Charmed-Meson Decay Constants in Three-Flavor Lattice QCD

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We present the first lattice QCD calculation with realistic sea quark content of the D^+-meson decay constant f_{D^+}. We use the MILC Collaboration's publicly available ensembles of lattice gauge fields, which have a quark sea with two flavors (up and down) much lighter than a third (strange). We obtain $f_{D^+} = 201 \pm 3 \pm 17$ MeV, where the errors are statistical and a combination of systematic errors. We also obtain $f_{D_s} = 249 \pm 3 \pm 16$ MeV for the D_s meson.

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Flavor physics currently plays a central role in elementary particle physics [1]. To aid the experimental search for physics beyond the standard model, several hadronic matrix elements must be calculated nonperturbatively from quantum chromodynamics (QCD). One of the most important of these is the decay constant of the B meson f_B [2]. Any framework for calculating f_B should, therefore, be subjected to stringent tests, and such a test is a key aim of this Letter.

The most promising method for these nonperturbative calculations is numerical lattice QCD. For many years the results suffered from an unrealistic treatment of the effects of sea quarks. In the last few years, however, this obstacle seems to have been removed: with three flavors of sea quarks lattice QCD now agrees with experiment for a wide variety of hadronic quantities [3]. This validation of lattice QCD has been realized, so far, only for so-called "gold-plated" quantities: masses and matrix elements of the simplest hadronic states. Note, however, that many of the hadronic matrix elements relevant to flavor physics are in this class, including f_B.

The challenges in computing f_B are essentially the same for the D^+-meson decay constant f_{D^+}. Experiments have observed the leptonic decay $D^+ \to l^+ \nu_l$, but not $B^+ \to l^+ \nu_l$. One can, thus, determine $|V_{cd}|f_{D^+}$, where V_{cd} is an element of the Cabibbo-Kobayashi-Maskawa (CKM) matrix. Taking $|V_{cd}|$ from elsewhere, one gets f_{D^+}. In 2004 the CLEO-c Collaboration mea-

sured f_{D^+} with a 20% error [4], and a more precise measurement is expected soon.

This Letter reports the first lattice-QCD calculation of f_{D^+} with three flavors of sea quarks [5]. We find

$$f_{D^+} = 201 \pm 3 \pm 6 \pm 9 \pm 13 \text{ MeV}, \qquad (1)$$

where the uncertainties are statistical, and a sequence of systematic effects, discussed below. We also obtain the decay constant of the D_s meson,

$$f_{D_s} = 249 \pm 3 \pm 7 \pm 11 \pm 10 \text{ MeV}. \qquad (2)$$

The second result is more precise than a recent lattice-QCD calculation with the same sea quark content but non-relativistic heavy quarks, which found $f_{D_s} = 290 \pm 20 \pm 41$ MeV [6]. These results are more reliable than older calculations [7] because we now incorporate (three) sea quarks and, for f_{D^+}, also because the light valence quark masses are smaller than before.

These results test the methods of Ref. [3] because they are predictions. The input parameters have been fixed previously [3, 8, 9, 10, 11], and, once comparably precise experimental measurements become available, one can see how Eqs. (1) and (2) fare. Indeed, this work is part of a program to calculate matrix elements for leptonic and semileptonic decays [10, 12, 13], neutral-meson mixing, and quarkonium [11, 14]. So far, these lattice QCD calculations agree with experiment for the normalization of

TABLE I: Notation for quark masses used in this Letter.

m	Description	Remark
m_c	Charmed quark	From m_{D_s} [10, 11]
m_s	Physical strange quark	From m_K^2 [8]
m_u	Physical up quark	$m_u = m_s/45.5$ [9]
m_d	Physical down quark	$m_d = m_s/19.6$ [9]
m_h	Simulation's heavier sea quark	$m_h \approx 1.1m_s$
m_l	Simulation's lighter sea quark	$0.1m_s \leq m_l \lesssim 0.8m_s$
m_q	Simulation's light valence quark	$0.1m_s \leq m_q \lesssim m_s$

D-meson semileptonic form factors [12, 15, 16]. They also have predicted correctly the form-factor shape [12, 17], as well as the mass of the B_c meson [14, 18].

