Abstract Using partially twisted boundary conditions we compute the $K \rightarrow \pi$ semi-leptonic form factors in the range of momentum transfers $0 \lesssim q^2 \leq q_{\text{max}}^2 = (m_K - m_\pi)^2$ in lattice QCD with $N_f = 2 + 1$ dynamical quark flavours. In this way we are able to determine $f_{+}^{K\pi}(0)$ without any interpolation in the momentum transfer, thus eliminating one source of systematic error. This study confirms our earlier phenomenological ansatz for the strange quark mass dependence of the scalar form factor. We identify and estimate potentially significant NNLO effects in the chiral expansion that guides the extrapolation of the data to the physical point. Our main result is $f_{+}^{K\pi}(0) = 0.9599(34)(^{33}_{-47})(14)$, where the first error is statistical, the second error is due to the uncertainties in the chiral extrapolation of the lattice data and the last error is an estimate of potential discretisation effects.

1 Introduction

The last five years have seen tremendous progress in high precision calculations from first principles of the $K \rightarrow \pi$ semi-leptonic vector form factor at vanishing momentum transfer, $f_{+}^{K\pi}(0)$. The results are combined with precise experimental measurements of $|f_{+}^{K\pi}(0)V_{us}|$ to obtain the CKM matrix element $V_{us}$. It has been shown in many numerical studies [1–7] that the observable $f_{+}^{K\pi}(0)$ can be computed with sub-percent level of precision on the lattice. All common efforts take advantage of the fact that the lattice prediction is necessarily unity in the $SU(3)$ limit in which $m_\pi^2 = m_K^2/4$. Thus leading lattice errors on the form factor are proportional to the mass difference and apply to the difference of the form factor from unity $f_{+}^{K\pi}(0) - 1 = \Delta f + f_2$, where $f_2$ is the analytically known $O(m_\pi^2, m_K^2, m_\pi^2)$ contribution to the form factor in $SU(3)$ chiral perturbation theory [8, 9]. The precision of current lattice computations is well represented by the result of the RBC-UKQCD collaboration [6],

\[ \Delta f = -0.0129(33)_{\text{stat}}(34)_{q^2,\chi}(14)_{a}. \] (1)

The first error is statistical, the second is due in approximately equal parts to the chiral extrapolation and to an interpolation in the momentum transfer $q^2$ and the final error is due to cut-off effects.

The primary purpose of this work is to remove completely the systematic error in $f_{+}^{K\pi}(0)$ due to the $q^2$-interpolation at the lightest quark masses. In addition we study in more detail the ansatz for the chiral extrapolation which was used to obtain the above result (1). To this end we build on our previous work on the $q^2$-dependence of meson form factors and stochastic quark propagators [10–12]. The chiral extrapolation error above includes a contribution from using a simulated strange quark which is a little heavier than the physical one. Here we confirm this estimate with new simulation results which allow us to interpolate directly in the valence strange quark mass. We also discuss phenomenological fits based on NLO $SU(2)$ [13] and on $SU(3)$ [8, 9] chiral perturbation theory for the vector form factor and we discuss potentially significant NNLO effects.

Our results reinforce the RBC-UKQCD collaboration’s computation of $f_{+}^{K\pi}(0)$ which constitutes a crucial input to precision tests of the Standard Model and for constraining its possible extensions [14]. The results presented should be interpreted as an intermediate step towards the extension of the RBC-UKQCD collaboration’s effort towards simulations at smaller quark masses and at a smaller lattice spacing which are under way.

After a brief discussion of the computational setup and a comparison of our current strategy with the conventional one, we summarise and discuss our results.
2 Strategy

The matrix element of the vector current between initial and final states consisting of pseudo-scalar mesons \( P_i \) and \( P_f \) respectively, is in general decomposed into two invariant form factors which parameterise non-perturbative effects,

\[
\langle P_f (p_f) | V_\mu | P_i (p_i) \rangle = f_+^{P_f, P_i} (q^2) (p_i + p_f)_\mu + f_-^{P_f, P_i} (q^2) (p_i - p_f)_\mu ,
\]

where \( q = p_f - p_i \) is the momentum transfer. For \( K \to \pi \) semi-leptonic decays \( V_\mu \) is the weak current \( \bar{q} \gamma_\mu u \), \( P_i = K \) and \( P_f = \pi \). We also introduce the scalar form factor

\[
f_0^{K\pi} (q^2) = f_+^{K\pi} (q^2) \frac{q^2}{m_K^2 - m_\pi^2} f_0^{K\pi} (q^2),
\]

