$D \rightarrow K, l\nu$ Semileptonic Decay Scalar Form Factor and $|V_{cs}|$ from Lattice QCD

Heechang Na, 1 Christine T. H. Davies, 2 Eduardo Follana, 3 G. Peter Lepage, 4 and Junko Shigemitsu 1
(HPQCD Collaboration)

1Department of Physics, The Ohio State University, Columbus, OH 43210, USA
2Department of Physics & Astronomy, University of Glasgow, Glasgow, G12 8QQ, UK
3Departamento de Física Teórica, Universidad de Zaragoza, Zaragoza, Spain
4Laboratory of Elementary Particle Physics, Cornell University, Ithaca, NY 14853, USA

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We present a new study of $D$ semileptonic decays on the lattice which employs the Highly Improved Staggered Quark (HISQ) action for both the charm and the light valence quarks. We work with MILC unquenched $N_f = 2 + 1$ lattices and determine the scalar form factor $f_0(q^2)$ for $D \rightarrow K, l\nu$ semileptonic decays. The form factor is obtained from a scalar current matrix element that does not require any operator matching. We develop a new approach to carrying out chiral/continuum extrapolations of $f_0(q^2)$. The method uses the kinematic “$z$” variable instead of $q^2$ or the kaon energy $E_K$ and is applicable over the entire physical $q^2$ range. We find $f_0^{D\rightarrow K}(0) \equiv f_0^{D\rightarrow K}(0) = 0.747(19)$ in the chiral plus continuum limit and hereby improve the theory error on this quantity by a factor of $\sim 4$ compared to previous lattice determinations. Combining the new theory result with recent experimental measurements of the product $f_0^{D\rightarrow K}(0)\cdot |V_{cs}|$ from BaBar and CLEO-c leads to a very precise direct determination of the CKM matrix element $|V_{cs}|$, $|V_{cs}| = 0.961(11)(24)$, where the first error comes from experiment and the second is the lattice QCD theory error. We calculate the ratio $f_0^{D\rightarrow K}(0)/f_{D^+}$ and find $2.986 \pm 0.087$ GeV$^{-1}$ and show that this agrees with experiment.

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I. INTRODUCTION

Independent determinations of each of the Cabibbo-Kobayashi-Maskawa (CKM) matrix elements and checks of three generation unitarity provide stringent consistency tests of the Standard Model and have become an important part of flavor physics. For instance, first row unitarity tests of the Standard Model and have become an important part of flavor physics. For instance, first row unitarity now has been checked to very high accuracy with $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 - 1 = -0.0001(6)$ 11. Such precision became possible when both experiment and lattice QCD theory inputs to the determination of $|V_{us}|$ reached subpercent levels of accuracy (the contribution from $|V_{ub}|$ to the unitarity sum is negligible and $|V_{ud}|$ is known with $\sim 0.02\%$ errors).

In contrast to the elements of the 1st row, direct determinations of the 2nd row matrix elements are still much less precise. The latest PDG summary 2 quotes 4.8%, 3.5% and 3.2% errors for $|V_{cd}|$, $|V_{cs}|$ and $|V_{cb}|$ respectively when one considers all ways of extracting the matrix elements. If one focuses just on determinations of $|V_{cd}|$ and $|V_{cs}|$ from semileptonic $D \rightarrow \pi, l\nu$ and $D \rightarrow K, l\nu$ decays then until recently the total error has been at the 10% level and dominated by lattice QCD theory errors. Furthermore tests of 2nd row unitarity stands at $|V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2 = 1.101 \pm 0.074$ and for the 2nd column at $|V_{us}|^2 + |V_{cb}|^2 + |V_{cs}|^2 = 1.099 \pm 0.074$ 2. In both cases the error is dominated by the uncertainty in $|V_{cs}|$. Clearly reducing the errors in $|V_{cs}|$ will have immediate and significant impact on flavor physics and on CKM unitarity tests. On the experimental front Belle $\mathcal{B}$, BaBar $\mathcal{B}$ and CLEO-c $\mathcal{B}$ have all recently published precise measurements of the combination $f_0^{D\rightarrow K}(0)*|V_{cs}|$ with 3.3%, 1.4% and 1.1% errors respectively. These precise measurements can be turned into accurate $|V_{cs}|$ determinations if and only if theory can provide the form factor $f_0^{D\rightarrow K}(0)$ with comparable precision. The main goal of the current work was to improve lattice QCD calculations of $f_0^{D\rightarrow K}(0)$ and the outcome is that we have now succeeded in reducing the theory errors from 10% down to 2.5%. Innovations that made this dramatic improvement in errors possible include the employment of a new and better action for charm quarks, the use of an absolutely normalized hadronic matrix element that does not require any operator matching, improved analysis tools for lattice data and a new method for carrying out chiral/continuum extrapolations.

One reason for the large disparity in the size of lattice QCD errors between kaon and $D$ meson systems in the past has been the challenge of simulating quarks with masses as large as that of the charm quark. If “$a$” is the lattice spacing and hence $\sim 1/a$ the cutoff in the theory, then for charm quarks it was thought to be difficult to satisfy $am_c = m_c/\text{cutoff} \ll 1$. In the past this problem was circumvented by employing effective theories to handle the charm quark, nonrelativistic (NR)QCD, HQET or the “heavy clover” action of the Fermilab lattice collaboration. The first $N_f = 2 + 1$ unquenched studies of $D$ semileptonic decays on the lattice were carried out by the Fermilab Lattice and MILC collaborations using an effective theory for charm $\mathcal{B}$. This pioneering work predicted the shape of the form factors as a function of $q^2$ prior to subsequent verification by experiment. The theory errors, however, were quite large at $\sim 10\%$. The calculations by the Fermilab Lattice and MILC collaborations are being improved upon and their theory errors should be reduced significantly soon $\mathcal{B}$. On the other
hand, working with effective theories typically leads to larger statistical and systematic errors than when employing “relativistic” quark actions as can be done for kaon physics. This includes uncertainties coming from matching of heavy-light currents responsible for heavy meson leptonic or semileptonic decays, and from the tuning of heavy quark masses, all procedures that are much more complicated in effective theories.

In recent years there has been a major shift in lattice simulations with charm quarks. With the advent of highly improved lattice quark actions the concerns described above of $m_c$/cutoff being too large have been overcome and several collaborations are now working on charm physics without resorting to effective theories. In 2007 the HPQCD collaboration introduced the “Highly Improved Staggered Quark” (HISQ) action \[8\]. Many lattice artifacts, including all $O((am_c)^2)$ discretization effects and all $O(\alpha_s(am_c))$ and $O((am_c)^4)$ effects at leading order in the charm quark velocity $\frac{v}{c}$ have been removed. It then becomes feasible to simulate charm quarks on the lattice in a fully relativistic setting without introducing large discretization errors as long as one works with lattice spacings $a \ll 0.15\text{fm}$. This last condition is easily met nowadays in typical lattice simulations. Another approach to charm meson leptonic and semileptonic decays using relativistic charm quarks is being pursued by the European Twisted Mass (ETM) collaboration \[9\]. They employ a special version of Wilson type quark action called the “Twisted Mass” quark action where discretization errors come in at $O(a^4)$.

The HPQCD collaboration has successfully applied HISQ charm quarks to studies of $D$ and $D_s$ meson leptonic decays \[11\]. This formalism significantly reduced lattice errors in decay constant calculations. We have now also initiated $D$ meson semileptonic decay studies based on HISQ charm and light valence quarks. In reference \[11\] we developed and tested our approach on a simpler test case of a fictitious $D_s \rightarrow \eta_s, lv$ semileptonic decay ($\eta_s$ refers to a pseudoscalar $s - \bar{s}$ bound state). In the current paper we present the first application of HISQ charm quarks to realistic $D$ meson semileptonic decays. More specifically we calculate the scalar form factor $f_0(q^2)$ for $D \rightarrow K, lv$ decays. As mentioned above already experiment provides us with the product $f_+(0) \ast |V_{cs}|$. Then using the kinematic relation $f_0(0) = f_+(0)$, an accurate calculation of $f_0(q^2)$ from the lattice leads to a precise determination of the CKM matrix element $|V_{cs}|$.

We have carried out simulations on three of the MILC “coarse” ensembles with lattice spacing $a \sim 0.12\text{fm}$ and two of the “fine” ensembles with $a \sim 0.09\text{fm}$. Details of these ensembles are listed in Table I. The five ensembles provide enough variation and information to allow sensible chiral and continuum extrapolations to the physical world.

In the next section we review the formalism for extracting semileptonic decay form factors from hadronic matrix elements of appropriate heavy-light currents. We describe the advantages of working with the same relativistic action for both the heavy and the light quarks and explain why the form factor at $q^2 = 0$ is most accurately extracted from hadronic matrix elements of the scalar current as opposed to from the vector current. In section III we introduce the HISQ action and describe how action parameters such as bare quark masses were tuned. Section IV provides further details of our simulations including benefits derived from using “random wall” sources, in particular when simulating kaons with nonzero momenta. Section V describes our fitting strategy. We have invested considerable effort into developing improved fitting methods in order to extract the form factors of interest with subpercent errors for each ensemble and for all kaon momenta needed to cover the physical $q^2$ range.

In section VI we take the form factor results from the five ensembles and extrapolate to the chiral/continuum limit. To this end we have developed a new extrapolation method that can be used over the entire physical $q^2$ range, $(M_D - M_K)^2 \geq q^2 \geq 0$. Since we are interested in the form factor at $q^2 = 0$, it is important that any extrapolation scheme work all the way down to $q^2 = 0$ where the kaon in the $D$ meson rest frame has energy $E_K \approx 1\text{GeV}$. The new approach uses the “z-expansion” of Refs. 13, 14 to parameterize the kinematics (the dependence on $E_k$ or equivalently on $q^2$). The coefficients of this expansion are then allowed to be functions of the light and strange quark masses and of the lattice spacing. We find that good fits to all our data are possible with such an ansatz and the resulting $f_0(0)$ in the chiral/continuum limit is very stable against higher order terms in this ansatz.

Section VII summarises our final results for $f_0(0)$ at the physical point and explains our error budget. We incorporate experimental input from BaBar 4 and CLEO-c 5 to determine the CKM matrix element $|V_{cs}|$ and compare with values listed in the PDG and with expectations from CKM unitarity. In Section VIII we

| Set | $r_1/a$ | $a^{0.12}m_{sea}$ | $a^{0.12}$ | $N_{con}$ | $N_{tsrc} L^3 \times N_t$ |
|-----|--------|-----------------|----------|----------|----------------------|
| C1  | 2.647  | 0.005/0.050     | 0.8678   | 600      | 2 $2^{+4}_{-1} \times 64$ |
| C2  | 2.618  | 0.010/0.050     | 0.8677   | 600      | 2 $2^{+3}_{-1} \times 64$ |
| C3  | 2.644  | 0.020/0.050     | 0.8688   | 600      | 2 $2^{+3}_{-1} \times 64$ |
| F1  | 3.699  | 0.0062/0.031    | 0.8782   | 600      | 4 $2^{+3}_{-1} \times 96$  |
| F2  | 3.712  | 0.0124/0.031    | 0.8788   | 600      | 4 $2^{+3}_{-1} \times 96$  |
collect results obtained as “side products” of our analysis of semileptonic decay three-point hadronic matrix elements, namely results coming from two-point correlators such as decay constants of the pion, kaon, D, and D mesons. These two-point results provide nontrivial tests of our mass tunings, fitting and chiral/continuum extrapolation strategies leading to greater confidence in our form factor (i.e. three-point) results as well. Finally section IX gives a summary and addresses future plans. Several appendices cover details of Bayesian fits employed in this article. And in Appendix C we carry out the chiral/continuum extrapolation of $f_0(q^2)$ using an approach that differs completely from the $z$-expansion method of section VI and is based instead on Chiral Perturbation theory. We show that the two extrapolation methods give results in very good agreement with each other.

