Nonperturbative renormalization of B_K with domain-wall valence quarks on the $a \approx 0.06$ fm MILC Asqtad ensembles

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Time Requested: The equivalent of 3.6 million Jpsi core-hours plus 1.7 Tbytes of tape storage (the equivalent of $\sim 4,500$ Jpsi core-hours) on D_s at Fermilab.

Abstract

We propose to compute domain-wall propagators on the $a \approx 0.06$ fm "superfine" MILC ensembles to be used for the nonperturbative renormalization of B_K.

Over the past few years we have obtained computing time through USQCD in order to calculate the kaon bag parameter B_K. Last year we published a two-lattice spacing result with a quoted $\sim 4\%$ precision [1]. This is currently the best published unquenched determination of B_K, and fulfills one of the key goals in flavor physics of the U.S. lattice QCD community stated in the 2007 white paper. Combined with the recent determinations of B_K from RBC/UKQCD and Bae *et al.* (with which we are in good agreement) there is now some tension in the unitarity triangle fits. This tension is driven primarily by the new precision in the constraint from kaon mixing. Given this situation, it is crucial to further reduce the uncertainty in B_K by simulating with lighter pion masses, adding a third lattice spacing, and improving the nonperturbative renormalization.

We therefore request an additional 3.6 million Jpsi core-hours and 1.7 Tbytes of tape storage (the equivalent of $\sim$ 4,500 Jpsi core-hours) for our mixed-action kaon physics project to calculate the nonperturbative renormalization factor for B_K on the superfine MILC Asqtad ensembles.

Scientific Objectives

Over the past few years we have carried out a successful project to calculate the kaon bag parameter B_K using USQCD resources. B_K parameterizes the hadronic contribution to mixing between K^0 and $\overline{K^0}$ mesons, and is one of the most sensitive probes of new physics beyond the Standard Model. Last year we published our result [1],

$$\hat{B}_K = 0.724(8)(29), \tag{1}$$

where the first error is statistical, and the second is the sum of all systematic errors in quadrature. This is currently the best published unquenched determination of B_K, with all systematic errors under control, and fulfills one of the key goals in flavor physics of the U.S. lattice QCD community stated in the 2007 white paper "Fundamental parameters from future lattice calculations" [2]. Combined with the recent determination of B_K from RBC/UKQCD [3] and Bae *et al.* [4] (with whom we are in good agreement) we confirm the earlier claim of Ref. [5] that there is some tension in the unitarity triangle fits [6]. This tension is driven mostly by the new precision in the constraint from kaon mixing. In particular, using the latest averages of all lattice inputs to the unitarity triangle fit, as well as some previously neglected corrections to ϵ_K [7], the fit prefers the value $\hat{B}_K = 0.98 \pm 0.10$ [5] when the lattice input for $\hat{B}_K$ is excluded from the fit. Given this tension, it is crucial to continue our precision studies of kaon physics using multiple methods including our mixed-action approach. We are requesting additional computing resources for our current mixed-action kaon physics project that would allow us to complete the nonperturbative renormalization of B_K at a third $a \approx 0.06$ fm lattice spacing and reduce the total error in B_K to $\lesssim 3\%$.

Our project combines staggered and domain-wall fermions in the method pioneered by the LHP Collaboration [8], and takes advantage of the best properties of both discretizations. This method uses domain-wall valence quarks on top of an improved staggered sea (the MILC configurations [9]). By using staggered sea quarks we can take advantage of the vast library of MILC ensembles. This allows us to simulate at multiple lattice spacings using "2+1" flavors of light sea quarks with masses as low as 1/10th of the strange quark mass. The use of domain-wall valence quarks allows us to minimize operator mixing and makes it much easier to implement nonperturbative renormalization. In the case of a purely staggered calculation, taste-breaking effects due to the finite lattice spacing introduce significant mixings between the desired four-fermion operator and a number of other operators with incorrect tastes [10]. This makes nonperturbative techniques difficult to apply, and thus far the impressive three-lattice spacing staggered B_K calculation of Bae *et al.* only uses lattice perturbation theory to compute the renormalization factor [4]. The taste-violating corrections to the $\Delta S = 2$ operator also greatly increase the number of undetermined coefficients in the staggered chiral perturbation theory expression for B_K, making the chiral and continuum extrapolation quite complicated [11]. Domain-wall quarks, on the other hand, have better chiral properties than staggered fermions, leading to qualitatively simpler lattice discretization errors. Although they do not possess an exact chiral symmetry on the lattice, the degree to which chiral symmetry is broken can be controlled through the length of the fifth dimension. Consequently, while the $\Delta S = 2$ operator still mixes with other operators, there are significantly fewer such operators and non-perturbative renormalization can be used more easily in the determination of B_K. Domain-wall quarks, however, are computationally expensive, and the most recent published results with 2+1 flavors [3], though impressive, use only one lattice spacing. Although an updated preliminary domain-wall result including data at a second lattice spacing was presented at Lattice 2009 [12], given the expense of dynamical domain-wall configuration generation, results at a third lattice spacing are unlikely to appear soon.