which satisfies \( f_0^{K\pi} (0) = f_+^{K\pi} (0) \). In this paper we are primarily interested in computing \( f_+^{K\pi} (q^2) \) for \( q^2 = 0 \) but we also present new results for other values of \( q^2 \). In contrast to previous calculations of the form factor in lattice QCD [1–7] we simulate directly at \( q^2 = 0 \) by using partially twisted boundary conditions [15, 16]. One combines gauge field configurations generated with sea quarks obeying periodic boundary conditions with valence quarks with twisted boundary conditions [15–24], i.e. the valence quarks satisfy

\[
\psi (x_k + L) = e^{i\theta_k} \psi (x_k) \quad (k = 1, 2, 3),
\]

where \( \psi \) is either a strange quark \( s \) or it represents one of the degenerate up or down quarks \( q \). The dispersion relation for a meson in a finite volume projected onto Fourier momentum \( p_{FT} \) then takes the form [18, 20],

\[
E = \sqrt{m^2 + (p_{FT} + \Delta \theta)^2},
\]

where \( m \) is the meson mass and where \( \Delta \theta \) is the difference between the twist angles of the two valence quarks.

In [10] we showed how this technique can be used to extract meson transition matrix elements at arbitrary values of the momentum transfer. In particular, for the matrix element with the valence quark flow diagram as in Fig. 1 with the initial and the final meson carrying 3-momenta \( p_i = p_{FT,i} + \theta_i / L \) and \( p_f = p_{FT,f} + \theta_f / L \), respectively, the momentum transfer between the initial and the final state meson is

\[
q^2 = (p_i - p_f)^2 = (E_i(p_i) - E_f(p_f))^2 - (p_i - p_f)^2.
\]

In our study it will be sufficient to set the twist of the spectator (anti-)quark \( q_3 \) to zero so that it satisfies periodic boundary conditions.

As will become clear below, the matrix element in (2) can be extracted from the time-dependence of combinations of Euclidean two- and three-point correlation functions which can be computed straightforwardly in lattice QCD. The two-point function is defined by

\[
C_i (t_f, p_i) = \sum_x e^{i p_i x} \langle O_i (t_f, x) O_i^\dagger (0, 0) \rangle
\]

\[
= \frac{|Z_i|^2}{2E_i} (e^{-E_i t_f} + e^{-E_i (T-t_f)}),
\]

where \( i = \pi \) or \( K \), and where \( O_i \) are pseudo-scalar interpolating operators for the corresponding mesons \( O_\pi = \bar{q} \gamma_5 q \) and \( O_K = \bar{s} \gamma_5 q \) and we assume that \( t \) and \( T - t \) (where \( T \) is the temporal extent of the lattice) are sufficiently large that the correlation function is dominated by the lightest state (i.e. the pion or kaon). The constants \( Z_i \) are given by

\[
Z_i = \langle P_i | O_i^\dagger (0, 0) | 0 \rangle.
\]

The three-point functions are defined by

\[
C_{P_i P_f} (t_f, t_i, t_f, p_i, p_f)
\]

\[
= Z_V \sum_{x_f} e^{i p_f (x_f - x)} e^{i p_i x} \langle O_f (t_f, x_f) V_\mu (t, x) O_i^\dagger (t_i, 0) \rangle
\]

\[
= Z_V \frac{Z_f Z_i}{4E_f E_i} \langle P_f (p_f) | V_\mu (0) \rangle \langle P_i (p_i) \rangle
\]

\[
\times \left\{ \theta (t_f - t_i) e^{-E_i (t_i - t_f)} e^{-E_f (t_i - t_f)}
\right.
\]

\[
+ c_{\mu} \theta (t_f - t_i) e^{-E_f (T + t_f - t_i)} e^{-E_i (t_i - t_f)} \right\},
\]

where \( P_i, f \) is a pion or a kaon, \( V_\mu \) is the vector current with flavour quantum numbers to allow the \( P_i \to P_f \) transition and we have defined \( Z_f = \langle 0 | O_f (0, 0) | P_f \rangle \). We have introduced the constant \( c_{\mu} \) which is \( c_0 = -1 \) (time-direction) and \( c_i = +1 \) for \( i = 1, 2, 3 \). Again we assume that all the time intervals are sufficiently large for the lightest hadrons to give the dominant contribution.

The vector current renormalisation factor \( Z_V \) can be obtained as follows. For illustration we take \( 0 < t < t_f < T/2 \), in which case \( Z_V \) is defined by

\[
Z_V = \frac{\tilde{C}_\pi (t_f, 0)}{C_\pi^{-(B,)} (t_i, t_f, 0, 0)}.
\]

In the numerator we use the function \( \tilde{C}_\pi (t, p) = C_\pi (t, p) - |Z_\pi|^2 e^{-E_\pi (T-t)} \) where \( Z_\pi \) and \( E_\pi \) are determined from fits to \( C_\pi (t, 0) \) and using (5) for \( t_f = T/2 \) it is natural instead to use \( \tilde{C}_\pi (t, p) = \frac{1}{2} C_\pi (t, p) \) in (9)). The superscript \( B \) in
the denominator indicates that we take the bare (unrenormalised) current in the three-point function.