II. FORMALISM

To study the process $D \to K, l\nu$ one needs to evaluate the matrix element of the charged electroweak current between the $D$ and the $K$ meson states, $\langle K|V_{\mu} - A^\mu|D \rangle$. Only the vector current $V_{\mu}$ contributes to the pseudoscalar-to-pseudoscalar amplitude and the matrix element can be written in terms of two form factors $f_+(q^2)$ and $f_0(q^2)$, where $q^\mu = p^\mu_D - p^\mu_K$ is the four-momentum of the emitted $W$-boson.

$$\langle K|V_{\mu}|D \rangle = f_+^{D\to K}(q^2) [p^\mu_D + p^\mu_K - \frac{M_D^2 - M_K^2}{q^2} q^\mu] + f_0^{D\to K}(q^2) \frac{M_D^2 - M_K^2}{q^2} q^\mu$$

(1)

with $V_{\mu} \equiv \bar{\Psi} \gamma_{\mu} \Psi$. As described below, we find it useful to consider also the matrix element of the scalar current $S \equiv \bar{\Psi} \gamma_5 \Psi$, 

$$\langle K|S|D \rangle = \frac{M_D^2 - M_K^2}{m_{0c} - m_{0s}} f_0^{D\to K}(q^2).$$

(2)

In continuum QCD one has the PCVC (partially conserved vector current) relation and the vector and scalar currents obey,

$$q^\mu (V_{\mu}^{\text{cont.}}) = (m_{0c} - m_{0s}) \langle S^{\text{cont.}} \rangle. \quad (3)$$

In fact PCVC is the reason why the same form factor $f_0^{D\to K}(q^2)$ appears in eqs. (1) and (2). On the lattice it is often much more convenient to simulate with vector currents $\bar{\Psi} Q_1 \gamma_{\mu} \Psi Q_2$ that are not exactly conserved at finite lattice spacings even for $Q_1 = Q_2$. Such non-exactly-conserved currents need to be renormalized and acquire $Z$-factors. We are able to carry out fully nonperturbative renormalization of the lattice vector current by imposing PCVC. In the $D$ meson rest frame the condition becomes,

$$(M_D - E_K) \langle V_0^{\text{latt.}} \rangle Z_t + \bar{p}_K \langle \bar{V}^{\text{latt.}} \rangle Z_s = (m_{0c} - m_{0s}) \langle S^{\text{latt.}} \rangle. \quad (4)$$

III. THE HISQ ACTION AND TUNING OF ACTION PARAMETERS

The HISQ action was introduced in Ref. [8] and represents the next level of improvement of staggered quarks beyond the AsqTad action. Relative to the latter, the HISQ action reduces taste breaking effects by approximately a factor of three on MILC coarse and fine lattices. For heavy quarks such as charm the HISQ action includes one adjustable parameter $\epsilon$ which modifies the “Naik” term already present in the AsqTad action $\frac{1}{6} g^2 \Delta_{\mu}^3 \rightarrow \frac{1}{6} g^2 \Delta_{\mu}^3 + \epsilon \frac{1}{6} g^2 \Delta_{\mu}^3$. In Ref. [8] $\epsilon$ was adjusted nonperturbatively to get the correct dispersion relation for the $\eta_c$ meson. It was found that one ends up with $\epsilon$'s close to estimates coming from requiring that the tree-level quark

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### Table II: Action parameters and $\eta_c$ and $\eta_s$ masses

| Set  | $a m_{0c}$ | $a m_{0s}$ | $a m_{0q}$ | $1 + \epsilon$ | $a M_{\eta_c}$ | $a M_{\eta_s}$ |
|------|------------|------------|------------|----------------|----------------|----------------|
| C1   | 0.6207     | 0.0489     | 0.0070     | 0.780          | 1.7887(1)      | 0.4111(2)      |
| C2   | 0.6300     | 0.0492     | 0.0123     | 0.774          | 1.8085(1)      | 0.4143(2)      |
| C3   | 0.6235     | 0.0491     | 0.0246     | 0.778          | 1.7907(1)      | 0.4118(2)      |
| F1   | 0.4130     | 0.0337     | 0.00674    | 0.893          | 1.2807(1)      | 0.2942(1)      |
| F2   | 0.4120     | 0.0336     | 0.01350    | 0.894          | 1.2751(1)      | 0.2931(2)      |

We have checked the feasibility of this renormalization scheme and extracted preliminary $Z_t$ and $Z_s$ values for the test case of $D_s \to \eta_c, l\nu$ mentioned above in Ref. [11]. We plan to apply this fully nonperturbative renormalization scheme to evaluate $\langle \pi|V_{\mu}|D \rangle$ and $\langle K|V_{\mu}|D \rangle$ relevant for realistic $D \to \pi, l\nu$ and $D \to K, l\nu$ semileptonic decays in the near future. In the present article, however, we will focus on the form factor $f_+(q^2)$ just at $q^2 = 0$, since this is all that is needed to extract $|V_{cs}|$. We do this by exploiting the kinematic identity $f_+(0) = f_0(0)$, and concentrating on determining the scalar form factor $f_0(q^2)$ as accurately as possible. The best way to proceed is to evaluate the hadronic matrix element of the scalar current rather than of the vector current. From eq. (2) one then has,

$$f_0^{D\to K}(q^2) = \frac{m_{0c} - m_{0s}}{M_D^2 - M_K^2} \langle K|S|D \rangle.$$
the data points reflect statistical and annihilation effects in the lattice simulations. The target value for the $\eta_s$ meson mass has been adjusted to take into account the lack of annihilation and electromagnetic effects in our lattice calculation.

We show results for the $\eta_c$ and $\eta_s$ masses on the five ensembles together with the target values. One sees that tuning has been achieved very accurately. For $\eta_c$ our target value is $M_{\eta_c}^{\text{target}} = 2.9852(34)$ GeV which differs slightly from the experimental $M_{\eta_c}^{\text{exp}} = 2.9803$ GeV since we adjust for the absence of electromagnetic and annihilation effects in the lattice simulations. The target value for the $\eta_s$ is $M_{\eta_s} = 0.6858(40)$ GeV. The data points in Figs. 1 and 2 show only statistical and $r_1/a$ errors. We first determine $r_1 \times M_{\text{meson}}$ using the precisely know $r_1/a$ for each ensemble. At this point our data points have errors coming from both statistics and from the $\sim 0.1\%$ uncertainty in $r_1/a$ (with the latter dominating). For the purposes of using a physical scale on the vertical axis we then convert $r_1 \times M_{\text{meson}}$ to MeV using $r_1 = 0.3133(23)$ fm ($r_1^{-1} = 0.6297(46)$ GeV). For reasons explained below, we find it more informative not to include the $\sim 0.7\%$ uncertainty in the physical value of $r_1$ in these plots. Including this error will affect all five data points in the same way without changing relative uncertainties.

Once the bare charm and strange quark masses have been fixed for each ensemble there are no adjustable parameters left when one goes on to determining other meson masses such as $M_D$ or $M_{D^*}$, decay constants $f_D$, $f_{D^*}$, $f_K$ etc. or semileptonic form factors. In Fig. 3 we show results for $M_D$ and $M_{D^*}$. Again the errors on the data points reflect statistical and $r_1/a$ errors only. Any changes in the physical value of $r_1$ will shift all five data points uniformly without affecting their relative positions. Furthermore chiral/continuum extrapolations would be carried out on $r_1 \times M_{\text{meson}}$ with $r_1$ and its error coming in only after having extracted the physical limit. By omitting the full $r_1$ errors in Fig. 3 one can more easily identify discretization effects and light quark mass dependence. For instance, for $M_D$, the difference between the coarse and fine ensemble results is at the $\sim 6$ MeV level or $\sim 0.3\%$ and the sea light quark mass dependence is essentially nonexistent. The $0.3\%$ discretization effect should be compared to the $\sim 0.7\%$ uncertainty in $r_1$. One lesson to be learnt from this is the importance of tuning quark masses accurately enough so that results on the different ensembles agree to within the smaller $r_1/a$ errors and not just to within the larger $r_1$ error. Otherwise it would not be possible to have data points lying along smooth curves as in Fig. 3 where discretization and light quark mass dependence can be clearly identified and distinguished from mass tuning and $r_1$ errors. Based on Figs. 1-3 we believe the HISQ action parameters have been fixed accurately enough in preparation for going on to D semileptonic decays. Further consistency checks, such as determinations of decay constants will be given in section VIII.

**IV. SIMULATION DETAILS**

The goal is to determine the hadronic matrix element $\langle K | S | D \rangle$ in eq. (5) via numerical simulations. The starting point is the three-point correlator,

$$C^{3\text{point}}(t_0, t, \bar{p}_K) = \frac{1}{L^3} \sum_{\tilde{x}} \sum_{\tilde{y}} \sum_{\tilde{z}} e^{i\bar{p}_K \cdot (\tilde{z} - \tilde{x})} \langle \Phi_K(\tilde{x}, t_0) \bar{S}(\tilde{z}; t) \Phi_D^\dagger(\tilde{y}, t_0 - T) \rangle. \quad (6)$$

$\Phi_D$ and $\Phi_K$ are interpolating operators that create a $D$ meson or annihilate a kaon respectively and $\bar{S} \equiv a^3 S$ is the scalar current in lattice units. We also work with dimensionless fermion fields. Eq. (6) corresponds to first

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1 Note that HISQ and AsqTad masses are not numerically the same, since the two actions are different.
creating a zero momentum $D$ meson at time $t_0 - T$ which propagates to time slice $t$ with $t_0 \geq t \geq t_0 - T$. At time slice $t$ the scalar current $S = \bar{\psi}_s \psi_c$ converts the charm quark inside the $D$ meson into a strange quark while inserting momentum $\vec{p}_K$. The resulting kaon is then annihilated at time $t_0$.

In our simulations we have picked $t_0$ the location of the kaon operator $\Phi_K$ randomly and differently for each configuration in order to reduce autocorrelations. We also worked with $N_{t_{src}}$ values of $t_0$ per configuration (see Table I) placed $N_t/N_{t_{src}}$ time slices apart ($N_t$ is the total number of time slices for our lattices). Once $t_0$ was fixed, for each configuration we obtained results for several $T$ values, $T = 15$ and $16$ on coarse and $T = 19$, $20$, and $23$ on fine lattices. We will see later that having data at many $T$ values significantly reduces errors in extracted three-point amplitudes. To further improve statistics, for each $t_0$ and $T$ value we also evaluated the time-reversed three-point correlator, essentially the same as eq. (9) but with $\Phi_{D/K}^\dagger$ acting on time slice $t_0 + T$ and the scalar current inserted at $T + t_0 \geq t \geq t_0$.

