# $B$-meson physics with domain-wall light quarks at their physical mass and relativistic heavy quarks

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**Time Requested:** The equivalent of 22.7 million jpsi core-hours on the Fermilab clusters plus 112 Tbytes of tape storage (the equivalent of $\sim 0.336$ million jpsi core-hours) and 0.4 Tbytes of disk storage (the equivalent of $\sim$ 12k jpsi core-hours) at Fermilab.
**Project webpage:** http://rbc.phys.columbia.edu/USQCD/B-physics/


### Abstract

We propose to extend our current $B$-physics program by computing $B$-meson weak matrix elements using the new 2+1 flavor domain-wall Iwasaki gauge field configurations with physical light quarks currently generated by the RBC and UKQCD Collaborations. The use of physical light quarks follows the roadmap outlined in USQCD's 2013 white paper and will allow us to significantly reduce the uncertainties resulting from the extrapolation using heavy meson chiral perturbation theory. It will help to improve upon the precision of our results: the $B$-meson leptonic decay constants $f_{B_d}$ and $f_{B_s}$, the $B^0-\overline{B^0}$ mixing matrix elements, and their ratio, $\xi \equiv f_{B_s}\sqrt{B_{B_s}}/f_{B_d}\sqrt{B_{B_d}}$, as well as the $B \to \pi\ell\nu$ form factor. The $SU(3)$-breaking ratio $\xi$ provides an important constraint on the apex of the CKM triangle and decreasing the error of this quantity was therefore already highlighted as a key goal in flavor physics in the USQCD Collaboration's 2007 white paper. The $B \to \pi\ell\nu$ form factor allows us to determine the CKM Matrix element $|V_{ub}|$. Calculations of $|V_{ub}|$ are particularly critical due to the worrisome $\approx 3\sigma$ tension between inclusive and exclusive determinations. For all of these $B$-meson weak matrix elements we expect to obtain precise results that are competitive with other approaches, and that will place strong constraints on the CKM unitarity triangle fits. Our calculations will provide independent and valuable crosschecks of the results by HPQCD and Fermilab/MILC who both use the same set of gauge field configurations with staggered fermions in the sea-sector. We request the equivalent of 22.7 million jpsi core-hours on the Fermilab clusters plus 112 Tbytes of tape storage (the equivalent of $\sim 0.336$ million jpsi core-hours) and 0.4 Tbytes of disk storage (the equivalent of $\sim$ 12k jpsi core-hours) for this project.

# 1 Scientific motivation

The calculation of $B$-meson weak matrix elements on the lattice enables precise determinations of CKM matrix elements, constraints on the CKM unitarity triangle, and tests of the Standard Model in the quark-flavor sector. The standard global unitarity-triangle fit uses lattice-QCD inputs for neutral $B$-meson mixing matrix elements, the $B \to D^{(*)}\ell\nu$ form factors, and the $B \to \pi\ell\nu$ form factor [1–3]. In addition, the constraint on the unitarity triangle from $B \to \tau\nu$ decay requires a determination of the decay constant $f_B$. Thus lattice-QCD $B$-physics calculations are of great phenomenological importance.

One quantity that places a key constraint on the apex of the CKM unitarity triangle is neutral $B$-meson mixing. Experimentally, $B_q^0 - \overline{B_q^0}$ mixing is measured in terms of mass differences (oscillation frequencies) $\Delta m_q$, where $q$ labels the light quark content of the $B$-meson and is either a $d$- or $s$-quark. Within the Standard Model these oscillation frequencies are parameterized as [4]

$$\Delta m_q = \frac{G_F^2 m_W^2}{6\pi^2} \eta_B S_0 m_{B_q} f_{B_q}^2 B_{B_q} |V_{tq}^* V_{tb}|^2, \tag{1}$$

where $m_{B_q}$ is the the mass of the $B_q$-meson, $V_{tq}^*$ and $V_{tb}$ are the relevant CKM matrix elements, and the Inami-Lim function $S_0$ [5] and QCD coefficient $\eta_B$ [4] can be calculated in perturbation theory. The hadronic matrix element $f_{B_q}^2 B_{B_q}$, where $f_{B_q}$ is the leptonic decay constant and $B_{B_q}$ is the $B$-meson bag parameter, must be computed via lattice QCD. The $SU(3)$-breaking ratio

$$\xi = \frac{f_{B_s}\sqrt{B_{B_s}}}{f_{B_d}\sqrt{B_{B_d}}} \tag{2}$$

can be obtained with especially high precision because the lattice statistical and systematic uncertainties largely cancel between the numerator and denominator. This quantity allows the determination of the ratio of CKM matrix elements $|V_{ts}|^2/|V_{td}|^2$ via [6]:

$$\frac{\Delta m_s}{\Delta m_d} = \frac{m_{B_s}}{m_{B_d}} \xi^2 \frac{|V_{ts}|^2}{|V_{td}|^2} \tag{3}$$

and currently places one of the single tightest constraints on the apex of the CKM unitarity triangle (second only to $\sin(2\beta)$, which does not involve lattice inputs). The precision of $|V_{ts}|^2/|V_{td}|^2$ is still limited, however, by the uncertainty in lattice-QCD calculations of $\xi$. Recent experimental measurements of the oscillation frequencies $\Delta m_d$ and $\Delta m_s$ have established an accuracy of $\sim 1\%$ [7], but the $SU(3)$-breaking ratio $\xi$ is only known to $\sim 3\%$ [8, 9]. Given the phenomenological importance of $\xi$, this quantity was already highlighted as one of three "key matrix elements" in the USQCD Collaboration's 2007 white paper "Fundamental parameters from future lattice calculations" [10].

