\section{Introduction}

From experiments it is known that the masses of the nine light pseudo-scalar mesons show an interesting pattern. Taking the quark model point of view, the three lightest mesons, the pions, contain only the two lightest quark flavours, the \textit{up} and \textit{down} quarks. The pion triplet has a mass of $M_\pi \approx 140$ MeV. For the other six, the \textit{strange} quark also contributes, and hence they are heavier. In contrast to what one might expect, five of them, the four kaons and the $\eta$
meson, have roughly equal mass around 500 to 600 MeV, while the last one, the $\eta'$ meson, is much heavier, with a mass of about 1 GeV. On the QCD level, the reason for this pattern is thought to be the breaking of the $U_A(1)$ symmetry by quantum effects. The $\eta'$ meson is, even in a world with three massless quarks, not a Goldstone boson.

In this paper, we present the first lattice study of $\eta$ and $\eta'$ meson masses using mass degenerate up, down as well as heavier, non-degenerate strange and charm dynamical quark flavours. The lattice QCD formulation is the Wilson twisted mass formulation [1] with $N_f = 2 + 1 + 1$ dynamical quark flavours. This will not only allow a study of the dependence of the $\eta, \eta'$ masses on the light quark mass value, but also an investigation of the charm quark contribution to both of these states. Moreover, the $\eta_c$ meson could be studied in the unitary case in principle.

$\eta$ and $\eta'$ states are difficult to treat in lattice QCD, because fermionic disconnected contributions appear and cannot be ignored. This is why the amount of available results for these states from lattice QCD is rather limited in range of pion mass values as well as values of the lattice spacing. For recent lattice studies in $N_f = 2 + 1$ flavour QCD see [2,3,4,5]. Some of these we will discuss in more detail later and compare with our results. A previous lattice study with Wilson twisted mass fermions has been performed with $N_f = 2$ dynamical quark flavours [6]. In this work we have developed particular noise reduction techniques, which we also used to obtain the results presented here for the $N_f = 2 + 1 + 1$ case.

The paper is organised as follows. In section 2 we introduce the lattice QCD framework we are using, the Wilson twisted mass formalism, followed by a discussion of how we deal with flavour singlet pseudo-scalar mesons in this framework in section 3. In section 4 we present our results and discuss them in the following final section. More details on our analysis procedure and data tables can be found in the appendix.

## 2 Lattice Action

The lattice QCD action for $N_f = 2 + 1 + 1$ Wilson twisted mass fermions reads

$$S = S_g + \bar{\chi}_\ell D_\ell \chi_\ell + \bar{\chi}_h D_h \chi_h.$$  \hspace{1cm} (1)

For the gauge action $S_g$ we use the Iwasaki gauge action [8]. The twisted mass Dirac operator for the light – i.e. up/down quark – doublet reads [1]

$$D_\ell = D_W + m_0 + i\bar{\mu}_\ell \gamma_5 \tau^3$$ \hspace{1cm} (2)
\[ D_h = D_W + m_0 + i \mu_\sigma \gamma_5 \tau^1 + \mu_\delta \tau^3, \]  

(3)

where \( D_W \) is the Wilson Dirac operator. The value of \( m_0 \) was tuned to its critical value \( m_{\text{crit}} \) as discussed in refs. [10,7] in order to realise automatic \( O(a) \) improvement at maximal twist [11]. This way of \( O(a) \) improvement was first shown to work in practice in refs. [12,13] in the quenched approximation, and later for \( N_f = 2 \) in ref. [14] (see also ref. [15]). For a review see ref. [16]. Also for \( N_f = 2 + 1 + 1 \) we have strong indications that the scaling properties of Wilson twisted mass lattice QCD at maximal twist are favourable [7]. For a discussion on how to determine kaon and D-meson masses see ref. [17]. The bare twisted masses \( \mu_\sigma \) and \( \mu_\delta \) are related to the bare strange and charm quark masses via the relation

\[ m_{c,s} = \mu_\sigma \pm Z \mu_\delta \]  