As is well known, with the HISQ action, each flavor of quark comes in $N_{taste}$ copies called “tastes”. One has $N_{taste} = 4$ when working with one-component staggered fields and $N_{taste} = 16$ for four-component “naive” fields. In the naive fields language the interpolating operators $\Phi_{D/K}$ and the scalar current $S$ become,

$$\Phi_{D/K}^\dagger = \frac{1}{4} \gamma_5 \Psi_i,$$

(7)

and

$$S = \bar{\Psi}_s \Psi_c.$$

(8)

These are all single site bilinears. $\Phi_{D/K}$ correspond to taste non-singlet “Goldstone” pseudoscalars and the factors of $\frac{1}{4} = \sqrt{N_{taste}}$ serve to divide out traces over taste space. The scalar current in eq. (8) is a taste singlet current. Carrying out the contractions over fermionic fields in $C_{3\text{pnt}}$ and using the well known relation between naive quark propagators $G_{\Psi}(x, y)$ and one-component field propagators $G_{\chi}(x, y)$,

$$G_{\Psi}(x, y) = \Omega(x)\Omega(1)^\dagger(y)G_{\chi}(x, y)$$

(9)

with

$$\Omega(x) = \prod_{\mu=0}^3 (\gamma_{5\mu})^{x_{5\mu}},$$

(10)

one obtains,

$$\langle \Phi_K(x) \tilde{S}(z) \Phi_D^\dagger(y) \rangle$$

$$= \frac{1}{16} Tr \{ G_{\psi,s}(x, z)G_{\psi,c}(z, y)\gamma_5 G_{\Psi,l}(y, x)\gamma_5 \}$$

$$= \frac{1}{16} Tr \{ [\Omega(x)\Omega(1)^\dagger(z)\Omega(z)\Omega(1)^\dagger(y)\gamma_5 \Omega(y)\Omega(1)^\dagger(x)]\gamma_5 \}$$

$$\times G_{\chi,s}(x, z)G_{\chi,c}(z, y)G_{\chi,l}(y, x) \}$$

$$= \frac{1}{4} \phi(y)\phi(x) Tr \{ G_{\chi,s}(x, z)G_{\chi,c}(z, y)G_{\chi,l}(y, x) \}$$

$$= \frac{1}{4} \phi(y)\phi(x) Tr \{ G_{\chi,s}^\dagger(x, z)G_{\chi,c}(z, y)G_{\chi,l}(y, x) \}.$$  

(11)

$\phi(y)$ stands for $(-1)^{\sum_{\mu} 5\mu}$ and similarly for $\phi(x)$ and $\phi(z)$. In the last step we have used $G_{\chi}(x, y) = \phi(x) \ast \phi(y)G_{\chi}^\dagger(y, x)$. “Tr” is the trace over spin and color.
“tr” the trace only over color. The three-point correlator can now be written as

\[
C^{3\text{pnt}}(t_0, t, \vec{p}_K) = \frac{1}{L^3} \sum_{\vec{x}} \sum_{\vec{y}} \sum_{\vec{z}} e^{i\vec{p}_K \cdot (\vec{z} - \vec{x})} \times \frac{1}{4} \phi(y)\phi(z) \langle tr \left\{ G_{\chi,s}^\dagger(z, x)G_{\chi,c}(y)G_{\chi,l}(y, x) \right\} \rangle,
\]

(12)

with \( x_0 \equiv t_0 \), \( y_0 \equiv t_0 - T \) and \( z_0 \equiv t \) and where \( \langle \cdot \rangle \) now stands for average over configurations. One sees from eq. (12) that strange HISQ propagators are needed going from \((\vec{x}, t_0)\) to general \( z \) and light propagators again from \((\vec{x}, t_0)\) to general \( y \). If one actually wanted to carry out the \( \frac{1}{L^3} \sum_{\vec{x}} \) one would need a strange and a light propagator from each spatial point on time slice \( t_0 \) and that would be prohibitively expensive. A common approach is to give up on doing the \( \frac{1}{L^3} \sum_{\vec{x}} \) and to use “local sources” where \( \vec{x} \) is fixed at some \( \vec{x}_0 \), e.g. \( \vec{x} = 0 \). One then has,

\[
C^{3\text{pnt}}_{\text{loc}}(t_0, t, \vec{p}_K) = \frac{1}{L^3} \sum_{\vec{y}} \sum_{\vec{z}} e^{i\vec{p}_K \cdot \vec{z}} \times \frac{1}{4} \phi(y)\phi(z) \langle tr \left\{ G_{\chi,s}^\dagger(z, x_{\text{loc}})G_{\chi,c}(y)G_{\chi,l}(y, x_{\text{loc}}) \right\} \rangle,
\]

(13)

with \( x_{\text{loc}} = (0, t_0) \). Momentum conservation will ensure that only kaons with momenta \( p_K \) contribute and be picked out at time slice \( t_0 \). On the other hand “random wall” sources allow us to carry out the \( \frac{1}{L^3} \sum_{\vec{x}} \) without having to invert at each spatial point. This can be seen by writing,

\[
C^{3\text{pnt}}_{\text{rw}}(t_0, t, \vec{p}_K) = \frac{1}{L^3} \sum_{\vec{x}} \sum_{\vec{y}} \sum_{\vec{z}} e^{i\vec{p}_K \cdot (\vec{z} - \vec{x})} \times \frac{1}{4} \phi(y)\phi(z) \langle tr \left\{ G_{\chi,s}^\dagger(z, x)G_{\chi,c}(y)G_{\chi,l}(y, x') \right\} \rangle \times \xi^*(\vec{x})\xi(\vec{x}') \rangle
\]

(14)

\( \xi(\vec{x}) \) is a field of random \( U(1) \) phases, and \( \langle \xi^*(\vec{x})\xi(\vec{x}') \rangle = \delta_{\vec{x},\vec{x}'} \) ensures that (14) reduces to (12) after averaging over gauge field configurations. So in the random wall source approach one calculates the light quark propagator \( G_{\chi,l} \) using the source \( \frac{1}{\sqrt{L^3}} \sum_{\vec{x}} \xi(\vec{x}) \) and \( G_{\chi,c} \), the strange propagator by using the source \( \frac{1}{\sqrt{L^3}} \sum_{\vec{x}} \xi(\vec{x}) e^{i\vec{p}_K \cdot \vec{x}} \). Only one light quark inversion is required in addition to a separate strange quark inversion for each \( p_K \). In this way one obtains the random wall propagators,

\[
G_{\chi,l}(y, t_0) = \frac{1}{\sqrt{L^3}} \sum_{\vec{x}} G_{\chi,l}(y, x') \xi(\vec{x})
\]

(15)

and

\[
G_{\chi,c}^{\text{rw}}(z, t_0; \vec{p}_K) = \frac{1}{\sqrt{L^3}} \sum_{\vec{x}} G_{\chi,c}(z, x) \xi(\vec{x}) e^{i\vec{p}_K \cdot \vec{x}}.
\]

(16)

The expression for the three-point correlator becomes,

\[
C^{3\text{pnt}}_{\text{rw}}(t_0, t, \vec{p}_K) = \sum_{\vec{y}} \sum_{\vec{z}} e^{i\vec{p}_K \cdot \vec{z}} \times \frac{1}{4} \phi(y)\phi(z) \langle tr \left\{ G_{\chi,s}^\dagger(z, t_0; \vec{p}_K)G_{\chi,c}(z, y)G_{\chi,l}^{\text{rw}}(y, t_0) \right\} \rangle,
\]

(17)

The charm propagator in eq. (17) is obtained by inverting at time slice \( y_0 = t_0 - T \) with source \( \sum_{\vec{x}} \phi(y)G_{\chi,c}^{\text{rw}}(z, y) \). In this way one gets the “sequential” charm propagator,

\[
G_{\chi,c}^{\text{seq}}(z, t_0, T) = \sum_{\vec{y}} \phi(y)G_{\chi,c}(z, y)G_{\chi,c}^{\text{seq}}(y, t_0),
\]

(18)

and

\[
C^{3\text{pnt}}_{\text{rw}}(t_0, t, \vec{p}_K) = \sum_{\vec{x}} e^{i\vec{p}_K \cdot \vec{x}} \times \frac{1}{4} \phi(z) \langle tr \left\{ G_{\chi,s}^\dagger(z, t_0; \vec{p}_K)G_{\chi,c}^{\text{seq}}(z, t_0, T) \right\} \rangle.
\]

(19)

The most costly part of our simulations is calculating the random wall strange quark propagators of eq. (18). A separate inversion is required for each \( p_K \) (e.g. 8 inversions for the different combinations \( (\pm 1, \pm 1, \pm 1) \)). On the other hand, when we change the \( T \) values only \( G_{\chi,c}^{\text{seq}} \) of eq. (18) needs to be recalculated and one inversion suffices for all momenta. This is one of the reasons why the full kaon momentum \( p_K \) is put into (18) and none into (14).

In Fig. 4 we show comparisons of percentage errors in three-point correlator data of local sources versus random
wall sources. One sees significant improvement coming from random wall sources. These tests were carried out in the test case \( D \rightarrow \eta_s, l\nu \) calculations and with less than the full statistics. For \( D \rightarrow K, l\nu \) we immediately went to random wall sources.

In addition to the three-point correlators, as we will show in the next section, several two-point correlators are needed in order to extract the matrix element \( \langle K|S|D \rangle \). They are,

\[
C^{2ptn}_D(t, t_0) = \frac{1}{L^3} \sum_{\vec{x}} \sum_{\vec{y}} (\Phi_D(\vec{y}, t) \Phi_D^\dagger(\vec{x}, t_0)),
\]

and

\[
C^{2ptn}_K(t, t_0; \vec{p}_K) = \frac{1}{L^3} \sum_{\vec{x}} \sum_{\vec{y}} e^{i\vec{p}_K \cdot (\vec{x} - \vec{y})} (\Phi_K(\vec{y}, t) \Phi_K^\dagger(\vec{x}, t_0)).
\]

The \( \frac{1}{L^3} \sum_{\vec{x}} \) can again be implemented via random wall sources. As already mentioned in the previous section we also calculated correlators for the \( \eta_s \), \( \eta_c \) and \( D \) mesons in exactly the same way as \( C^{2ptn}_D/K \) in order to carry out and check mass tunings. We have accumulated simulation data for the three- and two-point correlators described in this section for the ensembles of Table I. In the next section we explain how hadronic matrix elements such as \( \langle K|S|D \rangle \) and meson masses and decay constants are extracted from this data.

V. FITS AND DATA ANALYSIS

The interpolating operators \( \Phi_D \) and \( \Phi_K \) do not create just the ground state \( D \) meson or kaon that we are interested in but also excited states with the same quantum numbers. With staggered quarks there is the further complication that in addition to regular states so-called “parity partner” states can contribute, whose energies are measured relative to \( i\tau \) so that \( e^{-\xi \tau} \rightarrow (-1)^\tau e^{-\xi \tau} \). The \( D \) meson correlator, for instance, has the \( t \) dependence (we set \( t_0 = 0 \) for simplicity),

\[
C^{2ptn}_D(t) = \sum_{j=0}^{N_D-1} b^D_j (e^{-E^D_j t} + e^{-E^D_j (N_D-t)}) + \sum_{k=0}^{N_D-1} d^D_k (-1)^t (e^{-E^D_k t} + e^{-E^D_k (N_D-t)}).
\]

We are interested in the ground state \( D \) meson contribution with amplitude,

\[
b_0^D = \frac{|\langle \Phi_D|D \rangle|^2}{2M_D a^3}.
\]

Similar relations apply for other mesons. Only in the case of equal mass mesons (\( \pi \), \( \eta_s \) or \( \eta_c \)) at zero momentum are the oscillatory contributions absent. The three-point correlators such as eq. \([19]\) will have contributions from regular and oscillatory states for both the kaon and the \( D \) meson. The rather complicated \( t \) and \( T \) dependence is then given by,

\[
C^{3ptn}(t, T) = \sum_j \sum_k A_{jk} e^{-E^D_j t} e^{-E^D_k (T-t)}
\]

\[
\sum_j \sum_k B_{jk} e^{-E^D_j t} e^{-E^D_k (T-t)} (-1)^t
\]

\[
\sum_j \sum_k C_{jk} e^{-E^D_j t} e^{-E^D_k (T-t)} (-1)^t (-1)^t.
\]

We will only consider the region 0 \( \leq t \leq T \) and take \( T < \ll N_t \) so that any contributions from mesons propagating “around the lattice” due to periodic boundary conditions in time can be neglected. The relevant amplitude here is,

\[
A_{00} = \frac{\langle \Phi_K|K \rangle \langle K|S|D \rangle \langle D|\Phi_D \rangle}{(2E_K a^3) (2M_D a^3)} a^3.
\]

From eqs. \([24]\) and \([31]\) one sees that our sought after hadronic matrix element is given by,

\[
\langle K|S|D \rangle = 2\sqrt{M_D E_K} \frac{A_{00}}{b_0^D b_0^*}.
\]

So our goal is to extract the combination on the right-hand-side of \([36]\) as accurately as possible and with any correlations among the errors of the individual components, \( A_{00}, b_0^K/D, M_D \) and \( E_K \) taken properly into account.

