B^0-$\overline{B^0}$-Mixing with Domain-Wall Light Quarks and Relativistic Heavy Quarks

March 20, 2009

Participants: Yasumichi Aoki, Taku Izubuchi, Hao Peng, Amarjit Soni, Ruth S. Van de Water, Oliver Witzel (RBC and UKQCD Collaborations)

Time Requested: The equivalent of 2.7 million 6n node-hours on the Fermilab clusters plus 4.6 Tbytes of tape storage (the equivalent of ∼6000 6n node-hours) and 0.02 Tbytes of disk storage (the equivalent of ∼300 6n node-hours) at Fermilab.

Abstract

We propose a precise determination of the B^0-$\overline{B^0}$ mixing matrix elements and their ratio, $\xi \equiv f_{B_s}\sqrt{\hat{B}_{B_s}}/f_{B_d}\sqrt{\hat{B}_{B_d}}$, on the 2+1 flavor dynamical domain-wall configurations generated by the LHP, RBC, and UKQCD Collaborations. Our calculation will improve upon earlier work of the RBC and UKQCD Collaborations, which used a static b-quark, by using a relativistic action for the b-quark. We will use domain-wall fermions for the light d- and s-valence quarks. A precise determination of ξ will allow a strong constraint on the apex of the CKM unitarity triangle, and is one of the key goals in flavor physics of the U.S. lattice QCD community, as stated in the 2007 white paper. Our calculation will provide a valuable independent cross-check of the results of the HPQCD and Fermilab/MILC Collaborations, both of which rely upon the 2+1 flavor Asqtad-improved staggered lattices generated by the MILC Collaboration. We request the equivalent of 2.7 million 6n node-hours on the Fermilab clusters plus 4.6 Tbytes of tape storage (the equivalent of ∼6000 6n node-hours) and 0.02 Tbytes of disk storage (the equivalent of ∼300 6n node-hours) for this project.

Scientific Motivation

Recent experimental measurements of the mass-differences of the neutral B-meson mass eigenstates Δm_d and Δm_s to $\sim 1\%$ accuracy [1] now allow the possibility of precisely determining the ratio of the CKM matrix elements $|V_{td}|/|V_{ts}|$. The uncertainty in this ratio, however, is limited by the knowledge of the nonperturbative factor $\xi \equiv f_{B_s}\sqrt{\hat{B}_{B_s}}/f_{B_d}\sqrt{\hat{B}_{B_d}}$, which parameterizes the hadronic contribution to B^0-$\overline{B^0}$ mixing [2]. It is likely that new physics would give rise to new quark-flavor changing interactions and additional CP-violating phases; these would manifest themselves as apparent inconsistencies among different measurements of quantities which should be identical within the standard CKM picture. Thus a precise determination of the ratio ξ will help to constrain physics beyond the Standard Model. In fact, there are already possible indications of new physics in B_d-mixing at the $\sim$2.7-σ level, as pointed out in Ref. [3]. Because the importance of ξ to new physics searches is well known to the lattice community, this quantity was highlighted as one of three "key matrix elements" in the USQCD Collaboration's 2007 white paper "Fundamental parameters from future lattice calculations" [4]. We are therefore submitting a Type A proposal to calculate the B^0-$\overline{B^0}$ mixing matrix elements $f_{B_s}\sqrt{\hat{B}_{B_s}}$, $f_{B_d}\sqrt{\hat{B}_{B_d}}$, and ξ using dynamical domain wall fermions and relativistic b-quarks.

Both the HPQCD and Fermilab/MILC Collaborations are also computing the B^0-$\overline{B^0}$ mixing matrix elements. The HPQCD Collaboration has recently published a determination of ξ to 2.6% accuracy [5], and the Fermilab Lattice and MILC Collaborations expect to have a result with similar errors soon [6]. Both of these computations, however, rely on the 2+1 flavor Asqtad-improved staggered ensembles generated by the MILC Collaboration. Therefore, for such a phenomenologically-important quantity as ξ, it is valuable to have an independent crosscheck using a different light quark formulation.

