Leptonic decay-constant ratio $f_{K^+}/f_{\pi^+}$ from lattice QCD with physical light quarks

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A calculation of the ratio of leptonic decay constants $f_{K^+}/f_{\pi^+}$ makes possible a precise determination of the ratio of CKM matrix elements $|V_{us}|/|V_{ud}|$ in the Standard Model, and places a stringent constraint on the scale of new physics that would lead to deviations from unitarity in the first row of the CKM matrix. We compute $f_{K^+}/f_{\pi^+}$ numerically in unquenched lattice QCD using gauge-field ensembles recently generated that include four flavors of dynamical quarks: up, down, strange, and charm. We analyze data at four lattice spacings $a \approx 0.06, 0.09, 0.12,$ and 0.15 fm with simulated pion masses down to the physical value 135 MeV. We obtain $f_{K^+}/f_{\pi^+} = 1.947(26)(37)$, where the errors are statistical and total systematic, respectively. This is our first physics result from our $N_f = 2 + 1 + 1$ ensembles, and the first calculation of $f_{K^+}/f_{\pi^+}$ from lattice-QCD simulations at the physical point. Our result is the most precise lattice-QCD determination of $f_{K^+}/f_{\pi^+}$, with an error comparable to the current world average. When combined with experimental measurements of the leptonic branching fractions, it leads to a precise determination of $|V_{us}|/|V_{ud}| = 0.2309(9)(4)$ where the errors are theoretical and experimental, respectively.

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Motivation. — Leptonic decays of charged pseudoscalar mesons are sensitive probes of quark flavor-changing interactions. Experimental measurements of the leptonic decay widths, when combined with precise theoretical calculations of the leptonic decay constants, enable the determination of elements of the Cabibbo-Kobayashi-Maskawa (CKM) quark-mixing matrix. Further, when combined with independent determinations of the CKM matrix elements from other processes such as semileptonic meson decays, they make possible precise tests of the Standard-Model CKM framework. Here we present a lattice-QCD calculation of the decay-constant ratio $f_{K^+}/f_{\pi^+}$, which may be used to determine $|V_{us}|/|V_{ud}|$ via [1, 2]

$$\frac{\Gamma(K \rightarrow l\bar{\nu}l)}{\Gamma(\pi \rightarrow l\bar{\nu}l)} = \frac{|V_{us}|^2 f_{K^+}^2 m_K}{|V_{ud}|^2 f_{\pi^+}^2 m_{\pi}} \left( \frac{1 - m_{\pi}^2}{m_K^2} \right)^2 \left[ 1 + \delta_{\text{EM}} \right],$$

where $l = e, \mu$ and $\delta_{\text{EM}}$ is a known 1-loop QED correction [3, 4]. The ratio $f_{K^+}/f_{\pi^+}$ can be calculated to subpercent precision using numerical lattice-QCD simulations [5, 6] because the Monte Carlo statistical errors are correlated between the numerator and denominator and the explicit dependence on the lattice scale drops out.

Lattice QCD enables ab initio calculations of nonperturbative hadronic matter elements. The QCD Lagrangian is formulated in discrete Euclidean spacetime, after which the now finite-dimensional path integral can be solved numerically with Monte Carlo methods. Once the $N_f + 1$ parameters of the QCD action (quark masses and gauge coupling) are fixed by matching to an equal number of experimental measurements, all other outputs of the lattice simulation are predictions of the theory. In practice, currently available computing resources limit the lattice spacing in most recent simulations to $a \gtrsim 0.06$ fm, the spacetime volume of the lattice to $L^3 \sim (4 \text{ fm})^3$, and the pion mass to $m_{\pi} \gtrsim 200$ MeV. These choices introduce systematic errors that must be quantified, but the good agreement between lattice-QCD calculations and experiment for a wide range of observables [7, 8] demonstrates that the errors are controlled.

Many precise lattice-QCD weak-matrix element calcu-
lations relevant for quark-flavor physics have been obtained using our $N_f = 2 + 1 + 1$ flavor gauge-field ensembles generated using the asqtad-improved staggered quark action for the dynamical $u$, $d$, and $s$ quarks [9–11]. Our calculations of $f_{K^+}/f_{\pi^+}$ on those ensembles [2, 11, 12] ultimately reached a precision of $\sim 0.6\%$. We are now embarking on a new program of configuration generation using the highly-improved staggered quark (HISQ) action [13], which has two primary advantages. The most important staggered discretization errors are approximately 3 times smaller for the HISQ action than for the asqtad action at the same lattice spacing [14]; this makes it possible to undertake simulations at the physical pion mass, which require a box of approximately (5 fm)$^3$. The improved quark dispersion relation for the HISQ action also allows the inclusion of dynamical charm quarks in the simulations.