Another quantity that is in critical need of improvement from lattice-QCD is the $B \to \pi\ell\nu$ form factor, which enables the determination of the CKM matrix element $|V_{ub}|$ from the experimental branching fraction via

$$\frac{d\Gamma(B \to \pi\ell\nu)}{dq^2} = \frac{G_F^2 |V_{ub}|^2}{192\pi^3 m_B^3} \left[(m_B^2 + m_\pi^2 - q^2)^2 - 4m_B^2 m_\pi^2\right]^{3/2} |f_+(q^2)|^2. \tag{4}$$

Over the past several years there has been a persistent tension between the exclusive determination of $|V_{ub}|$ from $B \to \pi\ell\nu$ decay and the inclusive determination from semileptonic decays of the form $B \to X_u\ell\nu$ where $X_u$ is any charmless hadronic final state. This tension has recently grown in magnitude to more than a $3\sigma$ discrepancy [3]. Further, the value of $V_{ub}$ obtained from recent experimental measurements of $\mathrm{BR}(B \to \tau\nu)$ combined with lattice-QCD calculations of $f_B$ is higher than both $|V_{ub}|_{\mathrm{excl}}$ and $|V_{ub}|_{\mathrm{incl}}$, and disagrees with their average by more than $2\sigma$ [11]. Although there is no obvious source for these discrepancies, the decay $B \to \pi\ell\nu$ is not a particularly good candidate for large new-physics contributions because it occurs at tree-level in the Standard Model. Thus one suspects that the disagreement may be due to a combination of underestimated systematic uncertainties and unkind statistical fluctuations. Lattice-QCD calculations of the $B \to \pi\ell\nu$ form factor with improved precision are key elements needed to address this puzzle. Once the situation is resolved and $|V_{ub}|$ is under better control, the constraint on the apex of the CKM unitarity triangle from $|V_{ub}|$ will strengthen tests of the Standard Model and tighten constraints on new physics in the quark-flavor sector.

Currently, the Fermilab/MILC and HPQCD collaborations are also computing $B$-meson weak matrix elements using the $2+1$ flavor Asqtad-improved-staggered and the $2+1+1$ flavor HISQ ensembles generated by the MILC Collaboration [8, 9, 12–14]. Our project will provide essential independent crosschecks using different light-quark and heavy-quark formulations, and we expect to obtain competitive uncertainties. With the computing time requested in this proposal we expect to improve the precision of our computations of $B$-meson decay constants, mixing parameters and the $B \to \pi\ell\nu$ form factor due to using new gauge field ensembles with physical light quarks. This follows the future plans outlined for flavor physics in USQCD's 2013 white paper [15]. Our results will enable precise determinations of CKM matrix elements, place stringent constraints on the CKM unitarity triangle, and allow rigorous tests of the Standard Model in the quark-flavor sector.

## 2 Our project

Four years ago we initiated this project to compute $B$-meson physics using the 2+1 flavor dynamical domain-wall ensembles with Iwasaki gauge action generated by the LHP, RBC and UKQCD collaborations. We use the "coarse" $24^3$ ensembles with lattice spacing $a \approx 0.11$ fm ($a^{-1} = 1.73$ GeV) and the "fine" $32^3$ ensembles with lattice spacing $a \approx 0.08$ fm ($a^{-1} = 2.271$ GeV) as listed in Tab. 1 [16, 17]. The light quarks in our calculation are simulated by domain-wall fermions with Shamir-kernel [18, 19] and we use the relativistic heavy quark (RHQ) action developed by Christ, Li and Lin for the heavy $b$-quarks [20, 21]. The RHQ method extends the Fermilab approach [22] by tuning all of the parameters of the clover action nonperturbatively [23]. 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.

Choosing different actions for light and heavy quarks allows us to compute heavy-light physics preserving the chiral properties of the light quarks, while keeping the discretization errors of heavy quarks on relatively coarse lattices under control. A consequence of this choice is that the light quarks dominate the costs of our computation and the costs for heavy quarks become almost negligible. We address this fact by separating our computation in two parts:

1. Generation and saving of general purpose point-source domain-wall light quark propagators.

2. Nonperturbative tuning of the parameters in the RHQ $b$-quark action and computation of bottom-light 2-point and 3-point correlation functions to obtain matrix elements.

With the help of resources obtained from USQCD we have completed most of the numerical work for our initial project using the $24^3$ and $32^3$ ensembles. A library of domain-wall light quark propagators generated on these ensembles is available on tape at Fermilab (see Tab. 2). We published the details and results of our nonperturbative tuning method for $b$-quarks last year [24]. We have also performed most measurements of bottom-light 2-point and 3-point correlation functions and are currently in the process of analyzing the data, estimating systematic uncertainties and preparing publications. Preliminary results for the decay constants $f_B$ and $f_{B_S}$ as well as for the $B \to \pi\ell\nu$ form factor were presented at Lattice 2012 [25, 26]. Also the perturbative calculations entering the $O(a)$ operator improvement and

| L | $a$(fm) | $m^l_{\rm sea}$ | $m^h_{\rm sea}$ | $m^\pi_{\rm sea}$(MeV) | # configs. | trajectory # |
|---|---|---|---|---|---|---|
| 32 | $\approx 0.08$ | 0.004 | 0.030 | 289 | 628 | [290:5:3425] |
| 32 | $\approx 0.08$ | 0.006 | 0.030 | 345 | 445 | [272:8:3824] |
| 32 | $\approx 0.08$ | 0.008 | 0.030 | 394 | 544 | [250:5:2965] |
| 24 | $\approx 0.11$ | 0.005 | 0.040 | 329 | 1636 | [495:5:8670] |
| 24 | $\approx 0.11$ | 0.010 | 0.040 | 422 | 1419 | [1455:5:8545] |

**Table 1.** Analyzed RBC-UKQCD domain-wall gauge field configurations. The pion masses are taken from [16, 17]. The analyzed trajectories are specified in the last column where the number between the colons specifies the separation. On the finer ("$32^3$") ensembles 1 trajectory = 2 molecular dynamics time units, whereas on the coarser ("$24^3$") ensembles 1 trajectory = 1 molecular dynamics time unit.

| L | $m^l_{\rm sea}$ | $m_{\rm val}$ | # sources/config | # propagators |
|---|---|---|---|---|
| 32 | 0.004 | 0.004, 0.006, 0.008, 0.025, 0.0272, 0.030 | 2 | 1256 |
| 32 | 0.006 | 0.004, 0.006, 0.008, 0.025, 0.0272, 0.030 | 2 | 1778 |
| 32 | 0.008 | 0.004, 0.006, 0.008, 0.025, 0.0272, 0.030 | 2 | 1088 |
| 24 | 0.005 | 0.005, 0.010, 0.020, 0.030, 0.0343, 0.040 | 1 | 1636 |
| 24 | 0.010 | 0.005, 0.010, 0.020, 0.030, 0.0343, 0.040 | 1 | 1419 |

**Table 2.** Generated domain-wall valence-quark propagators. To compensate for the lower number of gauge field configurations on the $32^3$ ensembles we generate additional time source(s) per configuration. The propagators with masses $m_{\rm val} = 0.0272$ on the $32^3$ ensembles and $m_{\rm val} = 0.0343$ on the $24^3$ ensembles correspond to the physical strange quark [17]).

the mostly nonperturbative operator renormalization are in place. These calculations motivated the development of a new framework for automating lattice perturbation theory calculations [27].