Our calculation will use the 2+1 flavor dynamical domain wall ensembles generated by the LHP, RBC, and UKQCD Collaborations with lattice spacings of $a \approx 0.11$ fm and $a \approx 0.08$ fm. We will compute several partially-quenched light domain-wall valence quark propagators on each ensemble. This will allow us to extrapolate to the physical light quark masses and the continuum in a controlled manner using chiral perturbation theory (χPT), which is particularly simple for the case of domain-wall fermions. The leading light-quark discretization effects in our calculation will be of $\mathcal{O}(a^2p^2)$. We will use the relativistic heavy quark (RHQ) action developed by Christ, Li, and Lin for the heavy b-quarks [7, 8]. This will improve upon the B^0-$\overline{B^0}$ mixing calculation of the RBC and UKQCD Collaborations using static quarks by including relativistic corrections that are $\propto 1/m_b$ [9, 10].[1] The RHQ method extends the Fermilab approach [11] by tuning all of the parameters of the clover action nonperturbatively [12]. The RHQ action is accurate to $\mathcal{O}(a^2p^2)$, but to all orders in $(am_b)^n$; thus it allows the computation of heavy-light spectrum quantities with discretization errors of the same order as in light-light quantities.

With the resources requested in this proposal, we expect to determine the ratio ξ to an accuracy of $\sim 5\%$, with comparable systematic errors to those of the other dynamical calculations. In order to obtain total errors comparable to those of HPQCD and Fermilab/MILC, we will likely need to further reduce the statistical and chiral extrapolation errors by running on additional configurations or with additional operator time sources in the following allocation year.

---

[1] We are also submitting a Type B proposal to complete the static B^0-$\overline{B^0}$ mixing project. The calculation with static b-quarks will provide a valuable cross-check of the $SU(3)$-breaking ratio ξ because the $1/m_b$ corrections should be proportional to $(m_s - m_d)$.

Table 1: Available RBC/UKQCD 24^3 and 32^3 ensembles. The pion masses on the coarser 24^3 lattices are given in Ref. [13], while the pion masses on the finer 32^3 lattices are preliminary estimates. Most ensembles were recorded every five trajectories, but the $am_l/am_s = 0.006/0.030$ ensemble was recorded every 4 trajectories.

a(fm)	L	m_l	m_s	m_π(MeV)	approx. # configs.
≈ 0.08	32	0.004	0.030	307	600
≈ 0.08	32	0.006	0.030	366	900
≈ 0.08	32	0.008	0.030	418	600
≈ 0.11	24	0.005	0.040	331	1600
≈ 0.11	24	0.01	0.040	419	1700
≈ 0.11	24	0.02	0.040	558	700
≈ 0.11	24	0.03	0.040	672	600

Computation Method

We will use the 2+1 flavor dynamical domain wall lattices generated by the RBC, UKQCD, and LHP collaborations for the computation of the B^0-$\overline{B^0}$ mixing matrix elements. The available ensembles are shown in Table 1. We refer to these by their spatial volumes in lattice units; the coarser "24^3" ensembles have $a \approx 0.11$ fm and the finer "32^3" ensembles have $a \approx 0.08$ fm. We will generate domain-wall valence quark propagators on these configurations using the same values of the domain-wall height ($M_5 = 1.8$) and the fifth-dimensional extent ($L_s = 16$) as in the sea sector. This will allow us to use the determinations of the light and strange valence quark masses and the residual quark mass from RBC/UKQCD's analysis of the light-pseudoscalar meson masses and decay constants [13]. We will generate both unitary and partially quenched data points; the additional correlated data will give us better control over the extrapolation to the physical light quark masses. In order to best take advantage of the larger number of configurations available on the coarser 24^3 ensembles, we will fit the 24^3 and 32^2 data together and perform a simultaneous extrapolation to the physical light quark masses and the continuum using partially-quenched heavy-meson χPT [14] supplemented by analytic terms $\propto a^2$ to parameterize light-quark discretization effects.