One of the largest sources of uncertainty in lattice-QCD determinations of quantities such as $f_{K^+}/f_{\pi^+}$ is from the extrapolation of the simulation results to the physical up- and down-quark masses. In this work, we replace this error with a negligible interpolation error by simulating at light-quark masses very close to or even below their physical values. The calculation presented here, using the configurations with four flavors of dynamical HISQ quarks, lays the foundation for a larger quark flavor-physics program to compute pion, kaon, and charmed weak matrix elements, and eventually even those with bottom quarks, on these ensembles.

**Lattice-QCD Calculation.** — This calculation is based on a subset of our $(2+1+1)$-flavor ensembles described in Refs. [14, 15]. These ensembles use a one-loop Symanzik-improved gauge action for the gluons [16, 17], and the HISQ action for the dynamical $u$, $d$, $s$, and $c$ quarks. The simulated strange and charm sea-quark masses ($m_s$ and $m_c$) are fixed at approximately their physical values. The simulated up and down sea-quark masses are taken to be degenerate with a common mass $m_l \approx m_s/27$, such that the simulated pion mass is approximately the physical value 135 MeV [18]. Additional ensembles with slightly heavier pions ($m_l = m_s/10$) allow us to correct $f_{K^+}/f_{\pi^+}$ a posteriori for the slight mistuning of the simulated sea-quark masses. The spatial volumes are sufficiently large ($m_l L > 3.5$) that finite-volume corrections are expected to be at the subpercent level for light pseudoscalar meson masses and decay constants, and we confirm this with an explicit finite-volume study. We use four lattice spacings $a \approx 0.15, 0.12, 0.09$, and 0.06 fm to enable a controlled extrapolation to the continuum ($a \to 0$) limit. The specific numerical simulation parameters are given in Table I.

Naive lattice discretizations of the quark action suffer from the problem of fermion doubling. The staggered quark action only partly eliminates fermion doublers, reducing the number of species from 16 to 4. The remaining species are referred to as “tastes” to distinguish them from physical flavors. Quarks of different taste can interact by exchanging gluons with momentum components close to the lattice cutoff $p_l \approx \pi/a$. Taste-changing interactions split the mass degeneracy of pions composed of different quark tastes. The taste splittings are of $\mathcal{O}(a^2)$ for the HISQ action, and decrease rapidly with lattice spacing. The taste-Goldstone and root-mean-squared (RMS) sea-pion masses are given in Table I; the difference between the two is only about 10 MeV for the finest $a \approx 0.06$ fm ensembles used in this analysis. More details can be found in Ref. [15].

The dynamical HISQ simulations use the fourth-root procedure to remove the unwanted taste degrees of freedom. Due to taste-changing interactions, the rooted Dirac operator is nonlocal at nonzero lattice spacing, and leads to violations of unitarity [19–22]. Nevertheless, there are strong theoretical arguments and numerical evidence that the continuum limit of the rooted staggered lattice theory is indeed QCD [23–30].

We obtain the meson masses and decay constants from fits of two-point correlation functions with a pseudoscalar interpolating operator at both the source and sink. For each valence-quark mass combination, we compute the decay constant using a partially-conserved axial current relation:

$$F_{xy} = (m_x + m_y) \langle 0 | \bar{\psi}_x \gamma_5 \psi_y | 0 \rangle / M_{xy}^2,$$

where $M_{xy}$ is the mass of the pseudoscalar meson $P_{xy}$ with bare valence-quark masses $m_x$ and $m_y$. We choose a fitting range for the correlators such that, in the case of degenerate valence-quark masses, a single-exponential fit gives a good fit as measured by the correlated $\chi^2$/dof and $p$-value. We include both the ground state and an opposite-parity excited state for the nondegenerate correlators. Statistical errors are estimated by jackknifing. The ground-state mass and amplitudes are stable with respect to a reasonable reduction of the minimum time separation of the source and sink, and with the inclusion

