High Precision determination of the $\pi$, $K$, $D$ and $D_s$ decay constants from lattice QCD

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We determine $D$ and $D_s$ decay constants from lattice QCD with 2\% errors, 4 times better than experiment and previous theory: $f_D = 241(3)$ MeV, $f_{D_s} = 207(4)$ MeV and $f_{D_s}/f_D = 1.16(11)$. We also obtain $f_K/f_s = 1.189(7)$ and $(f_{D_s}/f_D)/(f_K/f_s) = 0.979(11)$. Combining with experiment gives $V_{us}=0.2262(14)$ and $V_{cd}/V_{ud}$ of 4.43(41). We use a highly improved quark discretisation on MILC gluon fields that include realistic sea quarks, fixing the $u/d$, $s$ and $c$ masses from the $\pi$, $K$, and $\eta$ meson masses. This allows a stringent test against experiment for $D$ and $D_s$ masses for the first time (to within 7 MeV).

The annihilation to a $W$ boson of the $D_s$, $D$, $\pi$ or $K$ meson is a ‘gold-plated’ process with leptonic width (for meson $P$ of quark content $q\bar{q}$) given up, to a calculated electromagnetic correction factor $\Gamma(P \rightarrow l\nu_l(\gamma)) = \frac{G_F^2|V_{ab}|^2}{8\pi} f_P m_P^2 m_P \left(1 - \frac{m_l^2}{m_P^2}\right)^2.$ (1)

$V_{ab}$ is from the Cabibbo-Kobayashi-Maskawa (CKM) matrix and $f_P$, the decay constant, parameterizes the amplitude for $W$ annihilation. If $V_{ab}$ is known from elsewhere an experimental value for $\Gamma$ gives $f_P$, to be compared to theory. If not, an accurate theoretical value for $f_P$, combined with experiment, can yield a value for $V_{ab}$.

$f_P$ is defined from $\langle 0|\bar{\pi}\gamma_\mu(\gamma_5)b|P(p)\rangle \equiv f_P P_{\mu}$ calculable in lattice QCD to handle quark confinement, and with QED effects omitted. The experimental leptonic decay rates for $K$ and $\pi$ are known very accurately and $D$ and $D_s$ less so, but with expected errors shortly of a few percent. Accurate predictions from lattice QCD can be made now, ahead of these results and comparison will then be a severe test of lattice QCD (and QCD itself).

This has impact on the confidence we have in similar matrix elements being calculated in lattice QCD for $B$ mesons that provide key unitarity triangle constraints.

A major error in lattice QCD until recently was missing sea quarks from the gluon field configurations on which calculations were done, because of numerical expense. This has now been overcome. The MILC collaboration$^3$ has made ensembles at several different values of the lattice spacing, $a$, that include sea $u$ and $d$ (taken to have the same mass) and $s$ quarks with the $u/d$ quark mass taking a range of values down to $m_s/10$. The sea quarks are implemented in the improved staggered (asqtad) formalism by use of the fourth root of the quark determinant. This procedure, although deemed ‘ugly’, appears to be a valid discretisation of QCD$^4$.

For $f_{D_s}$ a large error can arise from the inaccuracy of discretisations of QCD for $c$ quarks. Discretisation errors are set by powers of the mass in lattice units, $m_a$, and this is not negligible at typical values of $a$. However, $m_a$ is not so large that it can easily be removed from the problem using nonrelativistic methods as is done for $b$ quarks, for example$^5$. The key then to obtaining small errors for $c$ quarks is a highly improved relativistic action on reasonably fine lattices (where $m_c a \approx 1/2$).

The FNAL and MILC collaborations previously obtained a prediction for $f_D$ of 201(17) MeV and for $f_{D_s}$ of 249(16) MeV$^6$ using the ‘clover’ action for $c$ quarks. The 6\%-8\% error comes largely from discretization errors in the clover action. Our action is improved to a higher order in the lattice spacing and this means that

\begin{table}[h]
\centering
\begin{tabular}{ |c|c|c|c|c| }
\hline
Lattice/sea & valence & $m_{u, d, s, c, 1+\epsilon}$ & $r_1/a$ \\
\hline
sea & $u_{am}$, $u_{am}$ & $0.0194, 0.0484$, $0.0264, 0.066, 0.85, 0.66$ & $2.129(11)$ \hline
valence & $u_{am}$, $u_{am}$ & $0.0132, 0.066, 0.85, 0.66$ & $2.133(11)$ \hline
$20^3 \times 64$ & $0.02, 0.05$ & $0.0278, 0.0525, 0.648, 0.79$ & $2.650(8)$ \hline
$24^3 \times 64$ & $0.01, 0.05$ & $0.01365, 0.0546, 0.66, 0.79$ & $2.610(12)$ \hline
$28^3 \times 96$ & $0.005, 0.05$ & $0.0067, 0.0537, 0.65, 0.79$ & $2.632(13)$ \hline
$32^3 \times 96$ & $0.0124, 0.031$ & $0.01635, 0.03635, 0.427, 0.885$ & $3.711(13)$ \hline
$32^3 \times 96$ & $0.0062, 0.031$ & $0.00705, 0.0366, 0.43, 0.885$ & $3.684(12)$ \hline
\end{tabular}
\end{table}