We extract $B$-meson decay constants, mixing parameters and form factors by performing a combined chiral- and continuum-extrapolation using partially quenched heavy meson $\chi$PT [28] supplemented by analytic terms $\propto a^2$ parameterizing light-quark disctretization effects. This combined chiral- and continuum-extrapolation is one of the biggest sources of our uncertainty. By submitting this proposal we intend to improve upon the chiral part of the extrapolation proposing to compute $B$-meson quantities using physical light quarks on the newly generated Möbius domain-wall ensembles listed in Tab. 3 [29].

# 3 Details and status of our computations

We designed our computational setup to use the same, expensive light quark propagators for computing $B^0 - \overline{B^0}$ mixing matrix elements and the decay constants $f_B$ and $f_{B_s}$. Later we added the computation of the $B \to \pi\ell\nu$ form factor and the coupling constant $g_{B^*B\pi}$ to our list and implemented mostly nonperturbative operator renormalization for the heavy-light (axial-)vector current by computing additionally the flavor conserving renormalization vector $Z_v^{bb}$ nonperturbatively. All quantities are computed re-using the same point-source domain-wall light quark propagators.

We outline the basic elements of our computation of the decay constant as an example. On the lattice we compute the vacuum-to-meson matrix element of the axial-vector current operator. The lattice and continuum axial-current operator are related via a matching factor $Z_A^{hl}$ and a series of improvement coefficients $c_A^{(i)}$:

$$\mathcal{A}_\mu^{\rm cont.} \doteq Z_A^{bl} \left( A_\mu^{{\rm lat},(0)} + c_A^{(ap),i} A_\mu^{{\rm lat},(ap),i} + \dots \right) , \tag{5}$$

| $L^3 \times T$ | $L_s$ | $a$(fm) | $m^l_{\rm sea}$ | $m^h_{\rm sea}$ | |
|---|---|---|---|---|---|
| $64^3 \times 128$ | 12 | $\approx 0.08$ | 0.00066 | 0.02659 | in production |
| $48^3 \times 96$ | 24 | $\approx 0.11$ | 0.00078 | 0.0362 | in production |

**Table 3.** Currently generated 2+1 flavor dynamical Möbius domain-wall fermion (MDWF) ensembles by the RBC and UKQCD collaborations. The Möbius parameters ($b_5 = 1.5$ and $c_5 = 0.5$) are chosen such that the resulting MDWF [30] 4d-overlap operator agrees with the corresponding Shamir DWF 4d-overlap operator to $\approx 0.1\%$ accuracy. These configurations are generated with 1 trajectory = 1 molecular dynamics time unit.

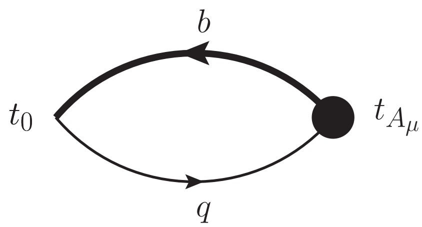


**Figure 1.** Two-point correlation function for computing the decay constant $f_{B_q}$ on the lattice.

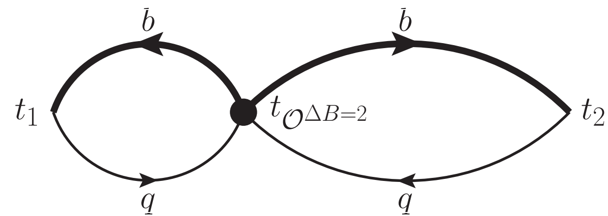


**Figure 2.** Three-point correlation function for computing $B^0_q\!-\!\overline{B^0_q}$ mixing on the lattice.

where the "$\doteq$" denotes equality of matrix elements and the "..." denote higher-order terms in the expansion parameter $ap$. The improvement coefficients enforce short-distance matching between the lattice and continuum calculations and are functions of the parameters in the RHQ action, while the renormalization factor $Z^{hl}_A$ matches to the continuum regularization and renormalization scheme. In order to reduce discretization errors in the current operators, we implement $O(a)$ operator improvement. In the case of the axial-vector current operator, only one additional matrix element is needed to improve the decay constant at $O(ap)$ to all orders in $\alpha_s$ because no momentum leaves the axial-current operator in Fig. 1. We compute the needed improvement coefficient $c^{(ap)}_A$ at 1-loop in tadpole improved lattice perturbation theory; this improves the decay constants through $O(\alpha_s ap)$, such that truncation errors are of $O(\alpha_s^2 ap, a^2p^2)$. To obtain a more precise determination of $Z^{hl}_A$, we implement mostly nonperturbative operator renormalization à la El Khadra *et al.* [31] instead of solely relying on 1-loop tadpole improved lattice perturbation theory. This approach takes advantage of rewriting the heavy-light axial-vector (or vector) current renormalization factor as the following product:

$$Z^{bl}_{A(V)} = \varrho^{bl}_{A(V)}\sqrt{Z^{bb}_V Z^{ll}_V}. \tag{6}$$

Because the flavor-conserving renormalization factors $Z^{bb}_V$ and $Z^{ll}_V$ can be obtained nonperturbatively from standard heavy-light and light-light meson charge normalization conditions, only the residual correction $\varrho^{bl}_{A(V)}$ needs to be computed perturbatively. The flavor-conserving factors $Z^{bb}_V$ and $Z^{ll}_V$ account for most of the operator renormalization, while $\varrho^{bl}_{A(V)}$ is expected to be close to unity because most of the radiative corrections, including contributions from tadpole graphs, cancel in the ratio $Z^{bl}_{A(V)}/\sqrt{Z^{bb}_V Z^{ll}_V}$ [32]. Therefore $\varrho^{bl}_{A(V)}$ has a more convergent series expansion in $\alpha_s$ than $Z^{bl}_{A(V)}$ and can be computed at 1-loop in tadpole improved lattice perturbation theory to few-percent precision. In practice, $Z^{ll}_V$ has already been obtained by the RBC/UKQCD Collaborations (see Ref. [17]), where we use the fact that $Z_A = Z_V$ for domain-wall fermions up to corrections of $\mathcal{O}(m_{\rm res})$. We therefore need only to calculate $Z^{bb}_V$ ourselves (see below). In the following we briefly sketch the computations and show preliminary results for the different quantities of interest.

