles. The errors are combined statistical and fitting uncertainty errors. More details on our fits are given in [21]. In Table I we also show results for $\langle OXj1 \rangle_{(sub)}$ the true relativistic corrections (after power law subtractions) from the dimension seven operators. By considering $\langle OXj1 \rangle_{(sub)}/\langle OX \rangle$, one finds the physical $\mathcal{O}(\Lambda_{QCD}/M)$ contribution to be -13% for $\langle OL \rangle$, 11% for $\langle OS \rangle$ and 6~8% for $\langle O3 \rangle$.

Having determined the matrix elements in the lattice theory we can plug the numbers into the RHS of (10).

For this matching we use $\alpha_s = \alpha_V(n_f=3)(2/a) = 0.32$ [13]. We set the scale for $\alpha_s$ to $q^* = 2/a$, which is close to $q^*$’s evaluated for heavy-light currents using other heavy and light quark actions. The matching coefficients $\rho_{XY}$ are generally functions of the $\overline{\text{MS}}$ scale $\mu$ through the combination log$(\frac{a}{\mu})$. We present results for $\mu = m_b$.

We evaluate the RHS of (10) for $\langle OL \rangle_{\overline{\text{MS}}}$, $\langle OS \rangle_{\overline{\text{MS}}}$ and $\langle O3 \rangle_{\overline{\text{MS}}}$ and combine with the definitions in (4) - (6) to obtain the main results of this article, namely,

\[
f^2_{B_s} B_{B_s}, \quad f^2_{B_s} B_{B_s} \frac{R^2}{f}, \quad f^2_{B_s} B_{B_s} \frac{R^2}{f}.
\]

(15)

The main errors in these quantities are listed in Table II. One sees that the two dominant errors are due to statistics + fitting and higher order matching uncertainties. We have also included a nonnegligible error coming from the uncertainty in the scale (lattice spacing) for the MILC ensembles used. At the final stage of extracting results for (15), one has to convert $a^3 f^2_{B_s} M_{B_s}$ into physical units. An uncertainty of $\sim 1.8\%$ in the lattice spacing turns at this point into a $\sim 5\%$ uncertainty for $a^{-3}$. The leading discretization error in the actions employed here comes in at $\mathcal{O}(a^2 \alpha_s) \sim 2\%$ and is believed to be dominated by taste-changing effects in the Asqtad action, an assumption that has been checked recently by comparing Asqtad valence quarks with more highly improved staggered quarks from the HISQ action [22]. We multiply the 2% by a factor of 2 to come up with a total discretization uncertainty of 4%, which should cover taste-changing effects in the sea as well, including the fourth root. This total error is consistent with scaling tests carried out via explicit simulations at two lattice spacings of other B physics quantities such as decay constants and semileptonic form factors employing the same actions as in the present article [6, 8]. In the future we plan to repeat the current calculations at finer lattice spacings in order to reduce discretization uncertainties and also to carry out tests with HISQ instead of Asqtad light valence quarks.

In Table II we take the operator matching error to be $1 \times \alpha_s^2$ since matching is done directly for the combination $f^2_{B_s} B_{B_s}$ (and for the other quantities in (15)). A naive attempt to deal separately with $f^2_{B_s}$ and $B_{B_s}$ in the formula for $\Delta M_s$ could increase the error estimate since the perturbative error for just $f_{B_s}$ alone (unsquared) is usually also taken as $1 \times \alpha_s^2$ coming from higher order matching of the heavy-light current. We avoid unnecessarily separating out the bag parameters and possibly introducing ambiguities in error estimates by always working with the relevant combination $f^2_{B_s} B_{B_s}$. Several years ago reference [23] also emphasized the virtues of working with physical combinations and never splitting off the bag parameters. The possibility of reducing errors by focusing on the combined $f^2_{B_s} B_{B_s}$ is also mentioned in [24].

Table III gives our final values for the square root of the quantities listed in (15) together with the scale invariant combination $f_{B_s} \sqrt{B_{B_s}}$. One sees that the light sea quark
TABLE III: Results for the square root of quantities listed in (15). The unhatted bag parameters are given at scale $\mu = m_b$. Errors quoted are combined statistical and systematic errors. Note that percentage errors here are smaller than those given in Table II by a factor of two due to the square root.

| $B_s$/$B_s$ [GeV] | $m_f/m_s = 0.25$ | $m_f/m_s = 0.50$ |
|------------------|------------------|------------------|
| $f_{B_s} \sqrt{B_{B_s}}$ | 0.281(21) | 0.289(22) |
| $f_{B_s} \sqrt{B_{B_s}(m_b)}$ [GeV] | 0.227(17) | 0.233(17) |
| $f_{B_s} \sqrt{B_{B_s}(m_b)}$ [GeV] | 0.295(22) | 0.301(23) |
| $f_{B_s} \sqrt{B_{B_s}(m_b)}$ [GeV] | 0.305(23) | 0.310(23) |