\textbf{Table I:} MILC configurations and mass parameters used for this analysis. The $16^3 \times 48$ lattices are ‘very coarse’, the $20^3 \times 64$ and $24^3 \times 64$, ‘coarse’ and the $28^3 \times 96$, ‘fine’. The sea asqtad quark masses ($l = u/d$) are given in the MILC convention with $u$ the plaquette tadpole parameter. Note that the $s$ quark mass on fine and coarse lattices are above the subsequently determined physical value$^3$. We make a small correction (with 50\% uncertainty) to our results for $f_{s,K,D,D_s}$ to allow for this, based on our studies of their sea quark mass dependence and MILC results in$^3$. It has negligible effect on our final numbers and errors. The lattice spacing values in units of $r_1$ after ‘smoothing’ are in the rightmost column$^3$. The central column gives the HISQ valence $u/d$, $s$ and $c$ masses along with the coefficient of the Naik term, $1 + \epsilon$, used for $c$ quarks$^4$. 

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our results are both more accurate for the $D$ and $D_s$ and more accurate for charmonium, allowing additional predictive power. In addition, our formalism has a partially conserved current so we do not have to renormalise the lattice $f_{D_s}$ to give a result for the continuous real world of experiment. We can then reduce the error on $f_{D_s}$ to 2% and the ratio of decay constants even further.

We use the Highly Improved Staggered Quark (HISQ) action, developed from the asqtad action by reducing by a factor of 3 the ‘taste-changing’ discretisation errors. Other discretisation errors are also small since, in common with asqtad, HISQ includes a ‘Naik’ term to cancel standard tree-level $a^2$ errors in the discretisation of the Dirac derivative. For $c$ quarks the largest remaining discretisation error comes from radiative and tree-level corrections to the Naik term and we remove these by tuning the coefficient of the Naik term to obtain a ‘speed of light’ of 1 in the meson dispersion relation. The hadron mass is then given accurately by its energy at zero momentum, unlike the case for the clover action.

In we tested the HISQ action extensively in the charmonium sector, fixing $m_c$ so that the mass of the ‘goldstone’ $\eta_c$ meson agreed with experiment. We showed that remaining discretisation errors are very small, being suppressed by powers of the velocity of the $c$ quark beyond the formal expectation of $\alpha_s(m_c a)^2$ and $(m_c a)^4$. The charm quark masses and Naik coefficients used for different ‘very coarse’, ‘coarse’ and ‘fine’ MILC ensembles are given in Table I. For the $s$ and $u/d$ valence quarks we also use the HISQ action with masses in Table II.

We calculate local two-point goldstone pseudoscalar correlators at zero momentum from a precessing random wall source and fit the average to:

$$C(t) = \sum_{i,ip} a_i e^{-M_{ip} t} + (-1)^i a_{ip} e^{-M_{ip} t} + (t \to T - t).$$

$T$ is the time length of the lattice and $t$ runs from 0 to $T$. $i$ denotes ‘ordinary’ exponential terms and $ip$, ‘oscillating’ terms from opposite parity states. Oscillating terms are significant for $D_q$ states because $m_c - m_q$ is relatively large, but not for $\pi$ or $K$. We use a number of exponentials, $i$ and $ip$, in the range 2-6 and loosely constrain higher order exponentials by the use of Bayesian priors. Constraining the $D$ and $D_s$ radial excitation energies to be similar improves the errors on the $D$. In lattice units, $M_P = M_0$ and $f_P$ is related to $a_0$ through the partially conserved axial current relation, which gives $f_P = (m_u + m_d) \sqrt{2 a_0 / M_0^2}$. The resulting fitting error for all states is less than 0.1% on $M_0$ in lattice units and less than 0.5% on decay constants. Full details will be given in a longer paper.