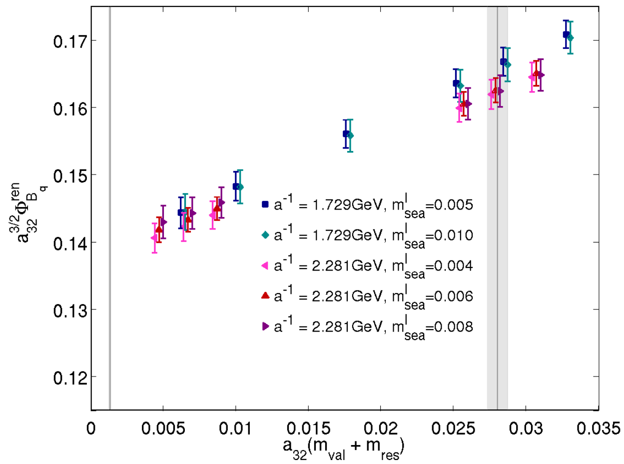


**Figure 3.** Preliminary results for the decay amplitude $\Phi^{\rm ren}_{B_q} = f_{B_q}\sqrt{M_{B_q}}$ in $a_{32}$ lattice units for all six valence quarks on all five ensembles.

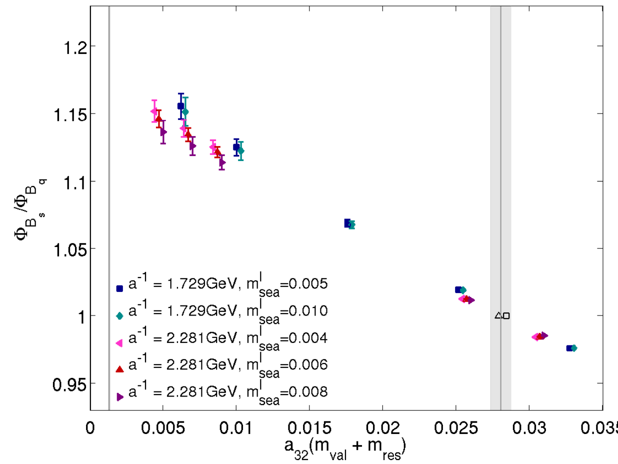


**Figure 4.** The ratio of the decay amplitudes $\Phi_{B_s}/\Phi_{B_q}$ obtained using our close to physical strange quark propagators.

## Decay constants $f_B$ and $f_{B_s}$

The decay constants $f_{B_q}$ are determined from the 2-point correlation function shown in Fig. 1. We combine a Gaussian-smeared source $b$-quark propagator originating at time $t_0$ with the existing point-source light-quark propagators to compute the vacuum-to-meson matrix element of the axial-vector current operator and the operator contributing for the $O(a)$-improvement. We compute decay constants $f_{B_q}$ for several values of the light-quark mass to aid in the chiral extrapolation to the physical $d$-quark mass. Our final results will be obtained by fitting data on the coarse "$24^3$" and fine "$32^3$" lattices together and performing a simultaneous extrapolation to the physical light-quark mass and the continuum using partially-quenched heavy-meson $\chi$PT [28] supplemented by analytic terms $\propto a^2$ to parameterize light-quark discretization effects. Fig. 3 shows our data obtained in terms of the renormalized and $O(a)$-improved decay amplitude $\Phi_{B_q}$ in lattice units for all five ensembles and Fig. 4 shows the ratio of the decay amplitudes $\Phi_{B_s}/\Phi_{B_q}$. Currently we are working on combined fits of our data and estimating systematic uncertainties.

## $B$-meson mixing matrix elements

The computation of the 3-point correlation used for measuring the $B^0_q - \overline{B^0_q}$ mixing matrix elements with the light quark content $q$ is shown in Fig. 2. Fixing the location of the effective four-quark operator $t_{\mathcal{O}^{\Delta B=2}}$, we vary the locations of the $B^0_q$ and $\overline{B^0_q}$ mesons, $t_1$ and $t_2$, over all possible time slices. Hence we require one point-source light quark and one point source $b$-quark propagator originating from $t_{\mathcal{O}^{\Delta B=2}}$ which can be used for both the $B^0_q$ as well as the $\overline{B^0_q}$ mesons. We project out the zero momentum component of the heavy $b$-quarks using a gauge-invariant Gaussian smeared sink. We optimized the Gaussian smearing such that the excited-state contamination for the $B_q$-meson correlators is minimal. Currently we are working on deriving and implementing the set of operators needed for the $O(a)$ operator improvement for Standard Model $B_q - \overline{B_q}$ mixing four quark operators. The computation then will make use of the full set of our propagators using all partially quenched data to aid in the chiral extrapolation to the physical $d$-quark mass. For the final result we intend to perform a combined fit of both $24^3$ and $32^3$ data sets. We hope to finish the numerical work within the present allocation period. Unfortunately, mostly nonperturbative renormalization is yet not available for $B$-meson mixing

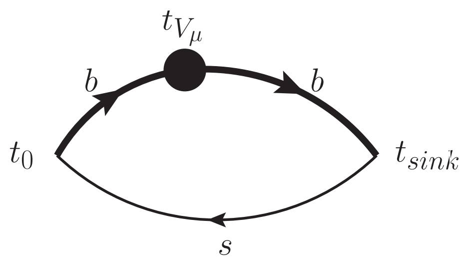


**Figure 5.** Three-point correlation function for computing $Z_V^{bb}$ on the lattice.

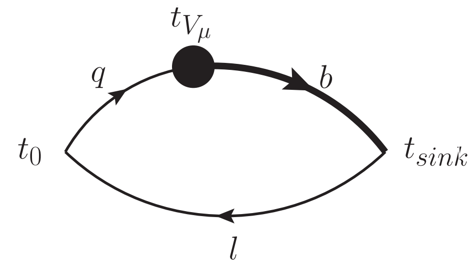


**Figure 6.** Three-point correlation function for computing the $B \to \pi\ell\nu$ form factor. The spectator quark is labeled $l$ and the daughter quark is labeled $q$.

| $a[fm]$ | $m^l_{\text{sea}}$ | $Z_v^{bb}$ |
|---|---|---|
| $\approx 0.11$ | 0.005 | 10.037(34) |
| $\approx 0.11$ | 0.010 | 10.042(27) |

| $a[fm]$ | $m^l_{\text{sea}}$ | $Z_v^{bb}$ |
|---|---|---|
| $\approx 0.08$ | 0.004 | 5.270(13) |
| $\approx 0.08$ | 0.006 | 5.237(12) |
| $\approx 0.08$ | 0.008 | 5.267(15) |

**Table 4.** Preliminary results for $Z_v^{bb}$ obtained on our two $24^3$ ensembles (left) and three $32^3$ ensembles (right) using the close to physical strange quark propagators as spectator quark.

operators. For the most important quantity $\xi$, the ratio of the $B_s$- over the $B_d$-meson mixing matrix element, much of the uncertainty due to the truncation of perturbation theory are expected to cancel in the ratio.