(4)

where \( Z \equiv (Z_P/Z_S) \) denotes the ratio of pseudo-scalar and scalar renormalisation constants \( Z_P \) and \( Z_S \). Quark fields in the twisted basis are denoted by \( \chi_\ell,h \) and in the physical basis by \( \psi_\ell,h \). They are related via the axial rotations

\[ \psi_\ell = e^{i \pi \gamma_5 \tau^3/4} \chi_\ell, \quad \bar{\psi}_\ell = \bar{\chi}_\ell e^{i \pi \gamma_5 \tau^3/4}, \]

\[ \psi_h = e^{i \pi \gamma_5 \tau^1/4} \chi_h, \quad \bar{\psi}_h = \bar{\chi}_h e^{i \pi \gamma_5 \tau^1/4}. \]  

(5)

With automatic \( O(a) \) improvement being the biggest advantage of twisted mass lattice QCD (tmQCD) at maximal twist, the downside is that flavour

| ensemble | \( \beta \) | \( \alpha_\mu \) | \( \alpha_\sigma \) | \( \alpha_\delta \) | \( L/a \) | \( N_{\text{conf}} \) | \( N_s \) | \( N_b \) |
|----------|---------|---------|---------|---------|---------|---------|---------|---------|
| A30.32   | 1.90    | 0.0030  | 0.150   | 0.190   | 32      | 1367    | 24      | 5       |
| A40.24   | 1.90    | 0.0040  | 0.150   | 0.190   | 24      | 2630    | 32      | 10      |
| A40.32   | 1.90    | 0.0040  | 0.150   | 0.190   | 32      | 863     | 24      | 4       |
| A60.24   | 1.90    | 0.0060  | 0.150   | 0.190   | 24      | 1251    | 32      | 5       |
| A80.24   | 1.90    | 0.0080  | 0.150   | 0.190   | 24      | 2449    | 32      | 10      |
| A80.24s  | 1.90    | 0.0080  | 0.150   | 0.197   | 24      | 2517    | 32      | 10      |
| A100.24  | 1.90    | 0.0100  | 0.150   | 0.190   | 24      | 2312    | 32      | 10      |
| B25.32   | 1.95    | 0.0025  | 0.135   | 0.170   | 32      | 1484    | 24      | 5       |
| B35.32   | 1.95    | 0.0035  | 0.135   | 0.170   | 32      | 1251    | 24      | 5       |
| B55.32   | 1.95    | 0.0055  | 0.135   | 0.170   | 32      | 1545    | 24      | 5       |
| B75.32   | 1.95    | 0.0075  | 0.135   | 0.170   | 32      | 922     | 24      | 4       |
| B85.24   | 1.95    | 0.0085  | 0.135   | 0.170   | 24      | 573     | 32      | 2       |
| D15.48   | 2.10    | 0.0015  | 0.120   | 0.1385  | 48      | 1045    | 24      | 10      |
| D45.32sc | 2.10    | 0.0045  | 0.0937  | 0.1077  | 32      | 1887    | 24      | 10      |

Table 1
The ensembles used in this investigation. The notation of ref. [7] is used for labeling the ensembles. In addition we give the number of configurations \( N_{\text{conf}} \), the number of stochastic samples \( N_s \) for all ensembles and the bootstrap block length \( N_b \).
(and parity) symmetry is broken at finite values of the lattice spacing. This was theoretically and numerically shown to affect mainly the mass value of the neutral pion [14,18,19], however, in the case of $N_f = 2+1+1$ dynamical quarks, it implies the complication of mixing between strange and charm quarks.

We use gauge configurations as produced by the European Twisted Mass Collaboration (ETMC) with action described above [7,17,20]. The details of the configurations are described in ref. [7] and the ensembles used in this investigation are summarised in table 1: we use ensembles denoted with A, B and D with values of the lattice spacing $a_A = 0.0863(4)$ fm, $a_B = 0.0779(4)$ fm and $a_D = 0.0607(2)$ fm, corresponding to $\beta_A = 1.90$, $\beta_B = 1.95$ and $\beta_D = 2.10$, respectively [20]. The physical volumes are with only a few exceptions larger than 3 fm. In the table we also compile the number of investigated gauge configurations and the number of stochastic samples per gauge configuration used to estimate the disconnected contributions.