To convert the results to physical units we use the scale determined by the MILC collaboration (Table I, II) in terms of the heavy quark potential parameter, $r_1$. $r_1/a$ is determined with an error of less than 0.5% and allows results to be tracked accurately as a function of sea $u/d$ quark mass and lattice spacing. At the end, however, there is a larger uncertainty from the physical value of $r_1$. This is obtained from the $T$ spectrum using the non-relativistic QCD action for $b$ quarks on the same MILC ensembles, giving $r_1 = 0.321(5)$ fm, $r_1^{-1} = 0.615(10)$ GeV.

Our results are obtained from $u/d$ masses larger than approximately three times the average $m_{u/d}$ of the physical $u$ and $d$ quark masses. We obtain physical answers by extrapolating our results to the correct $m_{u/d}$ using chiral perturbation theory. In addition we have systematic errors from the finite lattice spacing values used. Since our results are so accurate we can also fit them as a function of $a$ to extrapolate to the physical $a = 0$ limit. These two extrapolations are connected through the discretisation errors in the light quark action and one way to treat those is by modifying chiral perturbation theory to handle them explicitly. A more general approach, that allows us to handle light and heavy quark discretisation errors together, is to perform a simultaneous fit for both chiral and continuum extrapolations allowing for expected functional forms in both with a Bayesian analysis to constrain the coefficients. We tested this method by using it to analyze hundreds of different fake datasets, generated using formulas from staggered chiral perturbation theory with random couplings. As expected, we found that roughly 70% of the time the

![Fig. 1](image-url)
extrapolated results were within one standard deviation (computed using a Gaussian approximation to $\chi^2$ of the exact result from the formula, verifying the validity of our approach and of our error estimates.

We fit our results to the standard continuum chiral expansions through first order [13], augmented by second and third-order polynomial terms in $x_a \equiv B_0 m_q/(8\pi f_a)^2$, where $B_0 \equiv m^2_a/(m_u + m_d)$ to leading order in chiral perturbation theory. The polynomial corrections are required by the precision of our data [28]. We include $D^* - D$ mass difference terms in the $D/D_s$ chiral expansion and take the $DD^*\pi$ coupling to have the value inferred at leading order from the experimental $D^*$ width, allowing for a 30% error from higher order effects. We correct for the finite volume of our lattice from chiral perturbation theory, although only $f_K$ has corrections larger than 0.5%. Our corrections agree within 30% with those in Ref. [16] and we take a 50% uncertainty in the correction. We fit the couplings in the chiral expansions simultaneously to our $\pi$ and $K$ masses and decay constants. We do the same for the masses and decay constants of the $D$ and $D_s$. Given the couplings, we tune $m_{u/d}$ and $m_s$ so that our formulas give the experimental values for $m_K$ and $m_K^\star$ after correcting for the $u/d$ mass difference and electromagnetic effects [8, 17].

We find that finite $a$ errors are 2–3.5 times smaller with the HISQ quark action than with the asqtad action, but still visible in our results. We combine the extrapolation to $a = 0$ with the quark-mass extrapolation by adding $a^2$ dependence to our chiral formulas. We expect leading discretization errors of various types: $\alpha_s a^2$ and $a^4$ errors from conventional sources; and $\alpha_s^3 a^2$ and $\alpha_s^2 a^2 \log(x_{u,d})$ and $\alpha_s^3 a^2 x_{u,d}$ from residual taste-changing interactions among the valence and sea light quarks. We do not have sufficient data to distinguish between these different functional forms, but we include all of them (with appropriate priors for their coefficients) in our fits so that uncertainties in the functional dependence on $a^2$ are correctly reflected in our final error analysis. The $a^2$ extrapolations are sufficiently small with HISQ (1% or less for $\pi$ and $K$ from fine results to the continuum: 2% for $D$ and $D_s$) that the associated uncertainties in our final results are typically less than 0.5%. The combined chiral and continuum Bayesian fits have 45 parameters for $D/D_s$ and 48 for $\pi/K$ with 28 data points for each fit [27].

Fig. 1 shows the masses of the $D$ and $D_s$ as a function of $u/d$ quark mass. To reduce uncertainties from the scale and from $c$ quark mass tuning, the meson masses were obtained from $m_{D_s} - m_{\eta_c}/2 + m_{\eta_c,expt}/2$. The lines show our simultaneous chiral fits at each value of the lattice spacing and the dashed line the consequent extrapolation to $a = 0$. The shaded bands give our final results: $m_{D_s} = 1.962(6)$ GeV, $m_{D} = 1.868(7)$ GeV. Experimental results are 1.968 GeV and 1.869 GeV respectively. We also obtain $(2m_{D_s} - m_{\eta_c})/(2m_{D} - m_{\eta_c}) = 1.251(15)$, in excellent agreement with experiment, 1.260(2) [2]. This last quantity is a non-trivial test of lattice QCD, since we are accurately reproducing the difference in binding energies between a heavy-heavy state (the $\eta_c$ used to determine $m_{\eta_c}$) and a heavy-light state (the $D$ and $D_s$). Table II gives our complete error budget for this quantity.