### Mostly-nonperturbative operator renormalization ($Z_V^{bb}$)

We compute the flavor-conserving renormalization factor $Z_V^{bb}$ nonperturbatively from the 3-point correlation function shown in Fig. 5. On all ensembles we compute $Z_V^{bb}$ using the strange-quark mass as spectator-quark masses because we found (as expected) that $Z_V^{bb}$ is independent of the spectator mass within the statistical errors and the strange-quark spectator quark mass allowed to obtain $Z_V^{bb}$ with sub-percent accuracy. Tab. 4 lists the values of $Z_V^{bb}$ obtained on our five ensembles.

### The $B \to \pi\ell\nu$ form factor

We also calculate the $B \to \pi\ell\nu$ form factor using the same general setup. This requires computing the matrix element of the $b \to u$ vector current between a $B$-meson and a pion. The relevant 3-point correlation function is shown in Fig. 6. We fix the location of the pion at time $t_0$ and the location of the $B$-meson at a time separation $T = (t_{\text{sink}} - t_0)$. We then vary the location of the current operator $t_{V_\mu}$ over all time slices in between. We improve the operator at $\mathcal{O}(a)$, and compute the improvement coefficients at 1-loop in lattice perturbation theory, such that the residual errors are of $\mathcal{O}(\alpha_s^2 ap, a^2p^2)$. The $B$-meson is at rest, so we can use a Gaussian-smeared sequential $b$-quark to reduce excited-state contamination, and we inject momentum on the pion side to obtain the form factor's momentum dependence.

Because the 3-point correlation function in Fig. 6 requires a new $b$-quark inversion for every light spectator-quark mass, we compute the form factor only with a unitary spectator mass (*i.e.* equal to the lighter quark mass in the sea sector) but use, however, all available partially-quenched daughter-quark masses. These additional pion masses will help us to better resolve both the quark-mass dependence and the pion-energy dependence. As in the case of the $B$-mixing parameters and decay constants, we will extrapolate our data to the physical light-quark mass and continuum using next-to-leading order

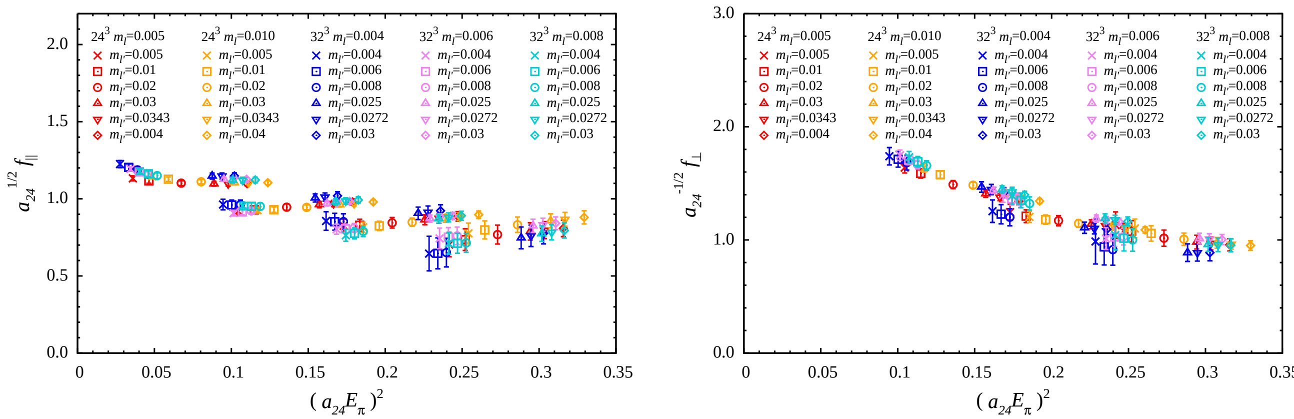


**Figure 7.** Form factors $f_\parallel$ and $f_\perp$ in coarse lattice units $a_{24}$. The red and orange symbols indicate data on the coarser $am^l_{\rm sea} = 0.005$ and $am^l_{\rm sea} = 0.010$ ensemble, blue, magenta and cyan symbols denote data on the finer $am^l_{\rm sea} = 0.004$, $am^l_{\rm sea} = 0.006$ and $am^l_{\rm sea} = 0.008$ ensemble, respectively. Different symbols indicate different partially quenched masses. Data shown do not include $O(a)$-improvement corrections.

partially-quenched heavy meson $\chi$PT supplemented by higher-order analytic terms [33, 34]. We will estimate the residual discretization errors from the RHQ action using heavy-quark power-counting.

The computation of the $B \to \pi\ell\nu$ form factor is performed using the same 3-point code as for $Z_V^{bb}$, but with momentum inserted on the pion side. We extract the $B \to \pi\ell\nu$ form factor from the ratio of the 3-point function shown in Fig. 6 over the pion and $B$-meson 2-point functions:

$$R_{3,\mu}^{B\to\pi}(t,T) = \frac{C_{3,\mu}^{B\to\pi}(t,T)}{\sqrt{C_2^\pi(t) C_2^B(T-t)}} \sqrt{\frac{2E_0^\pi}{\exp(-E_0^\pi t)\exp(-m_0^B t)}}\,, \tag{7}$$

where the phenomenologically-relevant form factor $f_+$ is a linear combination of the temporal form factor $f_\parallel \propto R_{3,0}^{B\to\pi}(t,T)$ and the spatial form factor $f_\perp \propto R_{3,i}^{B\to\pi}(t,T)$. We compute the ratios $R_{3,0}^{B\to\pi}(t,T)$ and $R_{3,i}^{B\to\pi}(t,T)$ including all four needed $O(a)$-improvement operators for the vector current and also obtain the corresponding coefficients in 1-loop tadpole improved lattice perturbation theory. Currently we are piecing the results together and will soon turn our attention to the combined chiral- and continuum extrapolation. Fig. 7 shows our preliminary results for $f_\parallel$ and $f_\perp$ obtained on our five ensembles.

