Semileptonic decays of $D$ mesons in three-flavor lattice QCD

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We present the first three-flavor lattice QCD calculations for $D \rightarrow \pi l \nu$ and $D \rightarrow K l \nu$ semileptonic decays. Simulations are carried out using ensembles of unquenched gauge fields generated by the MILC collaboration. With an improved staggered action for light quarks, we are able to simulate at light quark masses down to 1/8 of the strange mass. Consequently, the systematic error from the chiral extrapolation is much smaller than in previous calculations with Wilson-type light quarks. Our results for the form factors at $q^2 = 0$ are

$$f_{+}^{D \rightarrow \pi}(0) = 0.64(3)(6) \quad \text{and} \quad f_{+}^{D \rightarrow K}(0) = 0.73(3)(7),$$

where the first error is statistical and the second is systematic, added in quadrature. Combining our results with experimental branching ratios, we obtain the CKM matrix elements $|V_{ub}| = 0.239(10)(24)(20)$ and $|V_{cd}| = 0.969(39)(94)(24)$, where the last errors are from experimental uncertainties.

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Semileptonic decays of heavy-light mesons are of great interest because they can be used to determine CKM matrix elements such as $|V_{ub}|$, $|V_{cd}|$, and $|V_{cd}|$. The accuracy of one of the most important, $|V_{ub}|$, is currently limited by large theoretical uncertainty [1]. Lattice QCD provides a systematically improvable method of calculating the relevant hadronic amplitudes, making the determination of $|V_{ub}|$ and other CKM matrix elements more reliable and precise.

Semileptonic $D$ meson decays, such as $D \rightarrow K l \nu$ and $D \rightarrow \pi l \nu$, provide a good test of lattice calculations, because the corresponding CKM matrix elements $|V_{ub}|$ and $|V_{cd}|$ are known more accurately than $|V_{ub}|$. The decay rates and distributions are not yet very well known, but the CLEO-c experiment plans to measure them with an accuracy of a few per cent. Furthermore, measurements of leptonic and semileptonic $D_{(s)}$ decays can be combined so that the CKM matrix drops out, offering a direct and stringent check of lattice QCD.

Recently, dramatic progress has been achieved in lattice QCD, for a wide variety of hadronic quantities. Reference [2] showed agreement at the few per cent level between three-flavor lattice QCD and experiment for $f_{K}$, $f_{K}$, mass splittings of quarkonia, and masses of heavy-light mesons. The main characteristics of these quantities are that they have at most one stable hadron in the initial and final states, and that the chiral extrapolation from simulated to physical light quark masses is under control. This class can be called “gold-plated” [2], and many of the lattice calculations needed to test the Standard Model are in this class. The work reported here is part of a systematic effort to calculate the hadronic matrix elements needed for leptonic and semileptonic decays, and for neutral meson mixing [3, 4].

In this Letter we report results for $D \rightarrow K l \nu$ and $D \rightarrow \pi l \nu$ semileptonic decay amplitudes. All previous lattice calculations of heavy-light semileptonic decays have been done in quenched ($m_f = 0$) QCD. In addition to quenching, they also suffered from large uncertainties from the chiral extrapolation and, in some cases, from large heavy-quark discretization effects. Here we bring all three uncertainties under good-to-excellent control. Indeed, this Letter presents the first calculation in unquenched three-flavor lattice QCD, where the effect of dynamical $u$, $d$, and $s$ quarks is correctly included.

The relevant hadronic amplitude $\langle P | V_{u} | D \rangle$ ($P = \pi, K$) is conventionally parametrized by form factors $f_{+}$ and $f_{0}$ as

$$\langle P | V_{u} | D \rangle = f_{+}(q^2)(p_{D} + p_{P} - \Delta) + f_{0}(q^2)\Delta$$

where $q = p_{D} - p_{P}$, $\Delta = (m_{D}^{2} - m_{P}^{2})q^{2}/q^{2}$. The differential decay rate $d\Gamma/dq^{2}$ is proportional to $|V_{ux}|^{2}|f_{+}(q^{2})|^{2}$, $x = d, s$. (A contribution from $f_{0}$ is proportional to the lepton mass squared.) We calculate $f_{+}$ and $f_{0}$ as a function of $q^{2}$ and determine the decay rate $\Gamma$ and the CKM matrix $|V_{ux}|$ by integrating $|f_{+}(q^{2})|^{2}$ over $q^{2}$. Preliminary results have been reported in Ref. [4, 5].