We will use the relativistic heavy quark action for the b-quarks [7, 8]. The appropriate parameters have already been determined for the 24^3 lattices in Ref. [12], and we will tune the parameters on the 32^3 lattices in the same manner. By tuning the value of the hopping-parameter κ such that the kinetic meson mass M_2 is equal to the physical spin-averaged B-meson mass and tuning the value of the clover coefficient c_{SW} so that we reproduce the correct hyperfine splitting $m_{B_s^*} - m_{B_s}$, we match the lattice action onto the continuum action through $\mathcal{O}(pa)$, leaving errors of $\mathcal{O}(p^2a^2)$. Because the RHQ action treats the heavy-quark mass to all-orders in $m_b a$, the coefficient of the $\mathcal{O}(p^2a^2)$ heavy-quark discretization errors is a function of $m_b a$. Fortunately, however, El-Khadra, Kronfeld, and Mackenzie, showed that the function of $m_b a$ is always bounded to be of $\mathcal{O}(1)$ or less [11].

We will construct the B^0-$\overline{B^0}$ 3-point function in the manner shown in Fig. 1. We will fix the location of the effective four-fermion operator, $t_{\text{Op.}}$, and vary the locations of the B^0 and $\overline{B^0}$ mesons, t_1 and t_2, over all possible time slices. This requires one point-source light quark propagator and one point-source b-quark propagator originating from $t_{\text{Op.}}$. These propagators can be used for

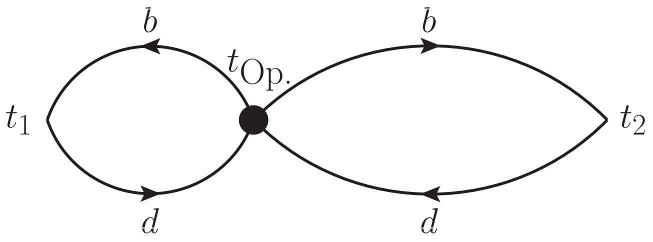

Figure 1: Three-point lattice correlation function for B^0-$\overline{B^0}$ mixing.

both the B^0 and $\overline{B^0}$ mesons, thereby reducing the computational cost. At the sink we will project out the zero-momentum component using a gauge-invariant Gaussian sink. We will compare the possibilities of using a smeared sink for only the heavy quark versus for both the heavy and light quarks on a smaller quenched ensemble. We will then optimize the Gaussian radius on the 24^3 and 32^3 dynamical ensembles.

We will reduce discretization errors in the four-fermion operator by rotating the b-quark at the source as in Ref. [6]. By computing the rotation parameter d_1 at tree-level in tadpole-improved lattice perturbation theory we will improve the operator to $\mathcal{O}(\alpha_s ap)$. We will calculate the renormalization factors needed to match the lattice operator onto the continuum using 1-loop tadpole-improved lattice perturbation theory, such that the truncation errors are of $\mathcal{O}(\alpha_s^2)$. At this order, the desired operator only mixes with one other lattice operator through $\mathcal{O}(1/m_b)$ [6]. Fortunately, because the additional operator resides at a single lattice site, we can reuse the point source light- and b-quark propagators to compute the additional 3-point correlation function. Because the quantity $\xi \equiv f_{B_s}\sqrt{\hat{B}_{B_s}}/f_{B_d}\sqrt{\hat{B}_{B_d}}$ is a ratio, much of the uncertainty due to the truncation of perturbation theory should cancel, even if the truncation errors in the numerator and denominator are more significant. Thus the quantity that is most important for phenomenology should also be the most reliable.

Run Plan and Resource Allocation

The most computationally intensive portion of this project will be the domain-wall propagator inversions, for which we will use the optimized domain-wall inverter in the Chroma lattice QCD software package [16]. We will use our own code, written using the Chroma and QDP++ libraries, to calculate the $\Delta B = 2$ operator. We have checked both the domain-wall and clover inverters against results from the Columbia Physics System [17]. We will check the matrix element code against FermiQCD [18], which is used for the current Fermilab/MILC calculation.