## Coupling constant $g_{B^*B\pi}$

Taking advantage of our saved domain-wall light quark propagators, Ben Samways and Jonathan Flynn in Southampton started the computation of the $B^*B\pi$ coupling constant using our RHQ action. The $B^*B\pi$ coupling constant enters $\chi$PT expressions used for fitting decay constants, $B \to \pi\ell\nu$ form factors or $B$-meson mixing matrix elements. In the past the literature exhibited a broad range of values mostly with incomplete error budget. Only recently Detmold et al. finished a computation in the static limit which accounts for all systematic uncertainties [35]. Our determination of $g_{B^*B\pi}$ using relativistic heavy quarks will further improve the quality of the coupling constant used in our chiral- and continuum-extrapolations. Fig. 8 shows our preliminary results obtained on the $24^3$ and $32^3$ ensembles.

## Lattice perturbation theory and operator improvement

Even though we will use a mostly nonperturbative framework for the operator renormalization, we need to employ lattice perturbation theory (LPT) to obtain improvement coefficients for the heavy-light (axial-) vector currents and four-quark operators. Although for the Tsukuba formulation of the

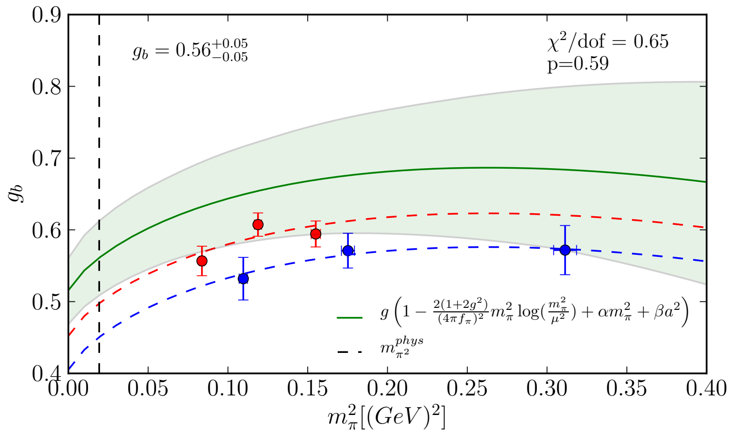


**Figure 8.** Chiral- and continuum extrapolation for the coupling constant $g_{B^*B\pi}$ obtained using the unitary light sea-quark mass on six different ensembles. Blue data points denote the "coarse" $24^3$ ensembles, red data points the "fine" $32^3$ ensembles.

RHQ action one-loop results for the matching of (axial-)vector currents are known [36], these results do not translate trivially to the Columbia formulation of RHQ [21] which we use. We have implemented an automated framework [27] to perform the necessary LPT calculations taking into account the complications introduced by non-trivial field rotations in the Columbia formulation. As a first test of the framework we extended the tadpole-improved 1-loop predictions of Ref. [37] for the RHQ parameter tuning to the Columbia formulation. Furthermore, the matching and $O(a)$-improvement of vector and axialvector heavy-light bilinear operators have been performed. Our automated LPT framework will allow for rapid progress for similar calculations in the future [27]. A publication containing these results is in preparation.

# 4 Run plan and resource allocation for including ensembles with physical light quarks

In order to improve the chiral part of our combined chiral- and continuum-extrapolation, we would like to compute $B$-meson quantities using physical light quarks on the newly generated $48^3$ and $64^3$ Möbius domain-wall ensembles.[1] Similar to our strategy on the $24^3$ and $32^3$ ensembles, we intend to first generate and save general purpose domain-wall propagators with a point source and in a second step generate heavy-quarks on the fly when we compute 2-point and 3-point correlation functions. This strategy suits best our computation because the costs for inverting a domain-wall light quark propagator is two orders of magnitude larger than for a heavy quark. In Tab. 5 we list the costs to create a single propagator on the Ds-cluster at Fermilab. These cost figures are obtained by measuring the time it takes to perform a propagator inversion on one sample configurations for each volume. We choose to create the Möbius domain-wall propagators using Andrew Pochinsky's `qlua` and `mdwf-1.3.3` [38–40] because this software is readily available and supposedly has the smallest overhead. Hence we are able to invert a $48^3$ ($64^3$) MDWF propagator on only 12 (18) Ds-nodes. The heavy quarks are generated with a variant of the Sheikohelsami-Wohlert (clover) action [41] and we use the standard inverter embedded in `Chroma` [42]. Using `Chroma` here allows us to re-use the same Chroma inline-functions we previously coded to perform the needed contractions for our 2-point and 3-point correlation functions on the $24^3$

[1] The parameters for the Möbius domain wall fermion (MDWF) action [30] are such that the resulting MDWF 4d-overlap operator agrees with the corresponding Shamir DWF 4d-overlap operator to $\approx 0.1\%$ accuracy.

| $a$(fm) | action | L | T | $L_s$ | $m_{\text{val}}$ | nodes (Ds) | time (hours) | jpsi core-hours | file size |
|---|---|---|---|---|---|---|---|---|---|
| $\approx 0.08$ | MDWF | 64 | 128 | 12 | 0.00066 | 18 | 100.0 | 76600 | 37 GB |
| $\approx 0.08$ | MDWF | 64 | 128 | 12 | 0.02659 | 18 | 6.5 | 5000 | 37 GB |
| $\approx 0.08$ | clover | 64 | 128 | — | 3.98 | 8 | 1.5 | 500 | — |
| $\approx 0.11$ | MDWF | 48 | 96 | 24 | 0.00078 | 12 | 82.0 | 42000 | 12 GB |
| $\approx 0.11$ | MDWF | 48 | 96 | 24 | 0.0362 | 12 | 4.5 | 2300 | 12 GB |
| $\approx 0.11$ | clover | 48 | 96 | — | 8.40 | 4 | 0.8 | 130 | — |

**Table 5.** Time to calculate a single $48^3$ (a $\approx$ 0.11 fm) or $64^3$ (a $\approx$ 0.08 fm) propagator on the new Möbius domain-wall and Iwasaki gauge field configuration. Timings are obtained for the Ds-cluster at Fermilab using the minimal number of nodes needed to meet the memory requirement. MDWF propagators are obtained using qlua and mdwf-1.3.3, whereas clover propagators are obtained using Chroma and timings include overhead for I/O, contractions and source smearing. The file sizes given refers to saving a propagator in single precision.

and $32^3$ ensembles. The number of Ds-nodes is chosen such that we can keep our desired number of propagators in memory to perform the contractions most efficiently and the timings include some overhead for I/O or creating the source.