In this set of calculations we use ensembles of unquenched lattice gauge fields generated by the MILC Collaboration [9, 19], with lattice spacing $a = 0.175$, 0.121, and 0.086 fm. The key feature of these ensembles is that they incorporate three flavors of sea quarks, one whose mass is close to that of the strange quark, and two with a common mass taken as light as possible.

For the sea quark and light valence quark we use the "Asqtad" staggered-fermion action [20]. Several different quark masses appear in this calculation; for convenience, they are defined in Table I. At $a = 0.175$, 0.121, and 0.086 fm there are, respectively, 4, 5, and 2 ensembles with various sea quark masses (m_l, m_h) [9, 19]. The larger simulation mass, m_h is close to the physical strange quark mass m_s. The light pair's mass m_l is not as small as those of the up and down quark in Nature, but the range $0.1m_s \leq m_l \lesssim 0.8m_s$ suffices to control the extrapolation in quark mass with chiral perturbation theory (χPT). For carrying out the chiral extrapolation, it is useful to allow the valence mass m_q to vary separately from the sea mass [21]. At $a = 0.175$, 0.121, and 0.086 fm we have, respectively, 6, 12, and 8 or 5 values of the valence mass, in the range $0.1m_s \leq m_q \lesssim m_s$.

A drawback of staggered fermions is that they come in four species, called tastes. The steps taken to eliminate three extra tastes per flavor are not (yet) proven, although there are several signs that they are valid. Calculations of f_{D^+} and f_{D_s} are sensitive to these steps: if Eqs. (1) and (2) agree with precise measurements, it should be more plausible that the techniques used to reduce four tastes to one are correct.

For the charmed quark we use the Fermilab action for heavy quarks [22]. Discretization effects are entangled with the heavy-quark expansion, so we use heavy-quark effective theory (HQET) as a theory of cutoff effects [23]. This provides good control, as discussed in Ref. [24], and the framework has been tested with the (successful) prediction of the B_c meson mass [14]. Nevertheless, heavy-quark discretization effects are the largest source of systematic error in f_{D_s}, and the second-largest in f_{D^+}.

The decay constant f_{D_q}, for a D_q meson with light valence quark q and momentum p_μ, is defined by [25]

$$\langle 0|A_\mu|D_q\rangle = if_{D_q}p_\mu, \qquad (3)$$

where $A_\mu = \bar{q}\gamma_\mu\gamma_5 c$ is an electroweak axial vector current. The combination $\phi_q = f_{D_q}\sqrt{m_{D_q}}$ emerges directly from the lattice Monte Carlo calculations. As usual in lattice gauge theory, we compute two-point correlation functions $C_2(t) = \langle O_{D_q}^\dagger(t)O_{D_q}(0)\rangle$, $C_A(t) = \langle A_4(t)O_{D_q}(0)\rangle$, where O_{D_q} is an operator with the quantum numbers of the charmed pseudoscalar meson, and A_4 is the (lattice) axial vector current. The operators are built from the heavy-quark and staggered-quark fields as in Ref. [26]. We extract the D_q mass and the amplitudes $\langle D|O_{D_q}|0\rangle$ and $\langle 0|A_4|D\rangle$ from fits to the known t dependence. Statistical errors are determined with the bootstrap method, which allows us to keep track of correlations.

The lattice axial vector current must be multiplied by a renormalization factor $Z_{A_4^{cq}}$. We write [27] $Z_{A_4^{cq}} = \rho_{A_4^{cq}}(Z_{V_4^{cc}}Z_{V_4^{qq}})^{1/2}$, because the flavor-conserving renormalization factors $Z_{V_4^{cc}}$ and $Z_{V_4^{qq}}$ are easy to compute nonperturbatively. The remaining factor $\rho_{A_4^{cq}}$ should be close to unity because the radiative corrections mostly cancel [28]. A one-loop calculation gives [29] $\rho_{A_4^{cq}} = 1.052$, 1.044, and 1.032 at $a = 0.175$, 0.121, and 0.086 fm. We estimate the uncertainty of higher-order corrections to be $2\alpha_s(\rho_{A_4^{cq}} - 1) \approx 1.3\%$; α_s is the strong coupling.