In our first year of running we plan to compute the B^0-$\overline{B^0}$ mixing matrix element on every 10^{th} trajectory on all of the available 32^3 ensembles and two of the available 24^3 ensembles. Because the 24^3 ensemble with $am_l = 0.02$ has many fewer configurations than the $am_l = 0.005, 0.01$ ensembles, we will compute the B^0-$\overline{B^0}$ mixing matrix element on every 5^{th} trajectory on this ensemble. We will not use the $am_l = 0.03$ 24^3 ensemble because the pion mass $m_\pi \approx 672$ MeV is very heavy on this ensemble. Table 2 summarizes our running plan. We plan to compute five valence quark masses per ensemble. The lightest three are equal to the light sea quark masses on the three ensembles per lattice spacing, and the heavier two bracket the physical strange quark mass to allow for an interpolation. An analysis of static B-meson data on the 24^3 lattices shows that 2-point correlators on configurations separated by 10 trajectories are essentially uncorrelated. In order to further reduce autocorrelations, we will move both the temporal and spatial positions of the operator from

Table 2: Proposed domain wall valence and sea quark mass combinations for the calculation of the $B^0 - \overline{B^0}$ matrix elements.

a(fm)	L	m_l	m_s	$m_{val.}^{\mathrm{dwf}}$	# configs.
≈ 0.08	32	0.004	0.030	0.004, 0.006, 0.008, 0.025, 0.030	300
≈ 0.08	32	0.006	0.030	0.004, 0.006, 0.008, 0.025, 0.030	450
≈ 0.08	32	0.008	0.030	0.004, 0.006, 0.008, 0.025, 0.030	300
≈ 0.11	24	0.005	0.040	0.005, 0.01, 0.02, 0.03, 0.04	800
≈ 0.11	24	0.01	0.040	0.005, 0.01, 0.02, 0.03, 0.04	850
≈ 0.11	24	0.02	0.040	0.005, 0.01, 0.02, 0.03, 0.04	700

Table 3: Time to calculate a single domain-wall propagator with $L_5 = 16$ using Chroma on the Fermilab "jpsi" cluster.

a(fm)	L	m_l	nodes (jpsi)	time (hours)	6n node-hours
≈ 0.08	32	0.004	32	4.06	525
≈ 0.08	32	0.006	32	3.07	397
≈ 0.08	32	0.008	32	2.46	318
≈ 0.08	32	0.025	32	0.96	124
≈ 0.08	32	0.03	32	0.84	109
≈ 0.11	24	0.005	16	1.91	123
≈ 0.11	24	0.01	16	1.27	82
≈ 0.11	24	0.02	16	0.79	51
≈ 0.11	24	0.03	16	0.59	38
≈ 0.11	24	0.04	16	0.48	31

configuration to configuration.

We have timed propagator inversions for the domain-wall valence quark masses listed in Table 2 on the 24^3 and 32^3 2+1 flavor domain wall lattices using Chroma on the Fermilab clusters; these are given in Tables 3. We have also timed clover inversions on the 24^3 lattices using the parameters determined in Ref. [12]; these are shown in Table 4. In order to propagate the errors in the nonperturbatively-tuned parameters of the RHQ action through the remainder of the calculation, we will compute the less expensive heavy-quark propagators with seven parameter sets on each ensemble. Using these timings, the total computing resources required to compute the B^0-$\overline{B^0}$ mixing matrix element using all of the light quark masses listed in Table 2 is given in Table 5. Our total computing request is 2.7 million 6n node-hours, and includes both the time needed to compute the quark propagators plus an additional 15% for testing code, optimizing sink smearings, calculating 2-point and 3-point correlation functions, and analysis.