Our calculations use ensembles of unquenched gauge fields generated by the MILC collaboration [6] with the “Asq-
“tad” improved staggered quark action and the Symanzik-improved gluon action [7]. The results are obtained on the “coarse” ensembles with sea quark masses \( a m^\text{sea}_s = 0.005, 0.007, 0.01, 0.02, \) and 0.03. The gauge coupling is adjusted to keep the same lattice cutoff (\( \alpha^{-1} \approx 1.6 \) GeV) and volume \([L^3 \times T \approx (2.5 \text{ fm})^3 \times 8.0 \text{ fm}].\) Each ensemble has about 400–500 configurations. For details of the gauge configurations, see Ref. [6].

For the light valence quarks, we adopt the same staggered action as for the dynamical quarks. The valence light \((u, d)\) quark mass \( m^\text{val}_i \) is always set equal to \( m^\text{sea}_i \). The valence strange quark mass is \( m^\text{val}_s = 0.0415 \), which is slightly larger than the physical value \( a m_s = 0.039 \) (at this lattice spacing) determined from fixing the masses of the light pseudoscalars [6]. We have repeated the calculations with a strange quark mass slightly too small, and find a negligible difference. Since the computation of the staggered propagator is fast, we can simulate with \( m_l \) as low as \( m_s/8 \). Consequently we are able to reduce the systematic error from the chiral extrapolation \( (m_l \to m^\text{ud}) \to \approx 3\% \), as we show below. In contrast, previous calculations with Wilson-type light quarks simulated at low\( \Lambda_{QCD} \) with the Fermilab interpretation [9]. The bare mass is fixed via errors from this source alone [8].

Another consequence of the extra tastes is that the 3- and 2-point functions receive contributions from states that oscillate in time, in addition to the ground state and non-oscillating excited state contributions. For example, the 3-point function’s time dependence takes the form

\[
C_{3,\mu}^{D \to P}(t_x, t_y; p) = A_0 e^{-E_p t_y} e^{-E_D(t_x-t_y)} + (-1)^t_y A_1 e^{-E' t_y} e^{-E_D(t_x-t_y)} + \ldots \tag{3}
\]

where \( A_0 \propto \langle P|V^\mu|D \rangle. \)

As usual, the desired hadronic amplitude is extracted from fitting the 3- and 2-point functions. We employ two methods. In the first method, we form the ratio \( R(t_y) = C_{3,\mu}^{D \to P}(t_x, t_y)/[C_D^2(t_x) C_P^2(t_x-t_y)], \) and fit to a constant in \( t_y \). The oscillating state contributions are partly canceled in the ratio, and further reduced by taking the average, \( \bar{R}(t_y) = |R(t_y) + R(t_y+1)/2 |. \) A plateau is then found for \( t_y \) around \( t_x/2 \). In the second method, we first fit \( C_{3,\mu}^{D \to P} \) and \( C_2^{P \to D} \) separately, using a multi-exponential form similar to Eq. (3), and then obtain \( \langle P|V^\mu|D \rangle \) from the fit results. The results from the two methods always agree within statistical errors. The difference between two results is less than 3% for the lower two momenta, and as large as 3% for the higher two momenta. We choose the first method for central values and take 3% as the systematic error from the fitting.

The lattice heavy-light vector current must be multiplied by a renormalization factor \( Z_{\mu}^{V^\mu} \). We follow the method in Ref. [8], writing \( Z_{\mu}^{V^\mu} = \rho_{V_i} (Z^{V^\mu}_V Z^{V^\mu}_V)^{1/2}. \) The flavor-conserving renormalization factors \( Z^{V^\mu}_V \) and \( Z^{V^\mu}_V \) are computed nonperturbatively from standard charge normalization conditions. The remaining factor \( \rho_{V_i} \) is expected to be close to unity because most of the radiative corrections are canceled in the ratio [11]. A one-loop calculation gives [12] \( \rho_{V_i} \approx 1.01 \) and \( \rho_{V_i} \approx 0.99 \) which we use in the analysis below. This perturbative calculation is preliminary, but it has been subjected to several non-trivial tests.

Rather than calculating the conventional form factors \( f_0 \) and \( f_+ \) directly, we first extract the form factors \( f_0 \) and \( f_+ \), as in Ref. [8], defined through

\[
\langle P|V^\mu|D \rangle = \sqrt{2m_D} \left[ v_\perp f_0(E) + p_\perp f_+ (E) \right],
\]

where \( v = p_D/m_D, p_\perp = p - Ev \) and \( E = v \cdot p_D \) is the energy of the light meson. \( f_0 \) and \( f_+ \) are more natural quantities in the heavy quark effective theory, and chiral expansions are given for them as a function of \( E \) [13, 14]. We therefore carry out the chiral extrapolation in \( m_l \) for \( f_0 \) and \( f_+ \) at fixed \( E \), and then convert to \( f_0 \) and \( f_+ \).
To perform the chiral extrapolation at fixed $E$, we interpolate and extrapolate the results for $f_\| \, f_\perp$ to common values of $E$. To this end, we fit $f_\| \, f_\perp$ simultaneously using the parametrization of Becirevic and Kaidalov (BK) \cite{15},