| $a$(fm) | $L$(fm) | $M_{\pi,5}$(MeV) | $M_{\pi,\text{RMS}}$(MeV) | $N_{\text{lats}}$ |
|--------|--------|-----------------|-----------------|-----------|
| 0.15   | 3.66   | 214             | 352             | 1000      |
| 0.15   | 4.82   | 133             | 311             | 1000      |
| 0.12   | (2.84,3.79,4.73) | 215           | 294             | 1000      |
| 0.12   | 5.83   | 133             | 241             | 1000      |
| 0.09   | 4.33   | 215             | 244             | 1000      |
| 0.09   | 5.63   | 128             | 173             | 707       |
| 0.06   | 3.79   | 223             | 229             | 678       |
| 0.06   | 5.45   | 134             | 143             | 310       |
of additional excited states; therefore the error due to excited-state contamination can be neglected compared with the statistical errors. Additional details of these fits can be found in Ref. [31].

Chiral perturbation theory ($\chi$PT) predicts that the finite-volume corrections to pion and kaon masses and decay constants are at the per mill level in our simulations, and are therefore comparable to the size of the statistical errors in our numerical data. We check this expectation with an explicit comparison of these quantities measured on three $a \approx 0.12$ fm ensembles with identical simulation parameters except for the spatial lattice volume (see Table I). We fit the data at the three volumes to the functional form:

$$aX(L) = A_X \left(1 + B_X(m_\pi, L)\right)$$

(3)

where $X = \{m_\pi, f_\pi, m_K, f_K\}$, $A_X$ is a free parameter, and the function $B_X$ is determined at a given order in $\chi$PT. We try both the NLO expression for $B_X$ in staggered $\chi$PT [32, 33], and the continuum NLO and resummed NNLO $\chi$PT expressions [34]. Figure 1 compares the numerical lattice data for $m_\pi$ and $f_\pi$ with these expressions. NLO staggered $\chi$PT describes the $f_\pi$ data very well at all three volumes, and describes the $m_\pi$, $m_K$, and $f_K$ data adequately (to $\sim 0.4\%$ or better). We therefore use NLO staggered finite-volume $\chi$PT to correct our simulation data in our central fit, and use the continuum NLO and NNLO finite-volume $\chi$PT corrections to estimate the systematic uncertainty.

Because our lattice-QCD simulations are isospin-symmetric (the up and down sea-quark masses are equal), we adjust the experimental inputs to what they would be in a world without electromagnetism or isospin violation before matching the simulation data to experiment to find the strange quark mass $m_s$ and the average light quark mass $m = (m_u + m_d)/2$. We follow the approach of Ref. [2], but with updated values for the EM correction to Dashen’s theorem. For the kaon, we consider the isospin-averaged mass $M_K^2 = (M_{K^+}^2 + M_{K^0}^2)_{\text{QCD}}/2$, where the subscript “QCD” indicates that the leading EM effects in the masses were removed from the experimental masses [18]; we take the parameter $\Delta_{\text{EM}} = 0.65(7)_{\text{stat}}(14)_{\text{syst}}$ that characterizes violations of Dashen’s theorem from our ongoing lattice QED+QCD simulations using asqtad sea quarks [35].