We would like to run on the Fermilab clusters. One of the authors (R.V.) is experienced in running on the Fermilab clusters, and the performance of the domain-wall inverter in Chroma on the Fermilab clusters is better than that of the domain-wall inverter in CPS on the QCDOC. The 24^3 propagators may be run efficiently either on kaon or on jpsi, but the 32^3 ensembles are sufficiently large that the propagators should be generated on jpsi. Thus we would like either a 40%-60% split between time on kaon and jpsi, or all of the time on jpsi. The smaller numbers of cores, decreased memory, and decreased scratch disk space make it impractical to compute the

Table 4: Time to calculate a single clover propagator using Chroma on the Fermilab "jpsi" cluster. The time for the 32^3 ensembles is an estimate based on scaling the 24^3 time by the ratio of the volumes.

a(fm)	L	nodes (jpsi)	time (hours)	6n node-hours
≈ 0.08	32	–	–	4
≈ 0.11	24	1	0.41	2

Table 5: Computer time needed to determine the B^0-$\overline{B^0}$ mixing matrix element using the sea quark ensembles, valence quark masses, and numbers of configurations listed in Table. 2.

24^3 $a = 0.12$ fm domain-wall propagators	0.764 $\times 10^6$ 6n node-hours
32^3 $a = 0.08$ fm domain-wall propagators	1.547 $\times 10^6$ 6n node-hours
24^3 $a = 0.12$ fm clover propagators	0.033 $\times 10^6$ 6n node-hours
32^3 $a = 0.08$ fm clover propagators	0.029 $\times 10^6$ 6n node-hours
code testing, sink optimization, 2-point and 3-point correlators, and analysis	0.356 $\times 10^6$ 6n node-hours
Total	2.729 $\times 10^6$ 6n node-hours

domain-wall propagators on pion, although we can use pion to generate the b-quark propagators, which are smaller by a factor of $L_s = 16$. The b-quark propagators, however, make up a small percentage of our allocation.

We would also like to save all of the domain-wall propagators to tape at Fermilab for enough time to allow their use in other projects and by other groups. Table 6 shows the file sizes of the domain-wall quark propagators for the two different lattice volumes, in both GB and 6n-equivalent node hours assuming that they are stored on tape. A comparison of Table 6 and Tables 3 reveals that calculating the domain-wall propagator is ~ 30 times more expensive than storing it for the cheapest propagator, and ~ 500 times more expensive for the costliest propagator. Thus it is more efficient to save and reuse the domain-wall propagators than to recalculate them. The total storage space needed to save all of the propagators listed in Table 2 is given in Table 7. Our total tape storage request is 4.59 TBytes of tape at Fermilab. We will also need a "/project" area at Fermilab to store our code, data, and logfiles. This, however, will be small and we estimate that we will only need 0.02 TBytes of disk space.

Summary

At the end of this project we expect to have a precise determination of the B^0-$\overline{B^0}$ mixing matrix elements along with a few-percent determination of their ratio ξ including dynamical light quark effects and relativistic heavy quark effects. This would fulfill one of the key goals in flavor physics of USQCD stated in the 2002 strategic plan and the 2007 white paper "Fundamental parameters from future lattice calculations" [4]. Use of two lattice spacings, multiple quark masses, and heavy meson chiral perturbation theory will give us control over the systematic errors associated with both the chiral and continuum extrapolations. This measurement, when used in a unitarity-triangle analysis, will place an important constraint on physics beyond the Standard Model.

With the resources requested we expect to determine ξ to $\sim 5\%$ accuracy. Given that we

Table 6: File sizes of domain-wall propagators for various spatial volumes. The equivalent cost to store the file on tape uses the conversion 1 Tbyte tape = 1,347 6n node-hours.

a(fm)	L	size (GB)	tape storage cost (6n node-hours)
≈ 0.08	32	2.25	3.0
≈ 0.11	24	0.95	1.3

Table 7: Mass storage needed to save all of the domain-wall propagators listed in Table 2. The equivalent cost to store the file on tape uses the conversion 1 Tbyte tape = 1,347 6n node-hours.

32^3 $a \approx 0.08$ fm propagators	2.36 TB
24^3 $a \approx 0.11$ fm propagators	2.23TB
Total	4.59 TB
	= 6183 6n node-hours

expect our systematic error budget to be similar to that of Fermilab/MILC, at this point we will likely be limited by statistical errors. If this is the case, we will request time to compute the matrix elements using additional time sources in a future allocation year. If not, we will work on reducing the dominant systematic errors. For example, if our largest systematic uncertainty in the B-meson decay constants is due to the use of perturbative operator matching, we can recompute the matching factors using the mostly-nonperturbative method of Fermilab/MILC. If there were a substantial increase in our allocation, we could easily use it to improve our statistics or to compute a lighter valence quark mass that is closer to the physical point. We could also run on the BG/P at Argonne, if necessary, since one of the authors is already running Chroma at this facility.

The domain-wall propagators that we will generate can be used for the calculation of other interesting physics quantities, and we encourage other members of the lattice QCD community to do so. Along with the B^0-$\overline{B^0}$ matrix elements, we will compute the B-meson decay constants f_B and f_{B_s}, as well as their ratio f_B/f_{Bs}. We would also like to retain exclusive rights to calculate the D- and D_s-meson decay constants using these propagators in the future. All of the propagators generated will be stored at Fermilab and will be made available immediately for non-competing analyses. Researchers who wish to use them should contact us to arrange access.

Acknowledgments

We thank Norman Christ, Elvira Gamiz, Andreas Kronfeld, Jack Laiho, Min Li, and Norikazu Yamada for useful conversations.

Table 8: Disk storage needed to save 2-point and 3-point correlation functions, logfiles, and analysis files in the "/project" area at Fermilab. Estimate is based on the sizes of the "/project" areas for other established projects. The equivalent cost to store the file on disk uses the conversion 1 Tbyte disk = 13,470 6n node-hours.

estimated	0.02 TB
Total	0.02 TB
	= 269 6n node-hours

References

[1] C. Amsler *et al.* [Particle Data Group], Phys. Lett. B **667**, 1 (2008).

[2] M. Bona *et al.*[UTfit Collaboration], http://utfit.roma1.infn.it/;
J. Charles *et al.*[CKMfitter Group], http://ckmfitter.in2p3.fr/.

[3] E. Lunghi and A. Soni, Phys. Lett. B **666**, 162 (2008) [arXiv:0803.4340 [hep-ph]].

[4] http://www.usqcd.org/documents/fundamental.pdf.

[5] E. Gamiz, C. T. H. Davies, G. P. Lepage, J. Shigemitsu and M. Wingate, arXiv:0902.1815 [hep-lat].

[6] R. Todd Evans, E. Gamiz, and A. X. El-Khadra, PoS **LAT2008**, 052 (2008).

[7] H. W. Lin and N. Christ, Phys. Rev. D **76**, 074506 (2007) [arXiv:hep-lat/0608005].

[8] N. H. Christ, M. Li and H. W. Lin, Phys. Rev. D **76**, 074505 (2007) [arXiv:hep-lat/0608006].

[9] C. Albertus *et al.* [RBC and UKQCD Collaborations], PoS **LAT2007**, 376 (2007).

[10] Y. Aoki and J. Wennekers [RBC and UKQCD Collaborations], PoS **LAT2007**, 345 (2007).

[11] A. X. El-Khadra, A. S. Kronfeld and P. B. Mackenzie, Phys. Rev. D **55**, 3933 (1997) [arXiv:hep-lat/9604004].

[12] M. Li [RBC and UKQCD Collaborations], PoS **LAT2008**, 120 (2008).

[13] C. Allton *et al.* [RBC-UKQCD Collaboration], Phys. Rev. D **78**, 114509 (2008) [arXiv:0804.0473 [hep-lat]].

[14] S. R. Sharpe and Y. Zhang, Nucl. Phys. Proc. Suppl. **47**, 441 (1996).

[15] A. Hasenfratz and F. Knechtli, Phys. Rev. D **64**, 034504 (2001) [arXiv:hep-lat/0103029].

[16] R. G. Edwards and B. Joo [SciDAC Collaboration and LHPC Collaboration and UKQCD Collaboration], Nucl. Phys. Proc. Suppl. **140**, 832 (2005) [arXiv:hep-lat/0409003].

[17] http://qcdoc.phys.columbia.edu/cps.html

[18] M. Di Pierro *et al.* [FermiQCD Collaboration], Nucl. Phys. Proc. Suppl. **129**, 832 (2004) [arXiv:hep-lat/0311027].