$$f_+(q^2) = \frac{F}{(1-q^2)(1-\alpha q^2)}, \quad f_0(q^2) = \frac{F}{1-q^2/\beta},$$

where $q^2 = q^2/m_{D^*}^2$, and $F = f_+(0)$, $\alpha$ and $\beta$ are fit parameters, and $f_+, f_0$ and $q^2$ are converted to $f_\|, f_\perp$ and $E$ before the fits. An advantage of the BK form is that it contains a pole in $f_+(q^2)$ at $q^2 = m_{D^*}^2$, where $m_{D^*}$ is the lattice mass of the charmed vector meson with daughter quark $x$. The BK fit for $f_\perp$ is shown in Fig. \[\text{FIG. 1}\] using data for all available momenta $p$. Excluding the data for the highest momentum $2\pi(1,1,1)/L$ gives indistinguishable results.

We perform the chiral extrapolation using recently obtained expressions \cite{13} for heavy-to-light form factors in staggered chiral perturbation theory ($\chi$PT) \cite{16}. Compared with the continuum $\chi$PT formulae \cite{13}, the $\chi$PT formulae include 6 new parameters (4 splittings and 2 taste-violating hairpins), which parameterize lattice discretization effects. The new parameters are fixed from the analysis of light pseudoscalars \cite{6}. As usual, low energy constants appear, such as the chiral coupling $f$ and heavy-to-light meson coupling $g$. We take $f = 130$ MeV and $g = 0.59$, but changing these constants by 10% has negligible effect. The fit form we adopt (“$\chi$PT+linear”) is

$$f_{\|,\perp}(E) = A[1 + \delta f_{\|,\perp}(E)] + Bm_t,$$

where $A$, $B$ are fit parameters, and $\delta f_{\|,\perp}$ is the $\chi$PT correction. To estimate the systematic error here, we try a simple linear fit and a “$\chi$PT+quadratic” fit with a term $Cm_t^2$ added to Eq. \[\text{5}\]. A comparison of the three fits is shown in Fig. \[\text{2}\].

For the $D \to \pi$ ($K$) decay, the linear fit gives $3\%$ ($2\%$) larger results at $m_t = m_{ud}$. The results from the $\chi$PT+quadratic fit typically lie between the results from the other two fits, with larger errors. We therefore take $3\%$ ($2\%$) as the systematic error from the chiral extrapolation for the $D \to \pi$ ($K$) decay.

We now convert the results for $f_\perp$ and $f_\|$ at $m_t = m_{ud}$, to $f_+ \, f_0$. To extend $f_+ \, f_0$ to functions of $q^2$, we again fit to the form Eq. \[\text{6}\]. The results are shown in Fig. \[\text{3}\] with statistical errors only. We then obtain the decay rates $\Gamma/[V_{x\ell}]^2$ by integrating (phase space) $\times |f_+(q^2)|^2$ over $q^2$. Finally, we determine the CKM matrix elements $|V_{cd}|$ and $|V_{cs}|$ using experimental lifetimes and branching ratios \cite{11}. These main results are summarized in Table \[\text{IV}\].

The results presented above rely on the $q^2$ dependence of BK parametrization, Eq. \[\text{6}\]. To estimate the associated systematic error, we make an alternative analysis without it. We perform a 2-dimensional fit in $(m_t, E)$ to the raw data employing a polynomial form plus the $\chi$PT correction $\delta f_{\|,\perp}$. The result from this fit agrees with the one from the fit with Eq. \[\text{5}\] within statistical errors. The deviation between the two fits is negligible at $q^2 \sim q_{max}^2$ and about $1\sigma$ at $q^2 \sim 0$ for $f_{\|,\perp}$, giving a $2\%$ difference for the CKM matrix elements.
TABLE I: Fit parameters in Eq. (4), decay rates and CKM matrix elements. The first errors are statistical, the second systematic, the third experimental.

| P   | F   | α   | β   | Γ/|V_{ck}|^2 [ps^{-1}] | |V_{ck}| |
|-----|-----|-----|-----|----------------|--------|
| π   | 0.64(3) | 0.44(4) | 1.41(6) | 0.154(12)(31) | 0.239(10)(24)(20) |
| K   | 0.73(3) | 0.50(4) | 1.31(7) | 0.093(07)(18) | 0.969(39)(94)(24) |