In this work, we tune the quark masses and lattice scale and determine $f_{K^+}/f_{\pi^+}$ in a single, self-contained analysis as follows. We begin with numerical lattice data for meson masses and decay constants for a selection of valence-quark masses that allow us to adjust for slight mistunings and interpolate or extrapolate to the physical values. In order to reduce autocorrelations below measurable levels, the single-elimination jackknife results are blocked by 20 lattices (100 or 120 molecular dynamics time units) before the final averaging. The physical-quark-mass $a \approx 0.06$ fm ensemble has an insufficient number of configurations for blocks that large. Instead, we block by 5 trajectories on that ensemble and rescale the resulting errors by a factor of 1.17, which is determined by comparing the errors at block sizes around 20 to those at block size 5 on the $m_l = 0.1m_s$, $a \approx 0.06$ fm ensemble, as well as an additional $m_l = 0.2m_s$, $a \approx 0.06$ fm ensemble not otherwise discussed here. We then construct the squared ratio of pseudoscalar-meson mass to decay constant, $M_{xx}^2/F_{xx}^2$, which $\chi$PT predicts to be approximately proportional to the valence-charge mass $m_x$. Using the lightest valence-quark mass on each ensemble, we interpolate or extrapolate data for this ratio linearly in $m_x$ to where it equals the experimental value for $M_{xx}^2/f_{\pi^+}^2$. This fixes the physical value of $\hat{m}$. We obtain the lattice spacing from requiring that the decay constant at this mass equal the experimental value for $f_{\pi^+}$ [36], where we use a quadratic interpolation/extrapolation through the lightest three valence-quark masses. We then
take nondegenerate “kaons” in which the strange valence-quark mass \( m_s \) is 1.0 or 0.8 times the strange sea-quark mass and the lighter valence-quark mass \( m_u \) is the lightest available, and linearly interpolate in the valence strange-quark mass to where 2\( M_{\pi y}^2 - M_{\pi x}^2 = 2M_{K}^2 - M_{\pi}^2 \); this fixes the physical strange-quark mass \( m_s \). Once we know \( m_s \), we obtain the \( u-d \) mass-splitting from the difference between the EM-subtracted neutral and charged kaon masses: \( m_d - m_u = (M_{K}^2 - M_{\pi}^2)_{QCD}/(\partial M_{\pi}^2/\partial m_x) \). Finally, we obtain \( f_{K^+} \) by linearly interpolating the decay constant \( F_{\pi y} \) in the light valence-quark mass to \( m_u \) and in the strange valence-quark mass to \( m_s \). In \( f_{K^+} \), we neglect isospin violations from the sea quarks, and we neglect all isospin violations in \( f_{\pi^+} \), because these effects are of NNLO in \( \chi PT \) [6]. We also slightly correct \( f_K \) \( a \ posteriori \) for sea-quark mass mistuning using the slope with respect to the light sea-quark mass, \( \partial f_K/\partial m_1 \), measured by comparing the value of \( f_K \) from the physical-mass ensembles with that from ensembles with \( m_1 \approx 0.1 m_s \). The results for \( f_{K^+}/f_{\pi^+} \) are shown versus \( a^2 \) in Fig. 2.

We extrapolate \( f_{K^+}/f_{\pi^+} \) at physical quark masses to the continuum limit quadratically in \( a^2 \). We estimate the uncertainty in the continuum extrapolation from alternative fits with different ansätze for the \( a^2 \) dependence and excluding the coarsest ensemble(s). Two reasonable choices are linear extrapolations of the three physical-mass data points with \( a \leq 0.12 \) fm, and a constant fit to the two physical-mass data points with \( a \leq 0.09 \) fm. Of these, the constant fit, shown in Fig. 2, gives the larger difference from the central extrapolation, 0.28%. Additional extrapolations have also been tried, including a quadratic-in-\( a^2 \), linear in \( m_1 \) fit to all the \( m_1 \approx m_s/27 \) and \( m_1 = 0.1 m_s \) data points, and a similar fit restricted to ensembles with \( a \leq 0.12 \) fm. These fits give differences from the central value that are comparable to or smaller than the difference seen above, as does a simple linear-in-\( a^2 \) extrapolation of the two finest \( a \leq 0.09 \) fm physical-mass points. We thus take 0.28% as our estimate of the discretization error. Note that, when the scale-setting procedure is changed by repeating the analysis using other quantities to fix the lattice scale instead of \( f_\pi \) (see Ref. [15] for further details), we find a 0.17% difference with the central value, well within the estimate for the continuum extrapolation error. To estimate the finite-volume error, we repeat the entire analysis using finite-volume corrections for the pion (kaon) masses and decay constants calculated at NNLO (NLO) in continuum \( \chi PT \). We propagate the statistical uncertainties in the tuned quark masses and lattice scale throughout the analysis via the jackknife method, so they are already folded into the statistical error. We estimate the systematic uncertainty from the quark-mass tuning and scale setting by taking the difference of our central tuning procedure with one where we interpolate/extrapolate the ratio \( M_{sx}^2/F_{sx}^2 \) quadratically in \( m_s \). For the physical-quark-mass ensembles (and hence for the continuum extrapolated result), the valence-quark masses are very close to the tuned physical values, so the choice of interpolation fit function makes a negligible difference. On the 0.1 \( m_s \) ensembles, however, valence masses as light as physical are not available, so the choice of fit function for the valence-quark extrapolation has a greater impact. The systematic errors from the tuning procedure are plotted as dotted error bars in Fig. 2. We estimate the uncertainty due to EM effects by varying the values of the EM-subtracted meson masses used in the quark-mass tuning; this primarily affects \( m_u \). We vary the parameter \( \Delta_{EM} \) by its total error [35]. We also repeat the tuning including a previously-neglected EM correction to the neutral kaon mass, \( \delta M_{K^0, EM} = 901(8)_{stat} \) MeV$^2$ [37]. Note that direct EM effects on the weak matrix elements are by definition removed from \( f_{\pi^+} \) and \( f_{K^+} \) [18].