In the following we drop the labels \( t_i \) and \( t_f \) (since they are fixed) and we combine the two- and three-point functions into the ratios

\[
P^{(\mu)}_{1,P_1P_f}(p_i, p_f) = \frac{C^{(\mu)}_{P_1P_f}(t, p_i, p_f) C^{(\mu)}_{P_fP_1}(t, p_f, p_i)}{\tilde{C}_{P_1}(t_f, p_i) \tilde{C}_{P_f}(t_f, p_f)},
\]

\[
P^{(\mu)}_{3,P_1P_f}(p_i, p_f) = \frac{C^{(\mu)}_{P_1P_f}(t, p_i, p_f)}{\tilde{C}_{P_f}(t_f, p_f)} \times \frac{C_{P_1}(t_f - t, p_i) C_{P_f}(t, p_f) \tilde{C}_{P_f}(t_f, p_f)}{C_{P_f}(t_f - t, p_f) C_{P_1}(t, p_i) \tilde{C}_{P_1}(t_f, p_i)},
\]  

where \( \mathcal{N} = 4Z \sqrt{E_i E_f} \) and the ratios are constructed such that

\[
P^{(\mu)}_{\alpha,P_1P_f}(p_i, p_f) = \int_{-\pi}^{\pi} (q^2) (p_i + p_f) \mu + \int_{-\pi}^{\pi} (q^2) (p_i - p_f) \mu,
\]  

for \( \alpha = 1, 3 \). For the ratios we use the naming convention of [10] but we have not made use of ratio \( R_2 \).  

Once these ratios have been computed for some choices for \( p_i \) and \( p_f \) while keeping \( q^2 \) constant (of course we are particularly interested in \( q^2 = 0 \)) the form factors \( f^{K\pi}_+(q^2) \) and \( f^{K\pi}_-(q^2) \) can be obtained as the solutions of the corresponding system of linear equations.

### 3 Simulation parameters

We simulate with \( N_f = 2 + 1 \) dynamical flavours generated with the Iwasaki gauge action [25, 26] at \( \beta = 2.13 \), which corresponds to an inverse lattice spacing \( a^{-1} = 1.73 \) GeV \( (a = 0.114(2) \) fm) [27, 28], and the domain wall fermion action [29, 30] with a residual mass of \( am_{\text{res}} = 0.00315(2) \) [27]. The simulated strange sea quark mass, \( am_{\text{sea}} = 0.04,^2 \) is close to its physical value [28], and here we choose the RBC-UKQCD configurations with the bare light sea quark mass \( am_{\text{sea}} = 0.005 \), which corresponds to a pion mass of 330 MeV [27, 28]. The calculations are performed on a lattice volume of \( 24^3 \times 64 \) sites with the fifth dimension having an extension of 16 lattice points. More details can be found in [28].

We distinguish three sets of correlation functions as summarised in Table 1. The correlation functions in set P4 (point source, 4 positions of the source) are identical to those on which the RBC-UKQCD prediction for \( f^{K\pi}_+(0) \) at \( am_q = 0.005 \) in [6] is based. The naming convention for the remaining two data sets, \( Z4PSs4 \) and \( Z4PSs3 \), is motivated as follows: spin-diluted \( \mathbb{Z}(2) \times \mathbb{Z}(2) \) [11, 12] noise source and point sink with strange quark mass \( am_s = 0.04 \) and \( am_s = 0.03, \) respectively. The data set \( Z4PSs4 \) with light quark mass \( am_q = 0.005 \) corresponds to a unitary simulation point, i.e. where the sea and valence quark masses are the same, while set \( Z4PSs3 \) corresponds to a partially quenched parameter choice. For \( Z4PSs3 \) and \( Z4PSs4 \) we started the measurement chains for eight different source time-slices. In each case we measured on every 40th trajectory and averaged the correlation functions over the chains into bins of eight. The correlation functions obtained in this way were computed with zero Fourier momentum and the momenta of the initial and/or final kaon/pion were induced by twisting one of the kaon’s and/or pion’s valence quarks. For each measurement we applied the full twist along one of the spatial directions. We changed this direction frequently as the measurements proceeded in order to reduce the correlations. Our choices for the twisting angles for \( Z4PSs4 \) and \( Z4PSs3 \) and the corresponding values of \( q^2 \) are summarised in Table 2. In order to obtain \( q^2 = 0 \) we make the following two choices of the twisting angles [10]:

\[
|\theta_K| = L \sqrt{\left( \frac{m_K^2 + m_\pi^2}{2m_\pi} \right)^2 - m_K^2} \quad \text{and} \quad \theta_\pi = 0, \quad \text{and} \quad |\theta_\pi| = L \sqrt{\left( \frac{m_K^2 + m_\pi^2}{2m_K} \right)^2 - m_\pi^2} \quad \text{and} \quad \theta_K = 0.
\]