We have carried out simultaneous fits to \( C_{2ptn}^{D/K}, \) \( C_{2ptn}^{D/K} \) and the three-point correlators with different \( T \) values, \( C^{3ptn}(t, T) \) \( i = 1, 2, ... \) following the fit ansatze of eqs. \([22]\) and \([24]\). Two (three) different \( T \) values are used for the coarse (fine) ensembles. This allows us to evaluate \([20]\) within one fit. The two-point correlators were fit for \( t \)-values between \( t_{\text{min}} = 2(2) \) and \( t_{\text{max}} = 30(20 \sim 30) \) for the \( K \) and \( D \) respectively for coarse lattices. For fine lattices, \( t \)-values were used between \( t_{\text{min}} = 2 \sim 4(2) \) and \( t_{\text{max}} = 30(30) \). For the three-point correlators we used all the data between \( t = 2 \) and \( t = T - 2 \) for coarse lattices, and \( t = 3 \) and \( t = T - 2 \) for fine lattices. Simultaneous fits with multiple \( T \) and taking different \( \chi^2 \) ranges for different correlators were also helpful to reduce the statistical errors, since it allows us to extract maximum information from both the three-point and two-point correlators. The number of exponentials in our fit ansatze was varied to test for stability of fit results. For our final fits we ended up
FIG. 5: $A_{00}$ versus the number $N_{D/K}$. In the left (right) plot
$N_K$ ($N_D$) is fixed at 3 (4).

choosing around $3 \sim 4$ for $N_D$ and $N_K$. $N_{D/K}'$ was taken
to be mostly $N_{D/K} - 1$. Figs 4 - 9 show some results for $A_{00}, M_D, b_0^D, E_K, b_0^K$ versus $N_D$ or $N_K$ for ensemble C1
at kaon momentum $\vec{p} = (0, 0, 0)$. All our fits are carried
out using Bayesian methods [21]. We describe choices for
priors and prior widths in the Appendix.

We have found that using data from several $C^{3\text{pnt}}$
with different $T$-values helps greatly in reducing statisti-
cal/fitting errors. Fig. 10 compares results for $f_0(q^2)$
for ensemble C2. One sees that having two rather than
just one $C^{3\text{pnt}}(t, T_i)$ involved in the simultaneous fit re-
duces errors and that this effect is most pronounced when
one combines an even $T$ with an odd $T$. It may not be
surprising that improvements are achieved from multi-$T$
fits. From the fit ansatz [21] one sees that having more
$C^{3\text{pnt}}$’s does not increase the number of fit parameters ($A_{jk}$ etc.)
although the amount of data and hence of information given to the minimizer is increased. Fur-
thermore if $T_1 + T_2$ is odd, then $(-1)^{T_1-t}$ and $(-1)^{T_2-1}$
have opposite signs and $C^{3\text{pnt}}(t, T_1)$ and $C^{3\text{pnt}}(t, T_2)$ will
provide more independent information.

Fig. 6 - 9 show some results for $A_{00}, M_D, b_0^D$
versus $N_D$ or $N_K$ for ensemble C1
at kaon momentum $\vec{p} = (0, 0, 0)$. All our fits are carried
out using Bayesian methods [21]. We describe choices for
priors and prior widths in the Appendix.

We have found that using data from several $C^{3\text{pnt}}$
with different $T$-values helps greatly in reducing statisti-
cal/fitting errors. Fig. 10 compares results for $f_0(q^2)$
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$C^{3\text{pnt}}$’s does not increase the number of fit parameters ($A_{jk}$ etc.)
although the amount of data and hence of information given to the minimizer is increased. Fur-
thermore if $T_1 + T_2$ is odd, then $(-1)^{T_1-t}$ and $(-1)^{T_2-1}$
have opposite signs and $C^{3\text{pnt}}(t, T_1)$ and $C^{3\text{pnt}}(t, T_2)$ will
provide more independent information.

Most of the fit parameters such as $M_D$ or $b_0^D$ etc. that
one gets from the simultaneous $C^{2\text{pnt}} - C^{3\text{pnt}}$ fits can also be determined by just fitting the two-point correla-
tors by themselves. Results from the $C^{2\text{pnt}}$ fits are also
shown on Figs. 6 - 9 and provide consistency checks. One
interesting outcome is that two-point correlator param-
eters are more accurately determined via simultaneous
fits with three-point correlators than when they are fit
alone. This is especially noticeable for $D$ meson corre-
lators, namely for $M_D$ and $b_0^D$ and has implications for
FIG. 9: Same as Fig. 6 for $b^K_0$ versus $N_K$.

FIG. 10: Effect of multi T-fits

determinations of the decay constant $f_D$. The latter is related to $b^K_0$ through,

$$a f_D = \frac{m_{0,L} + m_{0,J}}{M_D} \sqrt{\frac{2b^D_0}{a M_D}}.$$  \hspace{1cm} (27)

In Figs. 11 and 12 we compare results for $M_D$ and $f_D$ using either pure two-point fits or simultaneous fits. One sees the significant improvement coming from the simultaneous fit. Doing simultaneous fits gives a better handle on excited state contributions because they contribute differently to two-point and three-point correlators. This is effectively similar to adding smeerings to the correlators. In section VIII we will discuss extracting $f_D$ in the chiral/continuum limit. Having simultaneous fit results will make this determination more accurate than what can be achieved from pure two-point correlators. This appears to be a bonus side product of semileptonic decay studies.

In Tables III, IV and V we summarize our main fit results. One sees from Table V that we were able to determine $f_0(\bar{p}_K)$ with errors ranging from $\sim 0.2\%$ at zero momentum to $\sim 0.9\%$ at our highest momentum. In Fig. 13 we plot the square of the “speed of light” $c^2(\bar{p})$ for the kaon.

$$c^2(\bar{p}) = \frac{E^2_K(\bar{p}) - M^2_K}{\bar{p}^2}.$$  \hspace{1cm} (28)

One sees that the relativistic dispersion relation is satisfied to about $1 \sim 2\%$. We will check the effect of deviations from exact continuum dispersion relations on our final results for form factors in later sections.
TABLE III: Fit results for \(aM_D, a f_D, aM_{D^*}, \) and \(a f_{D^*}\). Numbers in brackets are from two-point fits, whereas the rest come from simultaneous fits.

| Set  | \(aM_D\)         | \(a f_D\)        | \(aM_{D^*}\)         | \(a f_{D^*}\)         |
|------|------------------|------------------|----------------------|----------------------|
| C1   | 1.1393(7)        | 0.1372(4)        | (1.1398(21))         | (0.1539(6))          |
| C2   | 1.1595(8)        | 0.1423(4)        | (1.1574(19))         | (0.1560(7))          |
| C3   | 1.1618(5)        | 0.1464(3)        | (1.1620(10))         | (0.1553(4))          |
| F1   | 0.8141(3)        | 0.0971(2)        | (0.8152(8))          | (0.1083(2))          |
| F2   | 0.8197(3)        | 0.1007(2)        | (0.8191(5))          | (0.1078(2))          |

TABLE IV: Fit results for \(aM_K, aE_K(\vec{p}), a f_K, a m_s\) and \(a f_s\). Numbers in brackets are from two-point fits, whereas the rest come from simultaneous fits.

| Set  | \(aM_K\)         | \(aE_K\)         | \(aE_K\)         | \(aE_K\)         |
|------|------------------|------------------|------------------|------------------|
|      | (1,0,0)          | (1,1,0)          | (1,1,1)          | (1,1,1)          |
| C1   | 0.3122(2)        | 0.4081(7)        | 0.4837(9)        | 0.5469(20)       |
| C2   | 0.3285(5)        | 0.4531(16)       | 0.5525(17)       | 0.6373(32)       |
| C3   | 0.3572(2)        | 0.4750(9)        | 0.5720(10)       | 0.6524(22)       |
| F1   | 0.2285(2)        | 0.3203(7)        | 0.3919(9)        | 0.4559(15)       |
| F2   | 0.2460(1)        | 0.3340(4)        | 0.4014(7)        | 0.4609(11)       |

| Set  | \(a f_K\)       | \(a m_s\)       | \(a f_s\)       |
|------|-----------------|-----------------|-----------------|
| C1   | 0.1011(1)       | (0.1599(2))     | (0.0893(1))     |
| C2   | 0.1044(1)       | (0.2108(2))     | (0.0949(1))     |
| C3   | 0.1079(1)       | (0.2931(2))     | (0.1023(1))     |
| F1   | 0.0721(1)       | (0.1344(2))     | (0.0645(1))     |
| F2   | 0.0748(1)       | (0.1873(1))     | (0.0697(1))     |

VI. CHIRAL AND CONTINUUM EXTRAPOLATIONS USING THE \(\varepsilon\)-EXPANSION

The twenty entries in Table V summarize our results for the form factor \(f_0(\vec{p}_K^2)\) evaluated on the five ensembles of Table III with four different momenta \(\vec{p}_K\) (including zero momentum) per ensemble. The kaon energy in the \(D\) rest frame, \(E_K\), is related to \(q^2\) via,

\[
q^2 = M_D^2 + M_K^2 - 2M_D E_K,
\]

and the physical region is \(0 \leq q^2 \leq q_{max}^2 = (M_D - M_K)^2\). \(M_K, E_K\) and \(M_D\) are given for the different ensembles in Tables III & IV. The next step is to extrapolate the data of Table V to the chiral/continuum physical limit. As is well known, chiral extrapolations for form factors are much more subtle than for static quantities such as masses or decay constants. The main reason for this is that form factors depend not only on meson/quark masses but also on a kinematic variable such as \(q^2\) (or equivalently on \(E_K\)). Kinematic variables are themselves functions of meson masses. It is not sufficient to parameterize just the light quark mass dependence of form factors. One must at the same time capture the kinematic variable dependence correctly for each value of the light quark mass and the lattice spacing (i.e. for each of our ensembles). Furthermore we are interested in a parameterization that works over the entire physical kinematic range. In the chiral limit, \(q^2\) ranges between \(0 \leq q^2 \leq 1.9\text{GeV}^2\) and \(E_K\) between \(0.495 \leq E_K \leq 1.0\text{GeV}\).
The z-expansion

In addition to $q^2$ and $E_K$ a third kinematic variable has proven to be convenient in semileptonic form factor studies, in particular in recent analysis of $B \to \pi, l\nu$ decays [13,15].

\[ z(q^2,t_0) = \frac{\sqrt{t_+ - q^2 - \sqrt{t_+ - t_0}}}{\sqrt{t_+ - q^2 + \sqrt{t_+ - t_0}}} \]

where $t_\pm = (M_D \pm M_K)^2$ and $t_0$ is a free parameter that defines the zero of the z-variable, $z(q^2,t_0,t_0) = 0$. By going to the z-variable one is mapping the cut region $t_+ < q^2 < \infty$ in the complex $q^2$ plane onto the circle $|z| = 1$ and $-\infty < q^2 < t_+$ onto $z \in [-1,1]$. The physical region $0 \leq q^2 \leq q_{\text{max}}^2 = t_-$ corresponds then to an even smaller region around $z = 0$. For instance for the choice $t_0 = 0.5t_-$ and for physical values of $M_D$ and $M_K$ one has $-0.057 \leq z \leq 0.046$. In other words one always has $|z| < 0.06$ in the physical region and this should make $z$ a good variable for a power series expansion. As discussed in the literature using analyticity properties of form factors one can write,

\[ f_0(q^2) = \frac{1}{P(q^2) \Phi_0(q^2,t_0)} \sum_{k=0}^{\infty} a_k(t_0) z(q^2,t_0)^k. \]

The function $P(q^2)$ in the denominator is there to factor out any isolated poles in the region $t_- < q^2 < t_+$ below the $DK$ threshold at $q^2 = t_+$. In the case of $D \to K$ semileptonic decays the charm-strange current has the same quantum numbers as the $D_s^*(2317) 0^+$ meson so that one choice for $P(q^2)$ would be $P(q^2) = (1 - q^2/(M_{D_s^*}^2))^2$. We have worked with both $P(q^2) = (1 - q^2/(M_{D_s^*}^2))^2$ and $P(q^2) = 1$ and find that although the expansion coefficients $a_k$ depend on the choice for $P(q^2)$, in either case the data can be reproduced very well with just a few terms (as we will discuss below, with just three terms) in the z-expansion.