**Results and Conclusions.** — We obtain the following determination of the ratio \( f_{K^+}/f_{\pi^+} \):

\[
\frac{f_{K^+}}{f_{\pi^+}} = 1.1947(26)_{stat}(33)_{a^2}(17)_{FV}(2)_{EM}, \tag{4}
\]

with an approximately 0.4% total uncertainty. Our result agrees with, but is more precise than, other independent lattice-QCD calculations \([12, 38–41]\), and its error is com-

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**FIG. 2:** Continuum extrapolation of \( f_{K^+}/f_{\pi^+} \). Our central value is obtained from a quadratic-in-\( a^2 \) fit to the physical-quark-mass data points (red circles), adjusted for tuning errors to the physical sea quark masses using the 0.1 \( m_s \) data points (blue squares). The size of the adjustments is too small to be visible on this plot. The black star shows \( f_{K^+}/f_{\pi^+} \) at the physical quark masses in the continuum, where the inner solid error bar is statistical and the outer dotted error bar includes the continuum-extrapolation error added in quadrature. An alternative, constant-in-\( a^2 \) fit to the two physical-mass data points, is shown by the dashed horizontal line. Its deviation from the central value gives our estimate of the continuum extrapolation error (see text). The dotted error bars on the 0.1 \( m_s \) data show the systematic error from the valence-quark mass tuning added in quadrature to the statistical error (see text); the tuning uncertainty on the physical-mass ensembles is negligible.
petitive with that of the current lattice-QCD world average [5, 6]. Because we use $f_\pi$ to set the lattice scale, we also obtain a result for $f_{K^+} = 155.80(34)_{\text{stat}}(48)_{\text{sys}}(24)_{f_\pi}$, where the errors are due to statistics, systematics in $f_K/f_\pi$, and the uncertainty in $f_\pi$. This agrees with the experimental determination of $f_{K^+}$ assuming CKM unitarity [36]. By combining $f_{K^+}/f_\pi$ with Eq. (4) with recent experimental results for the lepton branching fractions [42], we obtain $|V_{us}|/|V_{ud}| = 0.2309(9)_{\text{theo}}(4)_{\text{exp}}$. Taking $|V_{ud}|$ from nuclear $\beta$ decay [43], we also obtain $|V_{us}| = 0.2249(8)_{\text{theo}}(4)_{\text{exp}}(1)_{V_{ud}}$, which agrees with and has comparable errors to the determination from $K \to \pi\ell\nu$ semileptonic decay [42, 44–46]. Further, our result places stringent constraints on new-physics scenarios that would lead to deviations from unitarity in the first row of the CKM matrix. We find $1 - |V_{ud}|^2 - |V_{us}|^2 - |V_{ub}|^2 = 0.0003(6)$, which is in excellent agreement with the Standard-Model value of zero.

We are currently extending the ensemble with the physical pion mass at $a \approx 0.06$ fm as well as the other ensembles with fewer than 1000 equilibrated lattices. We will include this additional data in a longer work that updates this result and presents determinations of the charmed pseudoscalar decay constants. We will also perform a more sophisticated analysis using staggered chiral perturbation theory [32, 33, 47] to obtain the low-energy constants of $\chi$PT. Our result for $f_{K^+}/f_\pi$ lays the foundation for a new large-scale lattice-QCD physics program using the $N_f = 2+1+1$ flavor HISQ gauge-field ensembles with physical pion masses. These ensembles will enable calculations of light and heavy-light hadronic weak matrix elements with unprecedented precision, and will ultimately strengthen tests of the Standard Model and improve the reach of searches for new physics in the quark-flavor sector.

NB: After this work was submitted for peer review, another determination of $f_{K^+}/f_\pi$ using our HISQ ensembles and consistent with our result was posted by HPQCD [48].

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