As input to these formulae we have used the estimates for the central values of the kaon masses \( am_k = 0.2990 \) (\( Z4PS3 \)) and \( am_k = 0.3328 \) (\( Z4PS4 \)) and for the pion mass \( am_\pi = 0.1907 \) (for both data sets). These values had been determined from a previous study of the gauge field ensemble considered here. The momenta of the mesons are given by \( p_K = \theta_K/L \) and \( p_\pi = \theta_\pi/L. \) In addition to the values of \( \theta_\pi \) and \( \theta_K \) in (12), propagators were generated for other values of the twisting angle. In particular, for the kinematical situation where the kaon is at rest and the pion is moving

| Table 1 Some basic simulation parameters |
|-----------------|-------------------|-------------------|
|                 | P4                | Z4PSs4            | Z4PSs3            |
| \( am_q \)      | 0.04              | 0.04              | 0.03              |
| \# meas         | 700               | 1180              | 1180              |
| \# sources      | 4                 | 8                 | 8                 |

---

1We did not generate data for \( C^{(\mu)}_{P_iP_f}(t, p, p) \)\( \mu = 0 \) for \( P = \pi, \ K \) from which the forward matrix elements \( (P|V_\mu|P) \) relevant for the construction of \( R_2 \) can be extracted.

2When not indicated explicitly by the label ‘sea’ we always mean the valence quark mass.
due to the additional ad hoc twist angle \( \theta_\pi = 1.600 \) we determined the corresponding values for \( \theta_K \) which yield the same \( q^2 \) also when the pion is at rest. The contractions of these propagators into two- and three-point functions allow a computation of \( f_{K\pi}^+(q^2) \) for additional values of the momentum transfer in the range from about \( q^2 = 0 \) to \( q^2_{\text{max}} \) (cf. Table 2).

4 Data analysis

The results for the two- and three-point correlation functions for \( P4, Z4PSs \) and \( Z4PSs \) were analysed using the jack-knife as well as the boot-strap procedure. In all cases covariance matrices for the correlation functions and ratios \( R_1 \) and \( R_3 \) were generated in order to be used for the fits (frozen covariance matrix). Unfreezing the covariance matrix, i.e. using the covariance matrix computed individually for each jack-knife or boot-strap sample destabilised the fits. We interpret this as a reflection of the fact that we have an insufficient set of measurements and that the fluctuations of the covariance matrix are therefore large. We found that the results we get with the frozen covariance matrix agree within (similar) errors with the results we would get when neglecting any correlations.

We found that for the spatial component of the vector current in the three-point function, i.e. for \( R_1^{(i)} \) and \( R_3^{(i)} \), the plateaus are of comparable quality (cf. Fig. 2)—in the analysis we opted to use \( R_3^{(i)} \). For the time-component however in the cases where only one of the initial and final states carries a twist the quality of the ratios varies. Here we decided to use \( R_1^{(0)} \) for the case where only the pion carries the twist and \( R_3^{(0)} \) in all other cases (cf. Fig. 2).

Table 2 summarises the kinematical points which we analysed. The kaon masses for the full statistics of \( Z4PSs \) and \( Z4PSs4 \) turn out to be \( am_K = 0.2987(4) \) and \( am_K = 0.3327(4) \), respectively and the pion mass in both cases is \( am_\pi = 0.1903(4) \). From the table we see that there are degeneracies in \( q^2 \), i.e. we have data for the same \( q^2 \) but from three-point functions with different kinematical parameters for the kaon and pion. In the analysis we first compute the corresponding ratios \( R_1 \) and \( R_3 \) and then average them as indicated by the degeneracy.

\[ \text{Table 2: Table of twisting angles used in this study, together with the corresponding values of } q^2 \text{ and the results for the form factors} \]

\[ \begin{array}{cccccc}
\theta_\pi & \theta_K & q^2/\text{GeV}^2 & f_0^{K\pi}(q^2) & f_+^{K\pi}(q^2) & f_-^{K\pi}(q^2) \\
\hline
0 & 4.68 & 0.0002(2) & 0.9758(44) & 0.9758(44) & -0.0997(93) \\
2.682 & 0 & 0.0004(3) & 0.0216(2) & 0.9898(34) & 0.9975(42) & -0.081(17) \\
2.129 & 0 & 0.0381(2) & 1.0030(20) & 1.0213(32) & -0.108(11) \\
1.600 & 0 & 0.0607(2) & 1.0185(15) & & & \\
0 & 2.792 & 0.0382(2) & & & & \\
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\hline
\end{array} \]
5 Extrapolation models