Fig. 2 similarly shows our results for decay constants on each ensemble with complete error budgets in Table II. $f_K$ and $f_{\pi}$ show very small discretisation effects and good agreement with experiment when $V_{ud}$ is taken from nuclear $\beta$ decay and $V_{us}$ from $K_{l3}$ decays [2]. We obtain $f_{\pi} = 132(2)$ MeV and $f_K = 157(2)$ MeV. Alternatively our result for $f_K/f_{\pi}(1.189(7))$ can be used, with experimental leptonic branching fractions [8, 18] to give $V_{us}$. Using the recent KLOE result for the $K_{l3}$ we obtain $V_{us} = 0.2262(13)(4)$ where the first error is theoretical and the second experimental. This agrees with, but improves on, the $K_{l3}$ result. Then $1 - V_{ud}^2 - V_{us}^2 - V_{ub}^2 = 0.0006(8)$, a precise test of CKM matrix first-row unitarity.

$f_D$ and $f_{D_s}$ show larger discretisation effects but a more benign chiral extrapolation. Our final results are: $f_D = 241(3)$ MeV, $f_{D_s} = 207(4)$ MeV and $f_D/f_{D_s} = 1.164(11)$. These results are 4–5 times more accurate than previous full lattice QCD results [4] and existing experimental determinations. An interesting quantity is the double ratio $(f_D/f_{D_s})/(f_K/f_{\pi})$. It is estimated to be close to 1 from low order chiral perturbation theory [21]. We are able to make a strong quantitative statement with a value of 0.979(11). Equivalently $(\Phi_D/\Phi_{D_s})/(f_K/f_{\pi}) = 1.005(10)$, where $\Phi = f \sqrt{M}$. We also obtain $(f_D/f_{D_s})/(f_{B_s}/f_{B_s}) = 1.03(3)$ using our previous result for the $B$ ratio [22]. The $B$ ratio dominates the error but improvement of this is underway.

The results for $f_D$ and $f_{D_s}$ obtained from the experimental leptonic branching rates coupled with CKM ma-

| $r_1$ uncertainty | $a^2$ extrap. | finite vol. | $m_{u/d}$ extrap. | stat. errors | $m_s$ evoln. | $m_{d, QED}$ etc |
|-------------------|---------------|-------------|------------------|-------------|-------------|----------------|
| 0.3               | 0.2           | 0.4         | 0.2              | 0.4         | 0.1         | 0.0            |
| 1.1               | 0.2           | 0.5         | 0.3              | 0.5         | 0.3         | 0.0            |
| 1.4               | 0.4           | 0.6         | 0.3              | 0.6         | 0.3         | 0.5            |
| 1.0               | 1.0           | 0.5         | 0.3              | 0.0         | 0.1         | 0.5            |
| 1.4               | 0.7           |             |                  |             |             |                |
| $\Delta s/\Delta u$ |               |             |                  |             |             |                |
| 0.6               | 1.3           | 1.7         | 0.9              | 1.3         | 1.8         | 1.2            |

TABLE II: Error budget (in %) for our decay constants and mass ratio, where $\Delta s = 2 m_{D_s} - m_{\eta_c}$. The errors are defined so that it is easy to see how improvement will reduce them, e.g. the statistical uncertainty is the outcome of our fit, so that quadrupling statistics will halve it. The $a^2$ and $m_{u/d}$ extrapolation errors are the pieces of the Bayesian error that depend upon the prior widths in those extrapolations. ’$m_s$ evolution’ refers to the error in running the quark masses to the same scale from different values for the chiral extrapolation. The $r_1$ uncertainty comes from the error in the physical value of $r_1$ and the finite volume uncertainty allows for a 50% error in our finite volume adjustments described in the text.
The chiral fits are performed simultaneously with those of the corresponding meson masses, and the resulting continuum extrapolation curve is given by the dashed line. For $\pi$, $K$ we have $\chi^2/\text{dof} = 0.2$ and for $D, D_s$, $\chi^2/\text{dof} = 0.6$, each for 28 pieces of data. The shaded band gives our final result. At the left are experimental results from CLEO-c [25] and 283(23) MeV from BaBar [24].

Using our results for $f_D$, we have updated the result quoted by the PDG to 0.96(9) given by the PDG [2].

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