The heart of our analysis is the chiral extrapolation, from the simulated to the physical quark masses. It is necessary, and non-trivial, because the cloud of "pions" surrounding the simulated D_q mesons is not the same as for real pions. With staggered quarks the (squared) pseudoscalar meson masses are

$$M_{ab,\xi}^2 = (m_a + m_b)\mu + a^2\Delta_\xi, \qquad (4)$$

where m_a and m_b are quark masses, μ is a parameter of χPT, and the representation of the meson under the taste symmetry group is labeled by $\xi = P, A, T, V, I$ [30]. A symmetry as $m_a, m_b \to 0$ ensures that $\Delta_P = 0$. The "pion" cloud in the simulation includes all these pseudoscalars.

According to next-to-leading order χPT the decay constant takes the form

$$\phi_q = \Phi\left[1 + \Delta f_q(m_q, m_l, m_h) + p_q(m_q, m_l, m_h)\right], \quad (5)$$

where Φ is a quark-mass-independent parameter. Δf_q arises from loop processes involving light pseudoscalar mesons, and p_q is an analytic function. To obtain them one must take into account the flavor-taste symmetry of the simulation [30] and the inequality (in general) of the valence and sea quark masses [21]. One finds [31]

$$\Delta f_q = -\frac{1 + 3g^2}{2(4\pi f_\pi)^2}\left[\bar{h}_q + h_q^I + a^2\left(\delta_A' h_q^A + \delta_V' h_q^V\right)\right], \quad (6)$$

where $f_\pi \approx 131$ MeV is the pion decay constant, g is the D-D^*-π coupling [32], and δ'_A, δ'_V parametrize effects that arise only at non-zero lattice spacing [30]. The terms $\bar{h}_q$, h_q^I, h_q^A, and h_q^V are functions of the pseudoscalar meson masses. The last two, h_q^A and h_q^V, are too cumbersome to write out here. It is instructive to show the other two, $\bar{h}_q$ and h_q^I, when $m_q = m_l$ or m_h:

$$\bar{h}_q = \tfrac{1}{16}\sum_\xi n_\xi \left[2I(M_{ql,\xi}^2) + I(M_{qh,\xi}^2)\right], \qquad (7)$$

$$h_l^I = -\tfrac{1}{2}I(M_{ll,I}^2) + \tfrac{1}{6}I(M_{\eta,I}^2), \qquad (8)$$

$$h_h^I = -I(M_{hh,I}^2) + \tfrac{2}{3}I(M_{\eta,I}^2), \qquad (9)$$

where $I(M^2) = M^2 \ln M^2/\Lambda_\chi^2$ (with Λ_χ the chiral scale), and $M_{\eta,I}^2 = (M_{ll,I}^2 + 2M_{hh,I}^2)/3$. The term h_q^I receives contributions only from taste-singlet mesons (representation I). The term $\bar{h}_q$ receives contributions from all representations, with multiplicity $n_\xi = 1, 4, 6, 4, 1$ for $\xi = P, A, T, V, I$, respectively. The analytic function is

$$p_q = (2m_l + m_h)f_1(\Lambda_\chi) + m_q f_2(\Lambda_\chi) + O(a^2), \qquad (10)$$

where f_1 and f_2 are quark-mass-independent parameters. They are essentially couplings of the chiral Lagrangian, and their Λ_χ dependence must cancel that of Δf_q. This specifies $O(a^2)$ terms proportional to f_1 and f_2, which can be removed after our fit. We estimate the remaining $O(a^2)$ effects of light quarks to be small: around 4% at $a = 0.121$ fm and 1.4% at $a = 0.086$ fm.