In a previous analysis [6] we used results for the form factors at the lattice Fourier modes for four pion masses and one value of the (unitary) strange quark mass which post facto turned out to be slightly heavier than the physical one. At each simulated pion mass we first determined two estimates for $f_{K\pi}^0(0) = f_{K\pi}^0(0)$, one from an interpolation in $q^2$ with a pole ansatz,

$$f_{K\pi}^0(q^2)|_{\text{pole}} = \frac{f_{K\pi}^0(0)|_{\text{pole}}}{1 - q^2/M^2},$$

and one from an interpolation of $f_0(q^2)$ with a second order polynomial, $f_{K\pi}^0(0)|_{2\text{nd}}$ (cf. Table IV in [6]). We based the estimate of the systematic error due to the phenomenological interpolation on the difference between the two results.

The final central value was determined from a global fit ansatz incorporating pole dominance, the NLO expression for $f_{K\pi}^0(0)$ in [8],

$$f_{K\pi}^0(0)|_{\text{NLO}} = 1 + f_2 (f, m_\pi^2, m_K^2),$$

( $f$ is the pion decay constant), and modelling higher order contributions. The ansatz is

$$f_{K\pi}^0(q^2) = 1 + f_2 + (m_K^2 - m_\pi^2)^2 (A_0 + A_1 (m_K^2 + m_\pi^2)), 1 - q^2/(M_0 + M_1 (m_K^2 + m_\pi^2))^2,$$

where we use the $N_f = 2 + 1$ expression for $f_2$, partially quenched in the strange quark, as determined in [9]. Since the kaon mass appears explicitly, after fitting (15) to our lattice data, any values for $m_\pi$ and $m_K$ can be inserted into (15) to obtain a value for $f_{K\pi}^0(q^2)$. Hence, by inserting the physical values for $m_\pi$ and $m_K$, the strange quark mass is automatically corrected to its physical value. The data were well described with

$$A_0 = -0.34(9) \text{ GeV}^{-4}, \quad A_1 = 0.28(12) \text{ GeV}^{-6},$$

$$M_0 = 0.94(10) \text{ GeV}, \quad M_1 = 0.54(18) \text{ GeV}^{-1}.$$

In the meantime an expansion for $f_{K\pi}^0(0)$ in $SU(2)$ chiral perturbation theory has been derived [13]. In particular in view of the slow convergence of $SU(3)$ chiral perturbation theory observed for some quantities (cf. e.g. [28]) it seems useful to compare the present extrapolation strategy to one incorporating this new formula. Similarly to the case of $SU(3)$ chiral perturbation theory we use the ansatz,

$$f_{K\pi}^0(q^2) = \frac{F_+(1 - \frac{3}{2}L + c_2 m_\pi^2 + c_4 m_\pi^4)}{1 - q^2/(M_0 + M_1 m_\pi^2)^2},$$

where $L \equiv \frac{m_\pi^2}{16\pi^2 f_\pi^2} \log \frac{m_\pi^2}{\mu^2}$ with the normalisation scale $\mu$ and where in comparison to the original work we have added an additional term proportional to $m_\pi^4$. Note that the parameters in this fit ansatz depend on the value of the strange quark mass.

Reordering the chiral expansion We do not really know how light the quarks must be for the chiral expansion at a fixed order to represent the mass dependence of physical quantities to a given level of precision. In principle, (unrealistically expensive) lattice computations at very light quark masses, perhaps even lighter than the physical ones, could answer this question. Our present calculations however, involve masses in a regime where NNLO terms of the $SU(3)$ expansion are non-negligible, and yet we have insufficient data to determine these terms and all the corresponding low-energy constants (LECs). As discussed above, we therefore have to model the higher order contributions using an ansatz such as that in (15).

We observe that the interchange symmetry $f_{K\pi}^0(q^2) = f_{K\pi}^0(q^2)$ is held in the $SU(3)$ expansion order by order and also in non-perturbative data to all orders. The $SU(3)$ chiral expansion in terms of the unknown, but in principle unambiguous, LEC $f_0$ has this symmetry manifest in each term. However, we have the freedom to repartition terms of this expansion between different orders: for example to use an alternative expansion parameter $f$ differing from $f_0$ beyond leading order

$$f_{K\pi}^0(0) = 1 + f_2 (f, m_K^2, m_\pi^2) + \cdots.$$

In fact, the NLO term $f_2$ is usually quoted as $f_2(f_\pi, m_K^2, m_\pi^2) \simeq -0.023$, with the physical pion decay constant used in place of the unknown LEC $f_0$. For $SU(3)$ chiral perturbation theory to correspond to QCD when all terms are summed, this must be a passive transformation on the series making simultaneous but cancelling changes to different orders. There are several possible interpretations of the $f_\pi$ which appears in $f_2(f_\pi, m_K^2, m_\pi^2)$ that are consistent with QCD in the asymptotic light mass region.