For the “outer function” $\Phi_0$ we adopt the choice given in Ref. [14].

\[ \Phi_0(q^2,t_0) = \frac{3t_+ t_-}{32 \pi \chi_0} \left( \sqrt{t_+ - q^2 + \sqrt{t_+ - t_0}} \times \right) \]
\[ \left( t_+ - q^2 \right)^{1/2} \left( \sqrt{t_+ - q^2 + \sqrt{t_+ - t_0}} \right)^{1/2} \]
\[ \left( t_+ - t_0 \right)^{1/2} \left( \sqrt{t_+ - q^2 + \sqrt{t_+ - t_0}} \right)^{1/2}. \]

$\chi_0$ has been calculated in the literature using QCD perturbation theory and the Operator Product Expansion (OPE). An expression including $O(\alpha_s)$ and condensate contributions is given for instance in Ref. [14]. For fixed charm quark mass $\chi_0$ is a constant and affects just the overall normalization of the $a_k$’s. For simplicity we ignore the condensate contributions, which are of $O(m_c^{-3})$ and $O(m_c^{-4})$ respectively, and retain just the tree-level and $O(\alpha_s)$ contributions. Any other choice would just mean a common overall rescaling of the expansion coefficients $a_k$.

**Testing the z-expansion with individual fits**

In order to test the usefulness of the z-expansion we first fit $f_0(q^2)$ separately for each individual ensemble using the ansatz of eq. (31) with $\sum_k \to \sum_{k=0}^{\text{max}}$. In each case values used for $M_D$, $M_K$ and hence also for $t_\pm$ were those specific to that ensemble. We employed a common choice for $t_0$, $t_0 = 0.942 \text{GeV}^2$ corresponding to $t_0 = 0.5 \times t_\text{continuum}$. As is well known from z-expansions in general, other choices for $t_0$ made no difference in resulting fit curves. We find that good individual fits are possible once $k_{\text{max}}$ reaches $k_{\text{max}} = 2$ and that fit curves are then very stable with respect to further increases in $k_{\text{max}}$. In Fig. 14 we show representative results for two ensembles C2 and F1 for $f_0(q^2 = 0)$ versus $k_{\text{max}}$. We also show results for two different choices, $P(q^2) = 1$ and $P(q^2) = (1 - q^2/(M_{D_s^*}^2))^2$. One sees that fit results are very insensitive to these changes in $k_{\text{max}}$ or $P(q^2)$. At finite lattice spacing we have used $M_{D_s^*} = M_{D_s} + \delta M$ with $\delta M \equiv [M_{D_s}(0^+) - M_{D_s}(0^-)]_{\text{exp}}$. These individual z-expansion fit tests demonstrate (as advocated in the literature) the efficiency of z-expansions in capturing the kinematics of form factors with just a small number of parameters and in a model independent way.

In Fig. 15 we give examples of z-expansion fits to individual ensembles, specifically for ensembles C2 and F1.

**Simultaneous modified z-expansion fit**

Having verified the efficacy of the z-expansion in fits to individual ensembles we turn next to modifying the fit ansatz to enable extrapolation to the physical limit. All kinematic properties that depend on $q^2$ are absorbed
by $P, \Phi_0,$ and $z$. A natural way to distinguish between ensembles is to let $a_k \to a_k \ast D_k,$ where $D_k$ contains the light quark mass and lattice spacing dependence as shown below (we set $k_{\max} = 2$ and $P(q^2) = (1 - q^2/(M_{D_k}^2))^2$).

$$f_0(q^2) = \frac{1}{P(q^2)} \Phi_0 \left( a_0 D_0 + a_1 D_1 z + a_2 D_2 z^2 \right) \times (1 + b_1(a E_K)^2 + b_2(a E_K)^4),$$ (33)

where,

$$D_i = 1 + c_1 x_i + c_2 \delta x_s + c_3 x_i \log(x_i) + d_i (am_c)^2 + e_i (am_c)^4 + f_i \left( \frac{1}{2} \delta M^2_{\pi} + \delta M^2_{K} \right),$$ (34)

$$x_i = \frac{M_i^2}{(4\pi f_\pi)^2}$$ (35)

$$\delta x_s = \frac{M_{\pi}^2 - M_{\eta^0}^2}{(4\pi f_\pi)^2}$$ (36)

$$\delta M^2_{\pi} = \frac{1}{(4\pi f_\pi)^2} \left( (M_{\pi}^{AsqTad})^2 - (M_{\pi}^{HISQ})^2 \right)$$ (37)

In eq. 34, we put typical analytic terms for light valence ($x_i$ and $\delta x_s$ terms) and sea quark mass ($\delta M_\pi$ and $\delta M_K$ terms) dependence. We quote $M_{\pi}^{AsqTad}$ and $M_{\pi}^{HISQ}$ from ref. 22. For the chiral logs, we only include up/down quark contributions. The strange quark chiral logs are close to a constant that can be absorbed into the $a_i$’s. There are two distinct sources of lattice spacing dependence. ($am_c$)$^2$ and ($am_c$)$^4$ terms are due to the heavy quark discretization error, and ($a E_K$)$^2$ and ($a E_K$)$^4$ terms are introduced to estimate the discretization errors due to finite momentum. Since we want the $a_i D_i$ to be independent of the momentum, the $a E_K$ terms are placed separately outside the $z$-expansion. We include lattice spacing dependent terms up to fourth power, however, we tested with even higher terms and confirmed that the higher terms are negligible (see Fig. 22). We have carried out simultaneous fits to all the data of Table VI using the above ansatz and find that very good fits are possible.

Figs. 16 and 17 plot the resulting fit curves for each ensemble and the chiral/continuum extrapolated curve with its error band for $f_0(q^2)$ versus $E_K^2$ (we show separately the coarse and fine ensembles in order to avoid too much clutter). The fit is excellent and has $\chi^2/\text{dof} = 0.44$. In Table VII we summarize fit results for $a_k \ast D_k, k = 0,1,2$ coming from the simultaneous fit both for individual ensembles and in the physical limit. These are plotted in Figs. 15 - 20. In Fig. 21 we plot $f_0(q^2) = 0$ for the five ensembles and in the physical limit. One sees that within errors this quantity shows little light quark mass dependence and a $\sim 1.3\%$ lattice spacing dependence.

We call the chiral/continuum extrapolation based on the ansatz [33] - [35] and shown in Figs. 16, 17 and 21 the

![FIG. 15: Individual $z$-expansion fits for ensembles C2 and F1.](image)

![FIG. 16: Chiral/continuum extrapolation of $f_0(q^2)$ versus $E_K^2$ from the modified $z$-expansion ansatz. The data points are coarse lattice points. Three individual curves and the extrapolated band are from a fit to all five ensembles.](image)
FIG. 17: Chiral/continuum extrapolation of \( f_0(q^2) \) versus \( E_K^2 \) from the modified \( z \)-expansion ansatz. The data points are fine lattice points. Two individual curves and the extrapolated band are from a fit to all five ensembles.

FIG. 18: The expansion parameter \( a_0 * D_0 \) versus the light quark mass from a simultaneous fit to all data.

“simultaneous modified \( z \)-expansion extrapolation.” We have tested the stability of this extrapolation by adding further terms to the ansatz and/or modifying some of the fit parameters and checking for changes in the physical limit \( f_0(q^2 = 0) \). For example, we have,

1. added \( x_l^2 \) terms,
2. modified the lattice spacing dependent terms:
   (a) drop \( (am_c)^4 \) and \( (aE_K)^4 \) terms
   (b) drop \( (am_c)^4 \) term
   (c) drop \( (aE_K)^4 \) term
   (d) add \( (am_c)^6 \) term
   (e) add up to \( (am_c)^{10} \) terms
   (f) add \( (aE_K)^6 \) term,
3. used \( P(q^2) = 1 \) for the pole term,
4. used \( E_K \) from dispersion relations,
5. used an overall factor \( (1 + f(\frac{1}{2} \delta M_\pi + \delta M_K)) \) outside the \( \sum_k \) to incorporate sea quark effects, rather than include them in the \( D_i \)’s,
6. used an overall factor \( (1 + d(\frac{1}{2} (am_c) + e(\frac{1}{4} am_c)^4) \) outside the \( \sum_k \) to estimate the \( am_c \) errors, rather than include them in the \( D_i \)’s,
7. replaced \( \delta M_{\pi/K}^2 \to (M_{\pi/K}^{AsqTad})^2/(4\pi f_\pi)^2 \),
8. used a simpler \( D_i = 1 + d_1 x_l + d_2 x_s \),

FIG. 19: Same as Fig. 18 for \( a_1 * D_1 \).

FIG. 20: Same as Fig. 18 for \( a_2 * D_2 \).
error is stabilized. This also shows that the increasing, however after including the fourth powers the error is stabilized. The second item of the tests checks that we estimate the lattice spacing extrapolation error correctly. Until \((am_c)^4\) and \((aE_K)^4\) terms are included, the error is increasing, however after including the fourth powers the error is stabilized. This also shows that the \(am_c\) error of the HISQ action is under control in our simulations.

9. used an even simpler \(D_i = 1 + d'_i x_i\).

Fig. 22 summarizes the results of these tests. One sees that the standard \(z\)-expansion extrapolation result is very robust. The second item of the tests checks that we estimate the lattice spacing extrapolation error correctly. Until \((am_c)^4\) and \((aE_K)^4\) terms are included, the error is increasing, however after including the fourth powers the error is stabilized. This also shows that the \(am_c\) error of the HISQ action is under control in our simulations.

Fig. 21: \(f_0\) at \(q^2 = 0\) for the five ensembles and in the physical limit.

Fig. 22: Tests of the “simultaneous modified \(z\)-expansion extrapolation”. The red horizontal line is the central value of the fit shown in Figs. 16 and 17 and the orange lines indicate the error. The numbers under the data points correspond to the “test numbers” given in the text.