Throughout this paper we will use the Sommer parameter $r_0$ [21] to investigate the scaling of our results. We use the values of $r_0^\chi/a$ extrapolated to the massless limit at each $\beta$-value separately. For $\beta = 1.90$ and $\beta = 1.95$ we use the values quoted in ref. [7]. For $\beta = 2.10$ we did the extrapolation by ourselves. All values for $r_0^\chi/a$ are shown in table 2. For setting the physical scale we could use the results of ref. [20], where a chiral fit to data for $f_{PS}$ and $m_{PS}$ and the physical value of $f_\pi$ was used to set the scale. However, the fit in ref. [20] includes only two data points at $\beta = 2.10$, and hence, is rather preliminary. Therefore, we prefer to use a value of $r_0 = 0.45(2)$ fm in this paper to set the scale. The 5% error covers the statistical uncertainty and spread quoted in ref. [20] and allows room for systematic uncertainties. As soon as an update of the scale setting becomes available the results in this paper can be updated accordingly. For fixing the light and strange quark masses to their physical values we will use the experimental values of $M_{\pi^0} = 135$ MeV and $M_{K^0} = 498$ MeV. We use the masses of the neutral mesons to reduce uncertainties from the fact that we do not include electromagnetic effects in our simulation. See also ref. [22] and references therein for a discussion.

For every $\beta$-value the bare values of $a\mu_\sigma$ and $a\mu_\delta$ were kept fixed, and only the value of the light twisted mass parameter $a\mu_\ell$ is varied. The kaon masses measured on these ensembles are close to the physical value with a deviation of up to 10% [7] in particular for the A and D ensembles. The D-meson mass values have a large uncertainty, but they are also close to physical [7]. We will

| $\beta$  | 1.90  | 1.95  | 2.10  |
|----------|-------|-------|-------|
| $r_0^\chi/a$ | 5.231(38) | 5.710(41) | 7.538(58) |

Table 2
Values of $r_0^\chi/a$ for the three $\beta$-values.
discuss this point later in more detail.

For the ensembles \( A_{80.24} \) and \( A_{100.24} \) we have additional ensembles with retuned values of \( a \mu_\sigma \) and \( a \mu_\delta \) denoted by \( A_{80.24}s \) and \( A_{100.24}s \) (see table 1), which reproduce the physical kaon mass value more accurately than the original \( A_{80.24} \) and \( A_{100.24} \) ensembles (see figure 4). We will use these ensembles to estimate the strange quark mass dependence of the \( \eta \) mass.

3 Flavour singlet pseudo-scalar mesons

In order to compute masses of pseudo-scalar flavour singlet mesons we have to include light, strange and charm contributions to build the appropriate correlation functions. In the light sector, one appropriate operator is given by [6]

\[
\frac{1}{\sqrt{2}}(\bar{\psi}_u i\gamma_5 \psi_u + \bar{\psi}_d i\gamma_5 \psi_d) \rightarrow \frac{1}{\sqrt{2}}(-\bar{\chi}_u \chi_u + \bar{\chi}_d \chi_d) \equiv \mathcal{O}_\ell ,
\]

(6)
in the physical and the twisted basis, respectively. With twisted mass fermions we have to work with doublets of quarks, hence, in the strange and charm sector the corresponding operators read

\[
\left( \begin{array}{c} \bar{\psi}_c \\ \bar{\psi}_s \end{array} \right)^T i\gamma_5 \frac{1 \pm \tau^3}{2} \left( \begin{array}{c} \psi_c \\ \psi_s \end{array} \right) \rightarrow \left( \begin{array}{c} \bar{\chi}_c \\ \bar{\chi}_s \end{array} \right)^T \frac{-\tau^1 \pm i\gamma_5 \tau^3}{2} \left( \begin{array}{c} \chi_c \\ \chi_s \end{array} \right) \equiv \mathcal{O}_{c,s} .
\]

(7)
The sign in \( 1 \pm \tau^3 \) in the physical basis distinguishes the charm and strange quark contribution. As a consequence, working in the twisted basis we need to compute correlation functions of the following interpolating operators

\[
\mathcal{O}_c \equiv Z(\bar{\chi}_ci\gamma_5\chi_c - \bar{\chi}_si\gamma_5\chi_s)/2 - (\bar{\chi}_c\chi_c + \bar{\chi}_c\chi_s)/2 ,
\]

\[
\mathcal{O}_s \equiv Z(\bar{\chi}_si\gamma_5\chi_c - \bar{\chi}_ci\gamma_5\chi_c)/2 - (\bar{\chi}_s\chi_c + \bar{\chi}_c\chi_s)/2 .
\]