First, we may consider $f_\pi$ entering the expression to be simply an estimate of the true LEC $f_0$, and a rigorous error analysis must allow for $f_\pi$ to vary over a range of values. In order that the NNLO form is unchanged, and that the interchange symmetry remains manifest in our ansatz, we choose this first interpretation and vary the value of $f_0$ entering our expressions to estimate a systematic error.

Second, a mass dependent expression for $f_\pi(f_0, m_{ud}, m_s)$ may enter $f_2$ and the correction term

$$\delta_{\text{NNLO}} = f_2(f_\pi, m_K^2, m_\pi^2) - f_2(f_\pi(f_0, m_{ud}, m_s), m_K^2, m_\pi^2),$$

introduced at NNLO, passively repartitioning the series and possibly improving convergence. We note that this difference term now breaks the symmetry under $\pi \leftrightarrow K$ interchange, and the form of NNLO terms is changed to compensate the alternate expansion parameter.
A third but less helpful interpretation would be to consider adjusting the series to expand in terms of the physical decay constant $f_\pi \simeq 131$ MeV. Passive transformation requires that a correction term at NNLO be introduced with the same dependence on simulated masses

$$\delta_{\text{NNLO}} = f_2(f_0, m_K^2, m_\pi^2) - f_2(f_\pi = 131$ MeV, $m_K^2, m_\pi^2)$$.

This simply relabels the term involving the free parameter $f_0$ as NNLO. If $f_0$ is subsequently expanded in terms of $f_\pi$ and $m_{\text{phys}}$, this amounts to using a phenomenological estimate for $f_0$—with the associated systematic uncertainty.

Using $f_2(f_\pi = 131$ MeV, $m_K^2, m_\pi^2)$ but failing to adjust the forms appearing at NNLO is inconsistent with QCD in the true chiral limit as it actively changes the series. This discussion impacts our previous analysis in which we extrapolated the defect $\Delta f$, and did not admit variation in $f_0 \neq 131$ MeV, nor modified the form of our global fit ansatz at NNLO to admit breaking of the mass interchange symmetry. While we are concerned here with the context of the $K \to \pi$ decay, the considerations are applicable to practices used in the lattice study of many quantities if a chiral expansion parameters differing from $f_0$ is used to improve convergence of the truncated series.

6 Results

**Cost of the simulation** In Table 3 we compare the cost of the simulations for the two approaches to the computation of $f_+^{K\pi}(0)$. For $P4$, for each quark mass $am = am_q$, $am_s$ one normal and one extended propagator (cf. definition in [10]), one twist (periodic boundary conditions), four positions of the point source on 175 configurations and 12 spin-colour inversions were necessary. Since with point sources a Fourier transformation between the source and the point of the current insertion can be performed almost for free, one can directly interpolate to $q^2 = 0$ at no additional cost. This is not the case when using the noise source technique as for $Z4PSs4$ and $Z4PSs3$. We achieved a similar precision for $f_+^{K\pi}(0)$ at approximately the same total cost with the $Z4PS$-source type, where for each propagator of mass $am = am_q$ or $am = am_s$ four spin-colour inversions are necessary [11] for each choice of the twist angle. We note however that in general the quality of plateaus is significantly enhanced when using the stochastic volume source technique.

|       | $am$ | $n_{\text{props}}$ | $n_0$ | $n_{\text{arc}}$ | $n_{\text{config}}$ | $s-c$ | $N_{\text{tot}}$ |
|-------|------|-----------------|------|----------------|---------------------|------|--------------|
| $P4$  | 2 x 2 | 1 x 4           | 175  | 12             |                     |      | 33600        |
| $Z4PSs4$ | 2 x 2 | 2 x 8          | 147  | 4              |                     |      | 37632        |

*Table 3 Cost comparison*

![Fig. 3](https://example.com/f3.png)

Fig. 3 (Color online) Summary of simulation results of $f_+^{K\pi}(0)$. The black circles and the (dashed) pole interpolation correspond to the results of [6] while the results represented by the left- and right-pointing arrows, respectively, correspond to the results of this work for $am_q = 0.04$ and $am_s = 0.03$. The red and blue curve represent the result from the global fit in [6], once for $m_K^{0.03}$ and $m_K^{0.04}$.