VII. RESULTS IN THE PHYSICAL LIMIT: \(f_+(0)\), \(|V_{cs}|\) AND UNITARITY TESTS

This section summarizes the main results of this paper. We present our Standard Model prediction for the \(D \to K, \ell \nu\) decay form factor at \(q^2 = 0\), \(f_+(0) = f_0(0)\), determine the CKM matrix element \(|V_{cs}|\) using input from BaBar and CLEO-c and carry out unitarity tests.

\[ f_+(0) = f_0(0) \]

We have seen that the simultaneous modified \(z\)-expansion extrapolation method gives very stable results. It gives \(f_+(0) = 0.748 \pm 0.019\) in the physical limit for \(D^0 \to K^- \ell \nu\), and \(f_+(0) = 0.746 \pm 0.019\) for \(D^+ \to \bar{K}^0 \ell \nu\). We take an average over these two channels and our final result in the physical limit becomes,

\[ f_+^{D \to K}(0) = 0.747 \pm 0.011 \pm 0.015. \]

The first error comes from statistics and the second error represents systematic errors. Table VII summarizes the error budget. One sees that the largest contributions to the total error come from statistics followed by \((am_c)^2\) and \((aE_K)^2\) extrapolation errors.

In order to calculate the form factor, we have to put in meson masses from experiment and also from our lattice simulations. For example, we need experimental \(D\), \(K\), and \(\pi\) meson masses to get the form factor at the physical limit, and \(E_K\), \(D\), and \(K\) meson masses from the lattice calculations are used to fit at non-zero lattice spacing. In Table VII “Input meson mass” refers to errors induced from these input meson masses. In the fit ansatz, eq. (34), there are light quark \((c_1^i\) and \(c_2^i\)), strange quark \((c_3^i\)), and sea quark dependent terms \((f_i)\). Each systematic error due to these terms is shown on the fourth to sixth line in the table. Lattice spacing dependence errors are estimated separately for \((am_c)^2\) and \((aE_K)^2\) type contributions.

In the fit ansatz, \(x\log(x)\) is the most infrared sensitive term. We calculate the pion-tadpole loop integral both at finite volume and at infinite volume and compare these to estimate the finite volume effects. For the charm quark mass tuning error, we calculate the form factor with a different charm quark mass, \(am_c = 0.629\), on the C3 ensemble, and compare with the result with the tuned \(am_c = 0.6235\) of Table III. All but the last two entries in Table VII (finite volume and charm mass tuning) were calculated using methods introduced in reference [23]. The total error coming out of the chiral/continuum extrapolation can be decomposed into individual contributions, \(\sigma^2 = \sum c_i \sigma^2_i\), where the sum \(\sum c_i\) goes over the first 8 entries in Table VII. Details are described in Appendix B.

One might worry about other potential systematic errors, not listed in Table VII such as those due to missing sea charm quarks or electromagnetism/isospin breaking. The separate numbers given above eq. (39) for \(D^0 \to K^-\) and \(D^+ \to \bar{K}^0\) form factors take into account just the differences in masses of the charged versus neutral mesons.
This “kinematic” effect is seen to be less than $\sim 0.3\%$. It is much harder to assess the true dynamical electromagnetic effects. However no statistically significant differences have been observed experimentally [5] and we will ignore further electromagnetic/isospin breaking effects. Similarly we will assume that errors due to missing sea charm quarks are small enough so that they do not change the 2.5% total error when added in quadrature. This has been true in the case of several quantities where changes have been observed experimentally [5] and we will ignore further electromagnetic/isospin breaking effects. However no statistically significant differences have been observed experimentally [5] and we will ignore further electromagnetic/isospin breaking effects.

The total error for $f_+(0)$ is estimated here to be 2.5%. This is a factor of four times smaller than in the previous lattice calculation of Ref. [6]. This was achievable because of applying several new methods and techniques that were described in the text. We employ the HISQ action for both charm and light quark actions and a scalar current rather than the traditional vector current. Because of these new methods, we obtain results with smaller discretization errors and no operator matching. We also developed the modified $z$-expansion extrapolation method, which is crucial to decrease errors due to the discretization, chiral / continuum extrapolation and parameterization of the form factor. In order to decrease statistical errors, we apply random-wall sources and perform simultaneous fits with multiple correlators and $T$'s. If we compare with the error budget of Ref. [6], then we see the statistical errors reduced from 3% to 1.5% and the extrapolation and parameterization errors from 3% to 1.5% as well. The biggest improvement is in the discretization errors. The total discretization errors have now been reduced from 9% to 2%. We note that the concept of the discretization errors is different in Ref. [6] compared to here. In Ref. [6], they estimate the discretization errors by power counting, since they calculate at only one lattice spacing. However we actually perform continuum extrapolations with correction terms for the discretization effects. As a result, we do not have discretization errors per se, but instead extrapolation errors due to higher order correction terms.

In their papers both BaBar [4] and CLEO-c [5] have converted their measurements of $f_+(0) \cdot |V_{cs}|$ into results for $f_+(0)$ using values for $|V_{cs}|$ fixed by CKM unitarity. For this CLEO-c uses the 2008 PDG CKM unitarity value of $|V_{cs}| = 0.97334(23)$ [24] and obtains $f_+^{D\to K}(0) = 0.739(9)$ and BarBar uses $|V_{cs}| = 0.9729(3)$ leading to $f_+(0) = 0.737(10)$. In Fig. 23 we plot the new HPQCD result of this article, eq. (39), together with earlier theory results from the lattice [6] and from a recent sum rules calculation [24] and with the BaBar and CLEO-c numbers. One sees the very welcome reduction in theory errors which are now small enough so that the agreement between theory and experiment in Fig. 23 already provides a nontrivial indirect test of CKM unitarity. We can, however, do better and carry out more direct tests of unitarity by determining $|V_{cs}|$ without the assumption of unitarity.

Direct Determination of $|V_{cs}|$

As experimental input we take $f_+(0) \cdot |V_{cs}| = 0.719(8)$ from CLEO-c [5] and $f_+(0) \cdot |V_{cs}| = 0.717(10)$ from BaBar [4]. For the latter we have multiplied BaBar’s quoted $f_+(0)$ with their quoted CKM unitarity value for $|V_{cs}|$. Averaging between the two experiments we use $f_+(0) \cdot |V_{cs}| = 0.718(8)$ together with eq. (39) to extract $|V_{cs}|$. One finds, $|V_{cs}| = 0.961 \pm 0.011 \pm 0.024$, (40)
in good agreement (as expected from Fig. 23) with the CKM unitarity value of 0.97345(16) [2]. The first error in [40] is from experiment and the second from the lattice calculation of this article. This is a very precise direct determination of $|V_{cs}|$, made possible by the many advances in lattice QCD that are described in this article.

### Table VII: Total error budget.

| Type                        | Error   |
|-----------------------------|---------|
| Statistical                 | 1.5%    |
| Lattice scale ($r_1$ and $r_1/a$) | 0.2%    |
| Input meson mass            | 0.1%    |
| Light quark dependence      | 0.6%    |
| Strange quark dependence    | 0.7%    |
| Sea quark dependence        | 0.4%    |
| $aE_K$ extrapolation        | 1.4%    |
| Finite volume               | 0.01%   |
| Charm quark tuning          | 0.05%   |
| Total                       | 2.5%    |

![FIG. 23: Comparisons of $f_0(q^2 = 0)$ with other calculations and experiments.](image)
together with the tremendous progress in recent experimental studies of $D$ semileptonic decays \cite{4,5}. In Fig. 24, we plot several previous direct determinations of $|V_{cs}|$ from the 2010 PDG \cite{2} together with (40) and the CKM unitarity value.

In a companion paper \cite{20} where we update HPQCD’s $D_s$ meson decay constant $f_{D_s}$, we also determine $|V_{cs}|$ from $D_s \to \tau \nu$ and $D_s \to \mu \nu$ leptonic decays. One finds $|V_{cs}|_{\text{leptonic}} = 1.010(22)$ which is consistent with eq. (40) at the $1.4 \sigma$ level.

Further Unitarity Tests

Using the new value of $|V_{cs}|$, eq. (40), and the current PDG values $|V_{cd}| = 0.230(11)$ and $|V_{cb}| = 0.0406(13)$ one finds,

$$ |V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2 = 0.978(50) \quad (41) $$

for the 2nd row. And similarly for the 2nd column, with $|V_{us}| = 0.2252(9)$ and $|V_{ub}| = 0.0387(21)$ one gets,

$$ |V_{us}|^2 + |V_{cs}|^2 + |V_{ub}|^2 = 0.976(50) \quad (42) $$

These 2nd row and 2nd column unitarity test results are shown in Fig. 25 together with the PDG numbers mentioned already in the Introduction. Again one sees the improvement coming from the reduction in the uncertainty in $|V_{cs}|$.

VIII. FURTHER RESULTS FROM TWO-POINT CORRELATORS

In this section we summarize physics results extracted from two-point correlators that emerged as part of our analysis of $D$ meson semileptonic decays. This includes determinations of decay constants, $f_\pi$, $f_K$, $f_D$ and $f_{D_s}$.

These determinations serve mainly as consistency checks on our quark mass tunings and on our fitting and chiral/continuum extrapolation methods. More extensive studies of $f_{D_s}$ involving five lattice spacings are reported in \cite{20}. Here we present the first results for $f_D$ using HISQ charm and light quarks that employs the new HPQCD $r_1$ scale \cite{19} (the scale we use throughout in this article).

We use continuum partially quenched ChPT formulas augmented by discretization terms to extrapolate to the chiral/continuum limit. Error budgets are close to those in ref \cite{11} with, however, a decrease in the $r_1$ uncertainty. For $f_\pi$ and $f_K$, we find,

$$ f_\pi = 132.3 \pm 1.6 \text{ MeV} \quad (43) $$

$$ f_K = 157.9 \pm 1.5 \text{ MeV} \quad (44) $$

One sees that agreement with experiment \cite{2} is good and within $1 \sim 1.5\sigma$ (or 1.5%).

For $f_D$ we have results from the simultaneous fit with three-point correlators and also from just the two-point correlator fits. As we noted in section V, the former has smaller errors however they are consistent with each other.

$$ f_D^{\text{SimFit}} = 206.3 \pm 4.3 \text{ MeV} \quad (45) $$

$$ f_D^{\text{2pt}} = 211.1 \pm 5.7 \text{ MeV}. \quad (46) $$

Both values show good agreement with experiment \cite{2} as can be seen in Fig. 26.

For $f_{D_s}$, we find,

$$ f_{D_s} = 250.2 \pm 3.6 \text{ MeV}, \quad (47) $$
which agrees with (but is less precise than) our recent update in reference \[21\], \[f_{D_s} = 248.0 \pm 2.5 \text{ MeV}.\] One sees that with experimental values having come down in recent years and with the increase in the HPQCD value, there is no longer any discrepancy (beyond 1.6 \[\sigma\]) between theory and experiment. The current HFAG \[26\] number is \[f_{D_s} = 257.3 \pm 5.3 \text{ MeV}.\]

Finally we present the ratio,

\[
\frac{f_{D \to K}^+(0)}{f_{D_s}} = 2.986 \pm 0.087 \text{ GeV}^{-1}. \tag{48}
\]

This quantity can also be obtained from experimental measurements of \(D \to K, l\nu\) semileptonic and \(D_s\) leptonic decay branching fractions, and has the virtue that \(|V_{cs}|\) drops out in the ratio. We compare with experiment in Fig. 27 and good agreement is found.