(8)

Note that the sum of pseudo-scalar and scalar contributions appears with the ratio of renormalisation factors \( Z \), which needs to be taken into account properly. The renormalisation factors for eq. (7) are the non-singlet \( Z_P \) and \( Z_S \). While singlet and non-singlet \( Z_P \) are identical, the singlet and non-singlet \( Z_S \) differ at two loop order [23] in perturbation theory. Defining \( \vec{\mathcal{O}} = (\mathcal{O}_\ell, \mathcal{O}_c, \mathcal{O}_s)^T \), the correlation function matrix is given by

\[
\mathcal{C}(t) = \sum_x \langle \vec{\mathcal{O}}(x) \otimes \vec{\mathcal{O}}(0) \rangle .
\]

(9)

However, masses are independent of \( Z \) as well as the choice of basis, so, for the purpose of determining masses we can proceed as follows: starting from the
bilinears in eqs. (6) and (8) we change the operator basis via an appropriate rotation matrix $\mathcal{R}$

$$c_{\mathcal{R}}(t) = \left\langle \mathcal{R} \bar{\mathcal{O}}(t) \otimes \mathcal{R} \mathcal{O}(0) \right\rangle = \mathcal{R}c(0)\mathcal{R}^T,$$

where

$$c_{\mathcal{R}} = \begin{pmatrix} \eta_{O_O} & \eta_{O_S} & \eta_{O_P} \\ \eta_{S_O} & \eta_{S_S} & \eta_{S_P} \\ \eta_{P_O} & \eta_{P_S} & \eta_{P_P} \end{pmatrix},$$

(11)

is again a symmetric, real and positive definite correlation matrix with

$$\mathcal{P}_h \equiv (\bar{\chi}_c i\gamma_5 \chi_c - \bar{\chi}_s i\gamma_5 \chi_s)/2, \quad \mathcal{S}_h \equiv Z^{-1}(\bar{\chi}_s \chi_c + \bar{\chi}_c \chi_s)/2$$

(12)

and $\eta_{XY}$ denoting the corresponding correlation function. The rotation matrix $\mathcal{R}$ is given by

$$\mathcal{R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

(13)

Now we can drop the factor $Z^{-1}$, which appears only as a constant scaling factor for $\mathcal{S}_h$. We denote the corresponding correlation matrix by $\tilde{c}_{\mathcal{R}}$. This disentanglement of scalar and pseudo-scalar contributions greatly reduces the number of terms required for each element of the correlator matrix.

Solving the generalised eigenvalue problem [24,25,26]

$$\tilde{c}_{\mathcal{R}}(t) \eta^{(n)}(t, t_0) = \lambda^{(n)}(t, t_0) \tilde{c}_{\mathcal{R}}(t_0) \eta^{(n)}(t, t_0),$$

(14)

and taking into account the periodic boundary conditions for a meson, we can determine the effective masses by solving

$$\frac{\lambda^{(n)}(t, t_0)}{\lambda^{(n)}(t + 1, t_0)} = \frac{e^{-m^{(n)}t} + e^{-m^{(n)}(T - t)}}{e^{-m^{(n)}(t + 1)} + e^{-m^{(n)}(T - (t + 1))}}$$

(15)

for $m^{(n)}$, where $n$ counts the eigenvalues. The state with the lowest mass should correspond to the $\eta$ and the second state to the $\eta'$ meson. Alternatively, we use a factorising fit of the form

$$c_{qq}(t) = \sum_n \frac{A_{q,n} A_{q',n}}{2m^{(n)}} \left[ \exp(-m^{(n)}t) + \exp(-m^{(n)}(T - t)) \right]$$

(16)

to the correlation matrix matrix $\mathcal{C}$. For this we either first rotate $\tilde{c}_{\mathcal{R}}$ back taking the factor $Z$ into account, see below, or we directly