- **q^2-dependence of the form factor** The data generated for this paper complement our previous data $P4$ by a number of new points for $f_0^{K\pi}(q^2)$ in the range $0 \lesssim q^2 \lesssim q_{\text{max}}^2$ for two valence strange quark masses $am_q = 0.04$ (unitary) and $am_q = 0.03$ (partially quenched). The results are illustrated in the plot in Fig. 3 by the red/blue right/left-pointing arrows, respectively. The new data points for $am_q = 0.04$ nicely agree with both the pole dominance and polynomial fits (cf. (13) in [6]) as can be seen in the following comparison:

**results for amq = 0.005, amq = 0.04**

- $f_+^{K\pi}(0)|_{\text{pole}} = 0.9774(35)$ [6],
- $f_+^{K\pi}(0)|_{\text{polynomial}} = 0.9749(59)$ [6],
- $f_+^{K\pi}(0)|_{\text{this work}} = 0.9757(44)$

In [6] we used the spread $f_+^{K\pi}(0)|_{\text{pole}} - f_+^{K\pi}(0)|_{\text{polynomial}} \approx 0.0024$ as an estimate of the systematic due to the phenomenological $q^2$-interpolation. As simulations move closer to the physical pion mass, the value of $q_{\text{max}}^2 = (m_K - m_\pi)^2$ increases. Therefore the interpolation to $q^2 = 0$, which crucially depends on the high precision which one is able to achieve for the form factor at $q_{\text{max}}^2$, will be increasingly sensitive to the ansatz one makes. One therefore expects the systematic error due to the interpolation to increase. We emphasise that the approach advocated here entirely removes this uncertainty.
am the lattice data reliably only below $m_\pi$ dependence resides in the low-energy constants. The limit based on iterations, at this stage we refrain from presenting fit results to include data at heavier pion masses. However, fits of accept- ues of the pion mass below this cut-off and extrapolations contrast to our study in [28] here we only have data for two val-
ses. In contrast, in SU(3) chiral perturbation theory one ex-
strains the form factor around vanishing pion mass at a fixed
dependence on a partially quenched strange quark well.

Combining the data sets $P4$, $Z4PSs3$ and $Z4PSs4$ and
carrying out the global fit (15) we update the previous result
$f_+^{K\pi}(0) = 0.9644(33) \rightarrow f_+^{K\pi}(0) = 0.9630(34)$ (statistical
errors only) at the physical point. The result of the global fit
is also illustrated in Fig. 4 by the solid black line.

The chiral extrapolation of the lattice data is well con-
strained by the natural hinge-point $f_0^{K\pi}(0)|_{m_K=m_\pi} = 1$. As
can be seen in Fig. 4, our data as well as the global SU(3)
fit ansatz (15) nicely approach this point for $m_\pi \rightarrow m_K$.
In contrast, in SU(2) chiral perturbation theory one ex-
pands the form factor around vanishing pion mass at a fixed
strange quark mass [13] (in fact, all strange quark mass depen-
dence resides in the low-energy constants). The limit
$f_0^{K\pi}(0)|_{m_K=m_\pi} = 1$ is not naturally implemented in this
expansion. Given our experience with SU(2) fits to other pion
and kaon observables in [28] such an expansion describes the
lattice data reliably only below $m_\pi \approx 400$ MeV. In con-
trast to our study in [28] here we only have data for two val-
ues of the pion mass below this cut-off and extrapolations
are therefore not well constrained. Alternatively one can in-
clude data at heavier pion masses. However, fits of accept-
able quality can then only be obtained after adding an extra
term ($\propto c_4$) to the expression in [13]. Given these consi-
derations, at this stage we refrain from presenting fit results
based on SU(2) chiral perturbation theory.

**Quark mass dependence** Inserting the unitary and partially quenched kaon mass which we simulated here together with the parameters in (16) into the phenomenological ansatz (15) we can predict the form factor that is to be expected for $a_{\pi_0} = 0.03$ and $a_{\pi_0} = 0.04$ with $am_q = 0.005$ as illustrated in terms of the blue (dot-dashed) and red (dashed) curve in Fig. 3. Both curves are nicely compatible with the new blue and red data points, thus confirming that the ansatz paramet-
ises the dependence of the form factor on a partially
quenched strange quark well.