\section{IX. SUMMARY AND FUTURE OUTLOOK}

We have completed the first study of \(D \to K\) semileptonic decays using the HISQ action for the valence charm, strange and light quarks. The most important result of this article is given in eq. \[49\] and provides the form factor \(f_{D \to K}^+(q^2)\) at \(q^2 = 0\). We were able to determine this quantity with a 2.5\% total error which represents a four fold improvement in precision over earlier theory results. This is shown in Fig. 26. We then combined our form factor result with recent measurements of \(D \to K\) semileptonic decays by the BaBar and CLEO-c collaborations to extract a very accurate direct determination of the CKM matrix element \(|V_{cs}|\). This is given in eq. \[411\] and comparisons with previous determinations shown in Fig. 24. The new value for \(|V_{cs}|\) is consistent with the PDG value based on CKM unitarity. We carried out direct tests of 2nd row and 2nd column unitarity with results given in equations \[11\] and \[12\] and depicted in Fig. 26. Although still far from the accuracy achieved in 1st row unitarity tests, the reduction in errors on \(|V_{cs}|\) has made 2nd row and column unitarity tests much more relevant and interesting than in the past. In section VIII we give a lattice QCD value for \(f_{D \to K}^+(0)/f_{D_s}\) which is consistent with experiment. Within the current theory and experimental errors, this provides a highly nontrivial consistency check on how we treat \(D\) semileptonic and leptonic decays on the lattice and more generally in the Standard Model.

The calculations of this article can be improved upon and extended in several ways. The largest errors in Table \[7\] from statistics and continuum extrapolations can be reduced straightforwardly by working with more gauge configurations and time sources and at more values of the lattice spacing. An obvious extension of the current study is to investigate \(D \to \pi\) semileptonic decays and determine \(|V_{ud}|\). Work on this project has already begun. In a future project we also plan to calculate the vector current hadronic matrix elements \(\langle K(\pi)\rangle |V_c|D\rangle\). This will provide \(f_+(q^2)\) as a function of \(q^2\). As mentioned in section II we will be carrying out nonperturbative matching of the vector current based on PCVC for this project.

\section*{Acknowledgements}

We thank the MILC collaboration for making their Asq-Tad \(N_f = 2 + 1\) configurations available. This work was supported in part by the DOE and NSF in the US and
TABLE VIII: A sample set of the priors and prior widths for ensemble F1 with $\tilde{p} = (0, 0, 0)$ and $\tilde{p} = (1, 1, 0)$. We have tested with various priors and prior widths, and the fit results are not sensitive to reasonable variations. Note that $i = 1, 2, 3, \ldots$ and $j, k = 0, 1, 2, \ldots$.

| Prior width $\tilde{p} = (0, 0, 0)$ | Prior width $\tilde{p} = (1, 1, 0)$ |
|-----------------------------------|-----------------------------------|
| $A_{jk}$                          | 0.01                              | 0.01                              |
| $B_{jk}$                          | 0.01                              | 0.01                              |
| $C_{jk}$                          | 0.01                              | 0.01                              |
| $D_{jk}$                          | 0.01                              | 0.01                              |
| $E_{0}^{2}$                       | 0.815 $\pm 0.048$                | 0.8 $\pm 0.6$                    |
| $E_{i}^{1} - E_{i-1}^{1}$         | 0.12                              | 0.015                             |
| $b_{0}^{2}$                       | 0.1                                | 0.03                              |
| $d_{0}^{2}$                       | 0.01                               | 0.0028                           |
| $E_{K}^{2}$                       | 0.23 $\pm 0.12$                   | 0.39 $\pm 0.03$                  |
| $E_{i}^{1} - E_{i-1}^{1}$         | 0.5                                | 0.4                               |
| $b_{K}^{2}$                       | 0.15 $\pm 0.25$                   | 0.1                               |
| $E_{K}^{2}$                       | 0.4 $\pm 0.4$                     | 0.53 $\pm 0.05$                  |
| $E_{i}^{1} - E_{i-1}^{1}$         | 0.5                                | 0.4                               |
| $d_{K}^{2}$                       | 0.01                               | 0.001                             |

by STFC in the UK. Computations were carried out at the Ohio Supercomputer Center and on facilities of the USQCD collaboration funded by the Office of Science of the U.S. DOE.

Appendix A: Priors and Prior Widths for Section V

We list a sample set of priors and prior widths in Table VIII that have been used for the simultaneous fits to $C_{2pm}^{1}$, $C_{2pm}^{2}$, and three of the three-point correlators with $T = 19, 20$, and $23$ for ensemble F1. The fit ansatz and results have been presented in Section V.

Appendix B: Bayesian Fits in Section VI

From [23] - [25], one sees that the chiral/continuum extrapolation ansatz for $f_0(q^2)$ starts out with 23 basic fit parameters $c_n$, $n = 1, 2, \ldots, 23$.

$$c_i : a_0, a_1, a_2, b_1, b_2, c_1, c_2, c_3, d_1, e_1, f_1,$$

where $i = 0, 1, \text{and} 2$. In a Bayesian fit each of these fit parameters will have its own prior $\sigma_n$ and prior width $\sigma_n$, which we call “Group I.” Our choices for these priors will be discussed below. Our fit ansatz for $f_0$ includes in addition to the fit parameters $c_n$ also many input parameters such as $M_D, E_{K}, r_1$ etc. all of which have some uncertainty associated with them. Ref. [23] describes a method to include effects coming from these types of uncertainties into the final error in the extrapolated value for $f_0$. What one does is convert all these input parameters into additional fit parameters with priors and prior widths given by their known central values and errors. Using this approach we have changed 61 input parameters into new fit parameters $p_j$, $j = 1, 2, \ldots, 61$, which we call “Group II.”

$$p_j : (\frac{p_j}{a})^i, aM_D^i, aE_{K}^{i}(\tilde{p}), aM_{\pi}^i, aM_{\pi}^i, (aM_{K}^{asqtad})^i, (aM_{K}^{asqtad})^i, M_{D}^{2}, M_{D}^{2}, M_{D}^{2}, M_{D}^{2}.$$ (B2)

where $i = 1, 2, \ldots, 5$ goes over the 5 ensembles. The use of Group II parameters is a very efficient way to include errors coming from uncertainties in input parameters into our final total error. An alternative approach would require visiting each input parameter in turn, redoing the chiral/continuum extrapolation and coming up with an estimate for the systematic error coming from this input parameter. In our approach no additional systematic errors for these input parameters are called for and the effects from their uncertainties are included in the extrapolation error. For instance, this is very helpful to include the error from $E_{K}^{2}$. In Fig. [10] and [11] there are errors for $E_{K}^{2}$ on the lattice data as well as the extrapolated results, and estimating these errors is not a trivial task. However, introducing the Group II parameters incorporates all $E_{K}^{2}$ errors as part of the final vertical error.

In Bayesian fits one minimizes the augmented chi-squared,

$$\chi^2_{\text{aug}} = \chi^2_{\text{traditional}} + \chi^2_{\text{Group I}} + \chi^2_{\text{Group II}}$$

$$\chi^2_{\text{traditional}} = \sum_{i=1}^{20} \frac{(f_i^1 - f_0(\text{ansatz}))^2}{(\sigma_{f_i})^2}$$

$$\chi^2_{\text{Group I}} = \sum_{n=1}^{23} \frac{(c_n - \tau_n)^2}{\sigma_n^2}$$

$$\chi^2_{\text{Group II}} = \sum_{j=1}^{61} \frac{(p_j - \tau_j)^2}{\sigma_j^2}$$

When carrying out the chiral/continuum extrapolations we have expressed all dimensionful quantities in units of GeV. We give the set of priors and prior widths for the Group I parameters $c_n$ in Table X and for the Group II parameters $p_j$ in Table XI.

Setting priors and prior widths is straightforward. For Group I, the quark mass terms, such as $x_1$ and $x_2$, are normalized by the scale, $\Lambda \equiv 4\pi f_\pi$. Therefore, it is natural
| Group I | prior width | fit result | fit error |
|---------|-------------|------------|-----------|
| $a_0$   | 0 1         | 0.09766    | 0.0029    |
| $a_1$   | 0 1         | 0.08999    | 0.02      |
| $a_2$   | 0 1         | -0.07044   | 0.11      |
| $b_1$   | 0 0.3       | 0.03775    | 0.13      |
| $b_2$   | 0 0.3       | 0.07179    | 0.17      |
| $c_1^0$ | 0 1         | -0.52596   | 0.31      |
| $c_1^1$ | 0 1         | -0.19051   | 0.82      |
| $c_1^2$ | 0 1         | 0.02877    | 1         |
| $c_2^0$ | 0 1         | -0.09919   | 0.98      |
| $c_2^1$ | 0 1         | 0.00827    | 1         |
| $c_2^2$ | 0 1         | 0.00044    | 0.1       |
| $c_3^0$ | 0 1         | -0.02897   | 0.24      |
| $c_3^1$ | 0 1         | 0.32804    | 0.66      |
| $c_3^2$ | 0 1         | -0.03116   | 0.1       |
| $d_0$   | 0 0.3       | 0.00966    | 0.11      |
| $d_1$   | 0 0.3       | 0.01769    | 0.29      |
| $d_2$   | 0 0.3       | 0.00541    | 0.3       |
| $e_0$   | 0 0.2       | 0.01554    | 0.19      |
| $e_1$   | 0 0.2       | 0.00447    | 0.2       |
| $e_2$   | 0 0.2       | 0.00131    | 0.2       |
| $f_0$   | 0 0.3       | -0.10860   | 0.28      |
| $f_1$   | 0 0.3       | -0.00474   | 0.3       |
| $f_2$   | 0 0.3       | 0.00105    | 0.3       |

TABLE IX: Priors and prior width of the Group I parameters for the simultaneous modified z-expansion extrapolation fit

that we expect that the parameters vary between $-1$ to $1$. However, we know from other lattice calculations with the same gauge configurations and our lattice data that the sea quark mass contribution is smaller than that of valence quark. Thus, we take the priors and prior widths for the sea quark mass terms as $f_i = 0 \pm 0.3$. The leading heavy quark error is proportional to $\mathcal{O}(a_s(a_m c_i)^2)$ so we use $d_j = 0 \pm 0.3$ for the $(a m_c)^2$ terms. For the purposes of setting priors, we conservatively do not include a factor of $v^2/c^2$ here. On the other hand for the $(a m_c)^4$ terms we do take the expected factor of $v^2/c^2$ into account and choose $e_i = 0 \pm 0.2$. Similarly we use $b_j = 0 \pm 0.3$ for the $(a E_k^2)$ and $(a E_k^4)$ terms. This reflects a factor of $a_s$ for the $(a E_k^4)$ terms and the fact that higher powers of $(a p^?)$ typically come with smaller numerical factors relative to lower powers (such as in an expansion of $\frac{1}{2} \sinh(aE)$). For Group II, we use lattice results and experiments that we described in the text for the priors and prior widths.