Using USQCD computing resources on Intrepid at Argonne, we have already computed the unrenormalized K^0-$\overline{K^0}$ mixing matrix element with several valence quark masses on two $a \approx 0.06$ fm sea quark ensembles. In order to use this data, however, we also need to compute the renormalization factor Z_{B_K} at this lattice spacing. Because of the large spatial volumes ($48^3 \times 144$), generating domain-wall valence quark propagators on the "superfine" MILC lattices is well-suited to large machines such as the BG/P at Argonne and the soon-to-be available D_s at Fermilab. We therefore request additional time on D_s for our mixed-action kaon physics project in order compute the nonperturbative renormalization factor Z_{B_K} on the $a \approx 0.06$ fm MILC lattices. Use of a third lattice spacing will nail down the combined chiral-continuum extrapolation and reduce the total uncertainty in B_K. Given the requested resources, we expect to determine B_K to better than $\sim 3\%$ accuracy[1].

Nonperturbative Renormalization Method and Code

We are using the nonperturbative renormalization (NPR) method of Rome-Southampton [13] to obtain the renormalization factor Z_{B_K}. This approach requires the computation of Landau gauge-fixed propagators at several valence quark masses and on multiple ensembles in order to obtain Z_{B_K} in the chiral limit. We are implementing some significant improvements over the method used to determine Z_{B_K} in our publication which will reduce both the statistical and systematic errors. This is essential for reducing the total error in B_K, since the largest single source of uncertainty is from the NPR.

Recently, both the RBC/UKQCD Collaborations and Lytle (on behalf of Bae *et al.*) have begun using an improved volume source to significantly reduce the statistical errors in Z_{B_K} [14, 15]. Although the propagators require a momentum projection at the source, and thus require a new inversion for each momentum, the averaging over the spatial volume allows one to use many fewer configurations to get small statistical errors. (For example, Lytle showed that as few as 8 configurations was sufficient to obtain the quark mass renormalization factor Z_q on the coarse MILC lattices to sub-percent statistical accuracy [15].) Therefore, the use of gauge-fixed momentum sources is preferable for the larger-volume $a \approx 0.06$ fm lattices, and will allow us to reduce the percentage of computing time used for the NPR by approximately a factor of 5 while at the same time reducing the size of the statistical errors by an order or magnitude.

Stürm *et al.* have also developed a new "non-exceptional" momentum scheme for determining Z_{B_K} [16]. Use of non-exceptional kinematics significantly reduces the amount of chiral symmetry breaking between Λ_V and Λ_A [17]. Chiral symmetry breaking is currently one of the largest sources of systematic uncertainty in our published determination of Z_{B_K}, but with the use of non-exceptional kinematics it will soon be one of the smallest. Use of non-exceptional kinematics can also reduce the size of higher-order corrections in the conversion from the RI/MOM scheme to the $\overline{MS}$ scheme, as has been demonstrated for the quark mass renormalization factor Z_m [16].

The most computationally intensive portion of the NPR is the propagator inversions, for which we are using the optimized domain-wall inverter in the Chroma lattice QCD software package [18]. We are using our own code written using the Chroma and QDP++ libraries, to compute and write out the un-amputated momentum-space Greens Functions, and our own python/cython analysis code for off-line amputation and projection. We have checked our code by computing the renormalization factors on one of RBC/UKQCD's 16^3 domain-wall ensembles and comparing with the results presented in Ref. [17].

[1]Note that achieving this level of precision with current methods would also require a continuum two-loop matching calculation, which is in progress by Almeida and Stürm.

Run Plan and Resource Allocation

Using USQCD computing resources on Intrepid at Argonne, we have already generated Coulomb gauge-fixed wall source propagators on two $a \approx 0.06$ fm ensembles, and have computed all of the 2-point and 3-point contractions needed to obtain the K^0-$\overline{K^0}$ mixing matrix element. In order to use this data, however, we also need to compute the renormalization factor Z_{B_K} at this lattice spacing. Table 1 shows the valence and sea quark mass combinations with which we propose to calculate the renormalization factor Z_{B_K} on the superfine MILC ensembles. We only plan on generating additional NPR propagators on a less expensive, smaller volume 48^3 ensemble. Because it is relatively cheap to generate NPR data on the $a \approx 0.0125$ fm and $a \approx 0.09$ fm ensembles, we primarily need the $a \approx 0.06$ fm data to determine the central value of the renormalization factor Z_{B_K}. Hence we can rely upon the "coarse" and "fine" data to estimate systematic uncertainties in order to save computing time.