The salient feature [33] of the chiral extrapolation of ϕ_q is that Δf_q contains a "chiral log" $I(2m_q\mu) \sim m_q \ln m_q$, which has a characteristic curvature as $m_q \to 0$. Equations (4)–(8) show that the chiral log is diluted by discretization effects, because $a^2\Delta_\xi \neq 0$ for $\xi \neq P$.

We can now discuss how we carry out the chiral extrapolation. Recall that we compute ϕ_q for many combinations of the valence and light sea quark masses. At each lattice spacing, we fit all results for ϕ_q to the mass dependence prescribed by Eqs. (4)–(10). Of the twelve parameters, eight—μ, the four non-zero Δ_ξ, f_π, δ'_A, and δ'_V—appear in the χPT for light pseudoscalar mesons. We constrain them with prior distributions whose central value and width are taken from the χPT analysis of pseudoscalar meson masses and decay constants on the same ensembles of lattice gauge fields [9]. The rest—Φ, g^2, f_1, and f_2—appear only for charmed mesons. We constrain g^2 to its experimentally measured value, within its measured uncertainty [34]. Thus, only three parameters—Φ, f_1, and f_2—are determined solely by the ϕ_q fit. To obtain physical results we reconstitute the fit setting the light sea quark mass $m_l \to (m_u + m_d)/2$, and $\Delta_\xi = \delta'_{A,V} = 0$. For ϕ_d (ϕ_s) we set the light valence mass $m_q \to m_d$ (m_s).

To isolate the uncertainties of the chiral extrapolation from other sources of uncertainty, we consider the ratio $R_{q/s} = \phi_q/\phi_s$. Figure 1 shows $R_{q/s}$ at $a = 0.121$ fm as a function of m_q/m_s, projected onto $m_q = m_l$. The gray
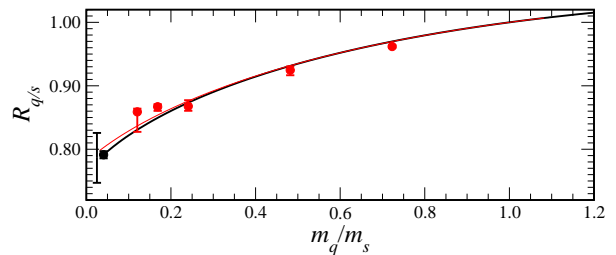

FIG. 1: Chiral extrapolation of $R_{q/s}$ at $a = 0.121$ fm. Data points show only statistical errors, but the systematic error of fitting is shown at left.
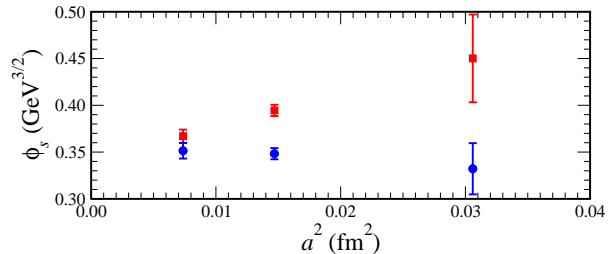

FIG. 2: Dependence of ϕ_s on a^2. Circles result from removing the $O(a^2)$ pieces in Eq. (10); squares omit this step.

(red) curve is the result of the full fit of ϕ_q to the separate sea- and valence-mass dependence. The black curve, and the extrapolated value at $m_q/m_s = 0.05$, results from setting $\Delta_\xi = \delta'_{A,V} = 0$ when reconstituting the fit. At the other lattice spacings we obtain similar results.

The precision after the chiral extrapolation is, however, a bit illusory. We tried several variations in the fit procedure: fitting the ratio directly; adding terms quadratic in the quark masses to Eq. (10); variations in the widths of the prior constraints of the parameters. When these possibilities are taken into account, the extrapolated value of $R_{d/s}$ varies by 5%, which we take as a systematic uncertainty. This variation could be reduced with higher statistics at the lightest sea quark masses.