As we stated above, all sources of systematic errors are already included in the fit ansatz, except the finite volume and charm quark mass tuning errors. We can consider the total error squared, $\sigma^2$, as a linear combina-

| Group II | prior width | fit result | fit error |
|----------|-------------|------------|-----------|
| $r_1$    | 0.3133      | 0.0023     | 0.313285  | 0.0023 |
| $M_{bc}^{phys}$ | 0.6858    | 0.0004     | 0.685799  | 0.0004 |
| $M_{bc}^{phys}$ | 0.1373    | 0.0023     | 0.1373    | 0.0023 |
| $M_{b}^{phys}$ | 1.8645     | 0.0004     | 1.8645    | 0.0004 |
| $M_{b}^{phys}$ | 0.4937     | 0.00016    | 0.4937    | 0.00016 |
| $M_{K}^{phys}$ | 2.3173     | 0.0006    | 2.3173    | 0.0006 |

TABLE X: Priors and prior width of the Group II parameters for the simultaneous modified z-expansion extrapolation fit. Parameters with five rows correspond to that on the five ensembles, C1, C2, C3, F1, and F2. |
TABLE XI: (Continued) Priors and prior width of the Group II parameters for the simultaneous modified z-expansion extrapolation fit. Parameters with five rows correspond to that on the five ensembles, C1, C2, C3, F1, and F2. We quote $M_{K_{\pi}q^4\text{ud}}$ and $M_{\pi q^4\text{ud}}$ from ref. [22].

| Group II | prior width | fit result | fit error |
|----------|-------------|------------|------------|
| $aM_{K_{\pi}q^4\text{ud}}$ | 0.3653 | 0.365304 | 0.00029 |
| $aM_{\pi q^4\text{ud}}$ | 0.1971 | 0.197174 | 0.00021 |
| $M_{D_{0}^+}$ | 2.32897 | 2.32897 | 0.00005 |

The chiral logs are contained in $\delta f$, the first term is for Group I ($c_n$), and the second term is for Group II ($p_j$). We actually calculate the contributions from each source, $C_{e_n}e_n^2$ and $C_{p_j}p_j$ using the method presented in [23], and they add up to the total error $\sigma^2$. We group together appropriate parameters, and list them in Table VII.

Appendix C: Chiral and Continuum Extrapolations based on Chiral Perturbation Theory

In this Appendix we carry out further consistency tests of the chiral/continuum extrapolation of section VI by working with a completely independent fit ansatz. We will use the partially quenched chiral perturbation theory (PQChPT) formulas developed in Refs. [16, 17] augmented by terms parameterizing discretization effects and $E_K$ dependence.

Heavy meson ChPT formulas are organized through form factors $f_{\parallel}$ and $f_{\perp}$ in terms of which $f_0(q^2)$ is given by,

$$f_0(q^2) = \frac{\sqrt{2M_D}}{M_D - M_K} \left[ (M_D - M_K) f_{\parallel} + (E_K^+ - M_K^+) f_{\perp} \right].$$  \hspace{1cm} (C1)

We follow very closely the approach and notation of Ref. [17], however with all the taste breaking effects turned off. $f_{\parallel}$ and $f_{\perp}$ are parameterized as,

$$f_{\parallel} = \frac{K}{f_{\pi}} \left[ 1 + \delta f_{\parallel} + c_{l}^\parallel m_l + c_{\gamma}^\parallel m_\gamma + c_{\text{sea}}^\parallel (2m_u + m_s + h_{\parallel}(E_K)^2) \right] (1 + c_0(am_\gamma)^2)$$  \hspace{1cm} (C2)

$$f_{\perp} = \frac{K}{f_{\pi}} \left[ 1 + \delta f_{\perp} + c_{l}^\perp m_l + c_{\gamma}^\perp m_\gamma + c_{\text{sea}}^\perp (2m_u + m_s + h_{\perp}(E_K)^2) \right] (1 + c_0(am_\gamma)^2 + c_1(am_\gamma)^4).$$  \hspace{1cm} (C3)

The chiral logs are contained in $\delta f_{\parallel}$, $\delta f_{\perp}$ and $D$. We give their explicit expressions in Appendix D. $m_l$ and $m_\gamma$ are valence and $m_u$ and $m_s$ the sea quark masses. $g_{\pi}$ is the $DD^*\pi$ coupling and $\Delta^*$ the $D^* - D$ mass splitting. $h_{\parallel}(E_K)$ and $h_{\perp}(E_K)$ are unknown functions of $E_K$. We will use polynomial expansions for them. $h_{\parallel}\perp(E_K) = c_{l\perp}^{\parallel,\perp} E_K + c_{\gamma}^{\parallel,\perp} E_K^2 + \ldots$. The first two terms are motivated by ChPT [17], however we view $h_{\parallel}\perp(E_K)$ as potentially parameterizing $f_0$ more generally, even beyond the regime of small $E_K$ where ChPT is assumed valid. Our data is fit very well ($\chi^2/\text{dof}=0.48$), however, all the way to $E_K \approx 1$GeV keeping just terms through $O(E_K^2)$ in $h_{\parallel}$ and $h_{\perp}$. Figs. 28 and 29 show results from a simultaneous fit to all our data points using the ChPT ansatz. These should be compared to Figs. 16 and 17 from the modified z-expansion ansatz.

In Fig. 30 we compare $f_0(q^2)$ in the physical limit coming from the z-expansion extrapolation of section VI and the ChPT extrapolation of this Appendix over the entire physical $q^2$ range. And in Fig. 31 we compare results at...
makes do with just a simple logx term. 

In this appendix we summarize partially quenched ChPT (PQChPT) expressions for the chiral logarithm terms \( \delta f_{\parallel}, \delta f_\perp \) and \( D \) that we employ in eqs. (C2) and (C3). The formulas for PQChPT in continuum QCD for heavy-to-light semileptonic decays were first developed in Ref.[16] for degenerate sea quarks. Ref.[17] generalized these results to nondegenerate 1+1+1 sea quarks and also to Staggered ChPT. We have started from the 1+1+1 continuum PQChPT expressions given in Ref.[17] for individual diagrams and for the \( D \) and kaon wave function renormalizations to obtain the full \( \delta f_{\parallel, \perp} \) in the 2+1 PQChPT case. For the convenience of the reader we give these reconstructed expressions below. We use the same notation as in Ref.[17]. “\( x \)" and “\( y \)" stand for the light valence quarks in the daughter meson (for the kaon \( x = l \) and \( y = s' \)) and “\( u \)" and “\( s \)" denote sea light and strange quarks. Furthermore \( m_{ab} \) is the mass of the pseudoscalar meson with quark content \( a \) and \( b \) and \( m_0^2 = \frac{1}{3}(m_{uu}^2 + m_{ss}^2) \).

\[
(4\pi f)^2 \delta f_{\parallel}^{D \rightarrow K} = \\
\left\{ \left[ I_1(m_{yu}) + \frac{1}{2} I_1(m_{ys}) \right] - 3g_\pi^2 \left[ I_1(m_{xu}) + \frac{1}{2} I_1(m_{xs}) \right] \right\} + [2I_2(m_{yu}) + I_2(m_{ys})] + \left[ \frac{1}{3} \left[ R^{[3,2]}_x(m_{xx}) (I_1(m_{xx}) + I_2(m_{xx})) + R^{[3,2]}_y(m_{yy}) (I_1(m_{yy}) + I_2(m_{yy})) + R^{[3,2]}_y(m_{yy}) (I_1(m_{yy}) + I_2(m_{yy})) \right] \right] + \left[ \frac{1}{6} \left[ DR^{[2,2]}(m_{yy}; I_1) \right] - 3g_\pi^2 \left[ DR^{[2,2]}(m_{xx}; I_1) \right] \right]
\]

\( q^2 = 0 \) for each ensemble and in the physical limit. One sees that the two extrapolations are nicely consistent with each other. We believe the consistency check of this Appendix has been very useful. It provides further support for the results of the \( z \)-expansion extrapolation and indicates that errors there were not underestimated. Note that the ChPT ansatz includes all the complicated chiral logs of Appendix D, whereas the \( z \)-expansion ansatz makes do with just a simple \( x \log x \) term.
\[ \begin{align*}
+ \frac{1}{3} \left[ DR^{[2,2]}(m_{yy}; I_2) \right] \\
(4\pi f)^2 \delta f^{D \to K}_{1} &= \\
\left\{ - I_1(m_{yu}) + \frac{1}{2} I_1(m_{ys}) - 3g_2^2 \left[ I_1(m_{xx}) + \frac{1}{2} I_1(m_{xs}) \right] \right. \\
& \left. - \frac{g_2^2}{3} \left[ R_y^{[3,2]}(m_{yy}) K_1(m_{xx}) + R_y^{[3,2]}(m_{yy}) K_1(m_{ys}) \right] \right. \\
& \left. - \frac{1}{6} \left[ DR^{[2,2]}(m_{yy}; I_1) - 3g_2^2 \frac{2}{6} \left[ DR^{[2,2]}(m_{xx}; I_1) \right] \right] \right\} \\
(4\pi f)^2 D^{D \to K} &= -3g_2^2 (v \cdot p) \times \\
\left\{ 2K_1(m_{yu}) + K_1(m_{ys}) \right\} + \frac{1}{3} \left[ DR^{[2,2]}(m_{yy}; I_1) \right] \\
\end{align*} \]

In the $D$ meson rest frame $v \cdot p = E_K$. Furthermore one has,

\[ I_1(m) = m^2 \log \frac{m^2}{\Lambda^2} \]

\[ I_2(m) = -2(v \cdot p)^2 \log \frac{m^2}{\Lambda^2} - 4(v \cdot p)^2 F \left( \frac{m}{v \cdot p} \right) + 2(v \cdot p)^2 \]

with

\[ F(x) = \begin{cases} 
\sqrt{1 - x^2} \tanh^{-1}(\sqrt{1 - x^2}) & 0 \leq x \leq 1 \\
-\sqrt{x^2 - 1} \tan^{-1}(\sqrt{x^2 - 1}) & x > 1 
\end{cases} \]

\[ K_1(m) = \left[ -m^2 + \frac{2}{3} (v \cdot p)^2 \right] \log \frac{m^2}{\Lambda^2} + \frac{4}{3} [(v \cdot p)^2 - m^2] \]

\[ + F \left( \frac{m}{v \cdot p} \right) - \frac{10}{9} (v \cdot p)^2 + \frac{4}{3} m^2 - \frac{2}{3} \frac{m^3}{v \cdot p} \]

\[ R_y^{[3,2]}(m) = \frac{(m^2_{uu} - m^2)(m^2_{ss} - m^2)}{(m^2_{yy} - m^2)(m^2_{yy} - m^2)} \]

\[ R_y^{[3,2]}(m) = \frac{(m^2_{uu} - m^2)(m^2_{ss} - m^2)}{(m^2_{yy} - m^2)(m^2_{yy} - m^2)} I(m) \]

\[ R_y^{[3,2]}(m) = \frac{(m^2_{uu} - m^2)(m^2_{ss} - m^2)}{(m^2_{yy} - m^2)(m^2_{yy} - m^2)} I(m) \]

We refer the reader to the original literature [16, 17] for further details. Here, for completeness, we give partially quenched formulas for the chiral logarithms in $D \to \pi$ decays. They will be used shortly in our own studies of $D \to \pi, \ell \nu$ decays. Some care is required in taking the $y \to x$ limit of (D11), (D2) and (D3), however in the end expressions simpler for $D \to \pi$ than for $D \to K$.

\[ (4\pi f)^2 \delta f^{D \to \pi}_{1} = \]

\[ \left\{ (1 - 3g_2^2) \left[ I_1(m_{xx}) \right] + \frac{1}{2} I_1(m_{xs}) \right\} + \frac{2}{6} \left[ DR^{[2,2]}(m_{xx}; I_1) \right] \]

\[ (4\pi f)^2 \delta f^{D \to \pi}_{1} = \]

\[ \left\{ -(1 - 3g_2^2) \left[ I_1(m_{xx}) \right] + \frac{1}{2} I_1(m_{xs}) \right\} + \frac{g_2^2}{3} \left[ DR^{[2,2]}(m_{xx}; K_1) \right] - \frac{1}{6} \frac{3g_2^2}{6} \left[ DR^{[2,2]}(m_{xx}; K_1) \right] \]

\[ (4\pi f)^2 D^{D \to \pi} = -3g_2^2 (v \cdot p) \times \\
\left\{ 2K_1(m_{yu}) + K_1(m_{ys}) \right\} + \frac{1}{3} \left[ DR^{[2,2]}(m_{xx}; K_1) \right] \]

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