It is hard to forecast how the configuration generation will proceed and how many configurations will be available at the beginning/during this allocation period. At the writing of this proposal about 80 thermalized configurations of the $48^3$ ensemble separated by five molecular dynamics time units are available and hopefully 200 more will follow within one year. In the end we would like to have at least 1000 measurements on both new ensembles. Here we propose to generate 500 domain-wall propagators on the $48^3$ ensemble with valence quark masses $m_{\text{val}} = 0.00078$ and 0.0362 which e.g. could be generated using four sources per configuration and configurations separated by 10 molecular dynamics time units. Given the much larger volume compared to the $24^3$ ensembles it seems to be safe to place four sources on one configuration and still have the full gain of "doubling the statistics". More investigation is needed to find out whether placing additional sources will preserve this. Concerns arise because on the $24^3$ ensembles we found for heavy quarks a Gaussian source corresponding to a diameter of about 16 lattice sites to be optimal and we fit heavy-light 2-point functions over a plateau range of 15 time slices. Depending on the number of sources placed per configurations, techniques like all mode averaging (AMA) [43] may turn out to be advantageous once the overhead costs get amortized. Unfortunately, AMA comes with a significantly increased memory consumption and likely 128 Ds-nodes (more than 1/4 of the entire cluster) are needed to perform AMA on the $48^3$ lattices. This would significantly limit the throughput and make it unfeasible to also use the older jpsi-cluster at Fermilab.

At the moment we are not fully conclusive about the optimal strategy and will continue to investigate. Maybe it turns out that other algorithmic improvements become available which are more suited for generating large volume domain-wall propagators on a cluster. One such candidate could be multigrid for domain-wall fermions [44] promised in the SciDAC3-proposal. Efforts at Boston University are very likely to resume given such a specific need. In this proposal, however, we estimate the costs for generating 500 Möbius domain-wall propagators on the $48^3$ ensembles separately using `qlua` and `mdwf-1.3.3`. We also estimated the time to generate heavy clover quarks and perform computations using our seven sets of RHQ parameters. Running our computation on the seven sets of RHQ parameters bears the advantage to "fine-tune" our RHQ parameters on the new ensemble, while at the same time allows us to cleanly propagate the statistical uncertainty of the RHQ parameters via single-elimination jackknife. The total amount of requested cluster time is 22.7 M jpsi-core hours (for details see Tab. 6).

We would like to continue running on the Fermilab clusters. Both jpsi and Ds have the capacity to perform the expensive domain-wall fermion inversions and are well-suited for the computation of

| | | |
|---|---|---|
| 500 | $48^3$ ($a \approx 0.11$ fm) domain-wall propagators with $m_{\rm val} = 0.00078$ | 21.0 $\times 10^6$ jpsi core-hours |
| 500 | $48^3$ ($a \approx 0.11$ fm) domain-wall propagators with $m_{\rm val} = 0.0362$ | 1.2 $\times 10^6$ jpsi core-hours |
| $7 \times 500$ | $48^3$ ($a \approx 0.11$ fm) clover propagators, 2- and 3-point correlators | 0.5 $\times 10^6$ jpsi core-hours |
| Total | | 22.7 $\times 10^6$ jpsi core-hours |

**Table 6.** Computer time needed for the first step to extend our $B$-physics project to include physical light quarks for the allocation period 2013/2014. Most of the time will be used to generate MDWF light quark propagators which will be made immediately available to other non-competing projects.

$b$-quarks and 2-point and 3-point correlation functions. Several of the proposal authors are experienced in running on the Fermilab clusters and our codes are compiled for both jpsi and Ds. We propose to save all generated domain-wall propagators on tape at Fermilab because the storage cost is only a fraction of the costs it takes to generate them. We are happy to share these propagators and will make them immediately available for non-competing projects on a per request basis. In order to save $2 \times 500$ domain-wall propagators on the $48^3$ ensemble, 12 TB additional tape storage will be needed. This amounts to an equivalent of 36 K jpsi-core hours. Currently we are using approximately 100 TB of tape to store our domain-wall propagators on the $24^3$ and $32^3$ ensembles which will then increase to a total use of 112 TB. In addition we need temporary space to store our propagators on the lustre file system at Fermilab while running, as well as storage for our data in the project area. We anticipate a typical use of approximately 30 TB of lustre space to hold domain-wall propagators while running and 0.4 TB of backed-up disc storage in the project area for our data.

# 5 Summary

By the end of the allocation period 2013/2014 we expect to have generated at least 500 Möbius domain-wall light quark propagators on the new $48^3 \times 96 \times 24$ domain-wall Iwasaki gauge field configurations. These propagators will enable us to improve our determinations of the $B$-meson decay constants $f_{B_d}$ and $f_{B_s}$, the $B^0 - \overline{B^0}$ mixing matrix elements and their ratio $\xi$, and the $B \to \pi \ell \nu$ form factor by essentially eliminating the need for a chiral extrapolation. Also they will help us to estimate which statistics is required to achieve statistical uncertainties around one percent e.g. for $f_B$ and $f_{B_s}$. Our calculation follows the direction of USQCD's 2013 white paper "Lattice QCD at the intensity frontier" [15] and, in particular, the computation of the $SU(3)$-breaking ratio $\xi$ will fulfill one of the key goals in flavor physics already listed in the 2002 strategic plan.

Our final results will be based on computations at two lattice spacings with physical light quarks and likely supplemented with multiple other quark masses generated in the past. This should allow us excellent control over the systematic errors associated with the chiral extrapolation. Our results will provide valuable independent and competitive crosschecks to results of Fermilab/MILC and HPQCD. When used in the unitarity triangle analysis, our results will place an important constraint on physics beyond the Standard Model. In the following year we may request further time to add statistics on this $48^3$ ensemble with $a^{-1} \approx 1.73$ GeV or start to take advantage of the finer $64^3$ ensemble ($a^{-1} \approx 2.21$ GeV) also generated with physical light quarks in the sea-sector.

We encourage other members of the lattice QCD community to make use of the domain-wall propagators we generate as part of this project in order to compute other physics quantities. Within this project we intend to compute the $B^0 - \overline{B^0}$ mixing matrix elements and their ratio $\xi$ , the decay constants $f_{B_d}$, $f_{B_s}$ and their ratio $f_{B_s}/f_{B_d}$, and the $B \to \pi \ell \nu$ form factor. We would also like to retain exclusive rights to calculate $D-$ and $D_s$-meson decay constants and beyond the Standard Model contributions to $B$- and $D$-meson mixing as well as the coupling constants $g_{B^* B \pi}$ and $g_{D^* D \pi}$ using these propagators in the future. All generated propagators will be stored at Fermilab and will be made available immediately for non-competing analysis. Researchers who wish to use them should contact us to arrange access.