With only one lattice spacing, the systematic error from discretization effects can be estimated only by power counting. The leading discretization errors from the Asqtad action are $O\left(\alpha_s (a\Lambda_{QCD})^2\right) \approx 2%$ (after removal of taste-violating effects with $\Sigma PT$), taking $\Lambda_{QCD} = 400$ MeV and $\alpha_s = 0.25$. In addition, there is a momentum-dependent error from the final state. The BK parameters are determined by the lower momentum data; in particular, the fits are insensitive to the highest momentum $2\pi (1, 1, 1)/L$. Therefore we estimate this effect to be $O\left(\alpha_s (a p)^2\right) \approx 5%$, taking the second-highest-momentum $p = 2\pi (1, 1, 0)/L$. The HQET theory of cutoff effects $\Delta \chi/\pi^2$ can be used to estimate the discretization error from the heavy charmed quark. In this way, we estimate the discretization error to be 4–7%, depending on the value chosen for $\Lambda_{QCD}$ (in the HQET context). This is consistent with the lattice spacing dependence seen in Ref. [8]. In future work we expect to reduce and understand better this uncertainty, so we shall adopt the maximum, 7%, here.

A summary of the systematic errors for the form factors $f_{+,0}$ or the CKM matrix elements $|V_{ck}|$ is as follows. The error from time fits is 3%; from chiral fits, 3% (2%) for $D \to \pi (K)$ decay; from BK parametrization, 2%. The 1-loop correction to $\rho_{l\nu}$ is only 1%, so 2-loop uncertainty is assumed to be negligible. The uncertainty for $a^{-1}$ is about 1.2% [4]; this leads to a 1% error for $|V_{ck}|$ (but not for the dimensionless form factors), from integrating over $q^2$ to get $\Gamma/|V_{ck}|^2$. Finally, we quote discretization uncertainties of 2%, 5%, and 7%, from light quarks, the final state energy, and the charmed quark, respectively. Adding all the systematic errors in quadrature, we find the total to be [3% + 3% (2%) + 2% + 1% + 2% + 5% + 7%] = 10%.

Incorporating the systematic uncertainties, we obtain

\[
\begin{align*}
 f_{+,0}^{D \to \pi} &= 0.64(3)(6), \\
 f_{+,0}^{D \to K} &= 0.73(3)(7),
\end{align*}
\]

and the ratio $f_{+,0}^{D \to \pi}/f_{+,0}^{D \to K} = 0.87(3)(9)$. Our results for the CKM matrix elements (Table I) are consistent with Particle Data Group averages $|V_{cd}| = 0.224(12)$ and $|V_{cs}| = 0.996(13)$ [1]; also with $|V_{ck}| = 0.9745(8)$ from CKM unitarity. If we instead use these CKM values as inputs, we obtain, for the total decay rates,

\[
\begin{align*}
 \Gamma(D^0 \to \pi^- l^+ \nu) &= (7.7 \pm 0.6 \pm 1.5 \pm 0.8) \times 10^{-3} \text{ps}^{-1}, \\
 \Gamma(D^0 \to K^- l^+ \nu) &= (9.2 \pm 0.7 \pm 1.8 \pm 0.2) \times 10^{-2} \text{ps}^{-1}, \\
 \Gamma(D^0 \to \pi^- l^+ \nu) &= 0.084 \pm 0.007 \pm 0.017 \pm 0.009,
\end{align*}
\]

where the first errors are statistical, the second systematic, and the third from uncertainties in the CKM matrix elements. We do not assume any cancellation of errors in the ratios, although some may be expected. Our results agree with recent experimental results, $f_{+,0}^{D \to \pi}(0) = 0.73(15)$, $f_{+,0}^{D \to K}(0) = 0.78(5)$ [17], $f_{+,0}^{D \to \pi}(0)/f_{+,0}^{D \to K}(0) = 0.86(9)$ and $\Gamma(D^0 \to \pi^- e^+ \nu_e)/\Gamma(D^0 \to K^- e^+ \nu_e) = 0.082 \pm 0.008$ [20].

This Letter presents the first three-flavor lattice calculations for semileptonic $D$ decays. With an improved staggered light quark, we have successfully reduced the two dominant uncertainties of previous works, i.e., the effect of the quenched approximation and the error from chiral extrapolation. Our results for the form factors, decay rates and CKM matrix, given in Table I and Eq. (8) are in agreement with experimental results. The total size of systematic uncertainty is 10%, which is dominated by the discretization errors. To reduce this error, calculations at finer lattice spacings and with more highly improved heavy-quark actions are necessary; these are underway. Finally, unquenched calculations of $B$ decays such as $B \to \pi l \nu$ and $B \to D l \nu$ are in progress, and will be presented in a separate paper.

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