Estimates of systematic errors As discussed in Sect. 5, a potential source of systematic error which to our knowledge has not been taken into account systematically in any previous computation of $f_+^{K\pi}(0)$ is the choice of the decay constant entering in the SU(3) NLO prediction for the form factor. Lacking a precise value of the decay constant in the chiral limit we repeated the global fit for the three choices $f = 100, 115, 131$ MeV which in our opinion cover a reason-
able range. For these choices we found for the central values of the form factor $f_+^{K\pi}(0) = 0.9556, 0.9599, 0.9630$,
respectively. In each case the fit was of very good quality.
This is quite a sizeable variation in the central value which is
illustrated in Fig. 5. We found that the choice of decay constant
particularly changes the slope of $f_+^{K\pi}(0)$ with respect to $m_\pi^2$ in the region of small pion masses where we do not have data. In order to study the behaviour at NNLO more systematically, one can use the FORTRAN computer code written by Bijnen-
s that can provide SU(3) NNLO terms in terms of numerical integration routines (see also [32] for form factor fits based on this code).
Our experience from using the code is that for our limited set of lattice data points there are too many free parameters (low-energy constants from the $O(p^4)$ and the $O(p^6)$ chiral Lagrangian) to be able to carry out reliable fits. Lacking a better analytical under-
standing of NNLO effects we prefer as the central value the
one corresponding to $f = 115$ MeV. As an estimate for the uncertainty in the chiral extrapolation we use the interval
defined by the result for $f_+^{K\pi}(0)$ as obtained when using
$f = 100$ MeV and $f = 131$ MeV, respectively. In this way we obtain $f_+^{K\pi}(0) = 0.9599(34)(^{+31}_{-43})(14)$.

The new data presented here confirm the ansatz for the $q^2$-interpolation for the smallest mass used in [6], i.e. $a_{m_q} = 0.005$. Since $q^{2\text{max}}$ increases as $m_q$ decreases, it is at this

4The programs for $f_+(q^2)$ and $f_-(q^2)$ used in [31] are available on request from Johan Bijnen.
mass that $q^2_{\text{max}}$ is the largest (and therefore furthest away from $q^2 = 0$) and hence the interpolation is the least constrained. We are therefore confident that the pole ansatz previously used in fits to our data [6] describes the form factor data well also for all the other simulation parameters where $q^2_{\text{max}}$ is closer to the origin. Further supporting evidence is provided by the result which one obtains when using a polynomial ansatz for the $q^2$-dependence rather than the pole ansatz (see (13) in [6]): In this case we obtain a result for the form factor which is by 0.002 smaller and we add this negative shift quadratically into the systematic error. With $\chi^2/\text{d.o.f.} = 0.8$ in both cases the fits are of good quality.

Our result is therefore,

$$f_+^{K\pi}(0) = 0.9599(34)^{+31}_{-47}(14), \quad (18)$$

where the first line the first error is statistical, the second is due to the chiral extrapolation and the third error is an estimate of lattice cut-off effects for which we stay with the previous estimate in [6]. We note that the quoted uncertainty due to the chiral extrapolation covers the central value of the result which one obtains when extrapolating instead with $f_2(f_\pi(m_{ud},m_s),m_K^2,m_\pi^2)$ in (15), i.e. with the decay constant as input that corresponds to each of our simulations points (cf. [28]). Adding all errors in quadrature we obtain

$$f_+^{K\pi}(0) = 0.960(5)_{-6}^{+7}. \quad (19)$$

We believe that the systematic error due to the chiral extrapolation discussed above is conservative but still a more rigid statement would be desirable. To this end a better understanding of the NNLO terms in the chiral expansion and additional simulation points at smaller pion masses are mandatory.

### 7 Summary and outlook

In this paper we present new data for the kaon semi-leptonic decay form factors computed in lattice QCD with $N_f = 2 + 1$ flavours of dynamical fermions. Using (partially) twisted boundary conditions we were able to directly simulate at the phenomenologically relevant kinematical point $q^2 = 0$, at a very small additional computational cost while at the same time making the computation independent of any phenomenological ansatz for the interpolation in the momentum transfer. In this way one significant systematic uncertainty in the computation of the form factors has been successfully removed.

We have reconsidered the estimates of the systematic uncertainties of our previous calculation presented in [6] and we present numerical evidence that our ansatz for the strange quark mass dependence of the form factor is under control by providing data at an additional partially quenched simulation point for the strange quark mass.

Currently, chiral extrapolations of lattice results for the kaon semi-leptonic form factor are based on NLO chiral perturbation theory. We show that ambiguities in the parametrisation of the NLO expression can lead to additional systematic effects which we include into our revised estimate of the systematic uncertainties. This ambiguity also applies to any other lattice computation of $f_+^{K\pi}(0)$.

We want to stress that the interpretation of lattice data for the $K \rightarrow \pi$ form factors would profit from the availability of their expressions at NNLO in chiral perturbation theory in a more transparent form.

The RBC-UKQCD collaboration is currently extending the set of data points presented here by simulations at lighter pion masses and at the same time at a finer lattice spacing. A combined analysis of all data is the next step in RBC-UKQCD’s program of a precise computation of the $K \rightarrow \pi$ form factors in $N_f = 2 + 1$ flavour lattice QCD.

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