The lattice spacing dependence of $\phi_s = f_{D_s}\sqrt{m_{D_s}}$ is shown in Fig. 2. The (blue) circles are the main results. In a preliminary report of this work [5] the $O(a^2)$ terms in ϕ_s were not removed. The (red) squares illustrate the effect of omitting this step. As one can see, the effect is small at $a = 0.086$ fm, but it is the main reason why the results in Eqs. (1) and (2) are smaller than in Ref. [5].

The χPT expressions for ϕ_q assume that the D_q meson is static. Since its mass is around 1900 MeV and the pseudoscalars are a few hundred MeV, this is a good starting point. Some corrections to this approximation can be absorbed into the fit parameters, with no real change in the analysis. A more interesting change arises in the one-loop self-energy diagrams, for which the function $I(M^2)$ is modified, and depends on $m_{D^*} - m_D$ as well as M. By replacing our standard extrapolation by one using the modified function, we estimate the associated

TABLE II: Error budget (in per cent) for $R_{d/s}$, ϕ_s, ϕ_d.

source	$R_{d/s}$	ϕ_s	ϕ_d
statistics	0.5	1.4	1.5
input parameters a and m_c	0.6	2.8	2.9
higher-order $\rho_{A_4^{cq}}$	0	1.3	1.3
heavy-quark discretization	0.5	4.2	4.2
light-quark discretization and χPT fits	5.0	3.9	6.3
static χPT	1.4	0.5	1.5
finite volume	1.4	0.5	1.5
total systematic	5.4	6.5	8.5

error to be 1.5% or less. Finite-volume effects also modify $I(M^2)$: based on our experience with f_π and f_K [9] and on continuum χPT [35], we estimate a further error of 1.5% or less.

Although χPT is able to remove (most of) the light-quark discretization errors, heavy-quark discretization effects remain. We estimate this uncertainty using HQET as a theory of cutoff effects [23, 24]. To arrive at a numerical estimate, one must choose a typical scale $\bar{\Lambda}$ for the soft interactions; we choose $\bar{\Lambda} \approx 500$–700 MeV. We then estimate a discretization uncertainty of 2.7–4.2% at $a = 0.086$ fm. Similarly, the results at $a = 0.121$ fm are expected to lie within 1–2% of those at $a = 0.086$ fm.

Because we cannot disentangle heavy- and light-quark discretization effects, to quote final results we average the results at $a = 0.086$ and 0.121 fm. We then find

$$R_{d/s} = 0.786(04)(05)(04)(42) \qquad (11)$$
$$\phi_s = 0.349(05)(10)(15)(14) \text{ GeV}^{3/2}, \qquad (12)$$

which are the principal results of this work. The uncertainties (in parentheses) are, respectively, from statistics, input parameters a and m_c, heavy-quark discretization effects, and chiral extrapolation. A full error budget is in Table II; all uncertainties are reducible in future work. The results for f_{D^+} and f_{D_s} in Eqs. (1) and (2) are obtained via $f_{D_s} = \phi_s/\sqrt{m_{D_s}}$, $f_{D^+} = R_{d/s}\phi_s/\sqrt{m_{D^+}}$, by inserting the physical meson masses.

Present experimental measurements, $f_{D^+} = 202 \pm 41 \pm 17$ MeV [4], $f_{D_s} = 267 \pm 33$ MeV [25], are not yet precise enough to put our results in Eqs. (1) and (2) to a stringent test. The anticipated measurements of f_{D^+} and, later, f_{D_s} from CLEO-c are therefore of great interest. If validated, our calculation of f_{D^+} has important implications for flavor physics. For B physics it is crucial to compute the decay constant f_B. To do so, we must simply change the heavy quark mass. In fact, heavy-quark discretization effects, with the Fermilab method, are expected to be smaller, about half as big.

Note added: After this Letter was submitted, the CLEO-c Collaboration announced a new measurement, $f_{D^+} = 223 \pm 16^{+7}_{-9}$ MeV [36].

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