mass dependence is small and not statistically significant. The largest difference between the central values of the $m_f/m_s = 0.25$ and $m_f/m_s = 0.5$ results is less than 3%, smaller than any of the other errors, and in particular significantly smaller than our current statistical errors. Any reasonable estimate of chiral extrapolation (in $m_{sea}$) uncertainties will not affect the total error in Table II. In the future we plan to use Staggered Chiral perturbation theory (SChPT) [22, 23] to extrapolate to the physical chiral limit. SChPT formulas for $B_s$ mixing with Asqtad light quarks are being worked out by Laiho and Van de Water [22] and will be important in $B_d$ mixing studies where one needs to extrapolate in both the valence and sea light quark masses. In the present case of $B_s$ mixing and until our statistical errors have been further reduced and more data points are available, we do not believe the whole machinery of SChPT is crucial. We note that in our studies of the $B_s$ meson decay constant, where we have data for $f_{B_s}$ at four different light sea quark masses on coarse MILC ensembles and for two sea quark masses on the fine MILC lattices, no sea quark mass dependence was observed [4, 28]. We do not attempt a chiral extrapolation in the light sea quark mass with the current data and take the $m_f/m_s = 0.25$ numbers as our best determinations of the hadronic matrix elements. In particular, this gives for the combination $f_{B_s} \sqrt{B_{B_s}}$, the crucial nonperturbative ingredient for $\Delta M_s$, the value quoted in the abstract:

$$f_{B_s} \sqrt{B_{B_s}} = 0.281(21) \text{ GeV}. \quad (16)$$

RESULTS FOR THE WIDTH DIFFERENCE $\Delta \Gamma_s$

We have emphasized our result [10] since this enters into $\Delta M_s$ for which a precision experimental measurement exists. The other entries in Table III for the four-fermion operators “OS” and “O3” are relevant for the width difference $\Delta \Gamma_s$ [31, 32], for which experimental errors are currently still greater than 50%. A recent measurement by the DØ Collaboration [33] gives, for instance, $\Delta \Gamma_s = [0.13 \pm 0.09] \text{ps}^{-1}$. On the theory side, the authors of [32] have recently shown that by going to a new basis employing operators “OL” & “O3”, as opposed to the old basis of “OL” & “OS”, theoretical uncertainties from $1/m_b$ and $\alpha_s$ corrections can be significantly reduced. We insert our results from Table III for $f_{B_s} \sqrt{B_{B_s}}$ and $f_{B_s} \sqrt{B_{B_s}}$, taking again the $m_f/m_s = 0.25$ data, into eq.(51) of reference [32] and obtain,

$$\Delta \Gamma_s = 0.10(3) \text{ps}^{-1}, \quad (19)$$

which is consistent with the DØ measurement. About half the error in [19] comes from lattice errors in $f_{B_s}^2 B_{B_s}$ and $f_{B_s}^2 B_{B_s}$ and the other half from remaining theoretical uncertainties in the formula of [32]. Both types of errors can be reduced through further work on the lattice and we plan to focus on obtaining a more accurate Standard Model theory prediction for $\Delta \Gamma_s$ while waiting for the experimental measurements to improve as well.

We argued above that there is no need to separate out the bag parameters when calculating $\Delta M_s$ or $\Delta \Gamma_s$. standard values for the other ingredients in [8] taken from recent reviews. We use $\eta_b^2 = 0.551(7)$, $\bar{m}_b(m_t) = 162.3(2.2) \text{GeV}$ (which leads to $\alpha_0(x_b) = 2.29(5)$) and $|V_{ts}^* V_{tb}| = 4.1(1) \times 10^{-2} [24, 30]$ together with [10] to obtain

$$\Delta M_s(\text{theory}) = 20.3(3)(0.8) \text{ps}^{-1}. \quad (17)$$
One might nevertheless be interested in doing so to judge how close we are to the “vacuum saturation” approximation. To convert to bag parameters we use the central value of the $B_s$ meson decay constant determined in\cite{3}, $f_{B_s} = 0.260(29)$GeV, together with (for $1/R^6$)\cite{32} $m_b = 4.25$GeV and $m_s = 85$MeV. One finds $B_{B_s}(m_b) = 0.76(11)$, $B_S(m_b) = 0.84(13)$ and $B_B(m_b) = 0.90(14)$, values consistent with earlier quenched\cite{18,34} and $N_f = 2$\cite{35} lattice determinations.

**SUMMARY**

This article presents full QCD results for hadronic matrix elements of four-fermion operators relevant for $B_s^0 - \overline{B_s^0}$ mixing. We give unquenched results including the effect of 2 + 1 flavors of sea quarks and calculate both leading and next-to-leading matrix elements in a nonrelativistic expansion of four-fermion operators for the first time. Using our nonperturbative QCD results one finds agreement between the recent Tevatron and Standard Model predictions. Our dominant errors for $f_{B_s}^2 \overline{B}_B$ come from statistics + fitting and from higher order operator matching uncertainties. Work is underway aimed at reducing these errors. This will allow even tighter constraints on any beyond the Standard Model effects entering $B_s^0 - \overline{B_s^0}$ mixing phenomena. We have also initiated studies of $B_d^0 - \overline{B_d^0}$ mixing. Our goal there is to obtain precision results for the important ratio $f_{B_s}^2 B_s^0/ f_{B_d}^2 B_d^0$, which will provide further consistency checks on the Standard Model and give us a handle on the CKM matrix element $|V_{td}|$. Some errors listed in Table II will cancel almost completely in this ratio, such as the $a^{-3}$ and the higher order matching uncertainties. Others, such as the statistical and fitting error, will cancel partially.

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