## References


[1] J. Charles *et al.* (CKMfitter Group), Eur.Phys.J. **C41**, 1 (2005), arXiv:hep-ph/0406184.
[2] M. Bona *et al.* (UTfit), JHEP **0507**, 028 (2005), arXiv:hep-ph/0501199.
[3] J. Laiho, E. Lunghi, and R. S. Van de Water, Phys.Rev. **D81**, 034503 (2010), arXiv:0910.2928 [hep-ph].
[4] A. J. Buras, M. Jamin, and P. H. Weisz, Nucl. Phys. **B347**, 491 (1990).
[5] T. Inami and C. S. Lim, Prog. Theor. Phys. **65**, 297 (1981).
[6] C. W. Bernard, T. Blum, and A. Soni, Phys.Rev. **D58**, 014501 (1998), arXiv:hep-lat/9801039.
[7] J. Beringer *et al.* (Particle Data Group), Phys.Rev. **D86**, 010001 (2012).
[8] E. Gamiz *et al.* (HPQCD), Phys. Rev. **D80**, 014503 (2009), arXiv:0902.1815 [hep-lat].
[9] A. Bazavov *et al.* (Fermilab Lattice and MILC), Phys.Rev. **D86**, 034503 (2012), arXiv:1205.7013 [hep-lat].
[10] USQCD, "Fundamental parameters from future lattice calculations," (2007), `http://www.usqcd.org/documents/fundamental.pdf`.
[11] E. Lunghi and A. Soni, Phys.Lett. **B697**, 323 (2011), arXiv:1010.6069 [hep-ph].
[12] H. Na *et al.* (HPQCD), Phys.Rev. **D86**, 034506 (2012), arXiv:1202.4914 [hep-lat].
[13] A. Bazavov *et al.* (Fermilab Lattice and MILC), Phys.Rev. **D85**, 114506 (2012), arXiv:1112.3051 [hep-lat].
[14] R. Dowdall *et al.*(2013), arXiv:1302.2644 [hep-lat].
[15] USQCD, "Lattice QCD at the intensity frontier," (2013), `http://www.usqcd.org/documents/13flavor.pdf`.
[16] C. Allton *et al.* (RBC and UKQCD), Phys. Rev. **D78**, 114509 (2008), arXiv:0804.0473 [hep-lat].
[17] Y. Aoki *et al.* (RBC and UKQCD), Phys.Rev. **D83**, 074508 (2011), arXiv:1011.0892 [hep-lat].
[18] D. B. Kaplan, Phys. Lett. **B288**, 342 (1992), arXiv:hep-lat/9206013.
[19] Y. Shamir, Nucl. Phys. **B406**, 90 (1993), arXiv:hep-lat/9303005.
[20] H.-W. Lin and N. Christ, Phys.Rev. **D76**, 074506 (2007), arXiv:hep-lat/0608005.
[21] N. H. Christ, M. Li, and H.-W. Lin, Phys.Rev. **D76**, 074505 (2007), arXiv:hep-lat/0608006.
[22] A. X. El-Khadra, A. S. Kronfeld, and P. B. Mackenzie, Phys. Rev. **D55**, 3933 (1997), arXiv:hep-lat/9604004.
[23] M. Li (RBC and UKQCD), PoS **LATTICE2008**, 120 (2008), arXiv:0810.0040 [hep-lat].
[24] Y. Aoki *et al.* (RBC and UKQCD), Phys.Rev. **D86**, 116003 (2012), arXiv:1206.2554 [hep-lat].
[25] O. Witzel, PoS **LATTICE2012**, 103 (2012), arXiv:1211.3180 [hep-lat].
[26] T. Kawanai, R. S. Van de Water, and O. Witzel, PoS **Lattice2012**, 109 (2012), arXiv:1211.0956 [hep-lat].
[27] C. Lehner, PoS **LATTICE2012**, 126 (2012), arXiv:1211.4013 [hep-lat].
[28] S. R. Sharpe and Y. Zhang, Nucl.Phys.Proc.Suppl. **47**, 441 (1996).
[29] RBC and UKQCD, "Generating ensembles with 2+1 flavors of domain wall fermions," (2013), USQCD proposal (PI Norman Christ).
[30] R. C. Brower, H. Neff, and K. Orginos(2012), arXiv:1206.5214 [hep-lat].
[31] A. X. El-Khadra *et al.*, Phys.Rev. **D64**, 014502 (2001), arXiv:hep-ph/0101023.
[32] J. Harada *et al.*, Phys.Rev. **D65**, 094513 (2002), arXiv:hep-lat/0112044 [hep-lat].
[33] D. Becirevic, S. Prelovsek, and J. Zupan, Phys.Rev. **D68**, 074003 (2003), arXiv:hep-lat/0305001 [hep-lat].
[34] C. Aubin and C. Bernard, Phys.Rev. **D76**, 014002 (2007), arXiv:0704.0795 [hep-lat].
[35] W. Detmold, C. D. Lin, and S. Meinel, Phys.Rev. **D85**, 114508 (2012), arXiv:1203.3378 [hep-lat].
[36] N. Yamada, S. Aoki, and Y. Kuramashi, Nucl. Phys. **B713**, 407 (2005), arXiv:hep-lat/0407031.
[37] S. Aoki, Y. Kayaba, and Y. Kuramashi, Nucl. Phys. **B697**, 271 (2004), arXiv:hep-lat/0309161.
[38] A. Pochinsky, PoS **LATTICE2008**, 040 (2008).
[39] A. Pochinsky and S. Syritsyn, `https://usqcd.lns.mit.edu/redmine/projects/mdwf`.
[40] A. Pochinsky, `https://usqcd.lns.mit.edu/w/index.php/QLUA`.
[41] B. Sheikholeslami and R. Wohlert, Nucl.Phys. **B259**, 572 (1985).
[42] R. G. Edwards and B. Joo (SciDAC, LHPC and UKQCD), Nucl.Phys.Proc.Suppl. **140**, 832 (2005), arXiv:hep-lat/0409003.
[43] T. Blum, T. Izubuchi, and E. Shintani(2012), arXiv:1208.4349 [hep-lat].
[44] S. D. Cohen *et al.*, PoS **LATTICE2011**, 030 (2011), arXiv:1205.2933 [hep-lat]