We have timed the propagator inversions for a number of valence quark masses on the $a \approx 0.06$ fm MILC lattices on the Argonne BG/P; these times are given in Table 2. The time to gauge-fix the lattices, and later to Fourier transform the propagators and compute the un-amputated Green's functions, are negligible as compared to the propagator inversions. Based on this estimate, the total computing time needed to compute Z_{B_K} on the superfine ensembles, and hence our current allocation request, is 3.6 million Jpsi core-hours.

We would like to save the Landau gauge-fixed domain-wall propagators to tape at Fermilab for enough time to allow their use in other projects (such as $K \to \pi\pi$ matrix elements) and by other groups. Table 3 shows the file sizes of the domain-wall quark propagators for the four different lattice volumes, in both GB and Jpsi-equivalent node hours assuming that they are stored on tape. A comparison of Table 3 and Table 2 reveals that calculating the domain-wall propagator is $\sim 100 - 200$ times more expensive than storing it. 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 1, plus the storage currently in use holding existing propagators is given in Table 4. Our total mass storage request is 1.7 TBytes of new tape at Fermilab. In order to save our correlators and other analysis files, we also require a small amount of additional disk space: ~ 0.02 TBytes in the "/project" area at Fermilab.

Summary

With the addition of data at a third lattice spacing, $a \approx 0.06$, we expect to have a precise determination of the neutral kaon mixing parameter B_K including dynamical quark effects with a total uncertainty below $\sim 3\%$. This will 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" [2]. At the level of precision we expect to achieve for B_K, it is also important to consider the effects of $K \to \pi\pi$ matrix elements in order to use ε_K as a constraint on new physics, and we are currently working on computing the necessary kaon matrix elements. (See our talk at the 2010 USQCD All Hands' meeting and our poster at Lattice 2010 for more information.) Other improvements needed to maximize the impact of our current proposal are the three-loop corrections to the Inami-Lim functions and an improved determination of $|V_{cb}|$, both of which are underway. The result of our published B_K calculation (along with that of RBC/UKQCD) has already made a significant impact on the global unitarity-triangle fit and revealed a tension with the Standard Model prediction; pursuing this lead by further reducing the uncertainties is essential and may ultimately lead to definitive evidence for new physics.

Acknowledgments

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Table 1: Proposed valence and sea quark mass combinations for the nonperturbative renormalization of B_K on the $a \approx 0.06$ fm ensembles.

a(fm)	L	m_l	m_s	$m_{val.}^{\rm dwf}$	# momenta	# configs.
≈ 0.06	48	0.0036	0.018	0.0036, 0.0072 0.0108, 0.033	5	10

Table 2: Time to calculate a single domain-wall propagator with $L_5 = 16$ using Chroma on the Argonne "intrepid" BG/P.

a(fm)	L	$m_{val.}^{\rm dwf}$	nodes (intrepid)	time (hours)	Jpsi core-hours
≈ 0.06	48	0.0036	1024	8.08	17,872
≈ 0.06	48	0.0072	1024	3.81	8,427
≈ 0.06	48	0.0108	1024	2.83	6,260
≈ 0.06	48	0.033	1024	1.56	3,450

Table 3: 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 = 2,694 Jpsi core-hours.

a(fm)	L	size (GB)	tape storage cost (Jpsi core-hours)
≈ 0.06	48	17	45

Table 4: Tape storage needed to save the Landau gauge-fixed domain-wall propagators used to compute the renormalization factor Z_{B_K}. This estimate based on the proposed new propagators in Table 1 and the file sizes in Table 3. The equivalent cost to store the file on tape uses the conversion 1 Tbyte tape = 2,694 Jpsi core-hours.

in use as of 11/02/2010	$\approx$ 147.6 TB
additional space for new runs	1.7 TB
Total	149.3 TB
	= 0.402 $\times 10^6$ Jpsi core-hours

Table 5: Disk storage needed to save 2-point and 3-point correlators, logfiles, and analysis files in the "/project" area at Fermilab. The current storage determination reflects actual usage, while the future storage requirement is an estimate. The equivalent cost to store the file on disk uses the conversion 1 Tbyte tape = 26,940 Jpsi core-hours.

currently in use	0.25 TB
additional space for new runs	0.02 TB
Total	0.27 TB
	= 7,300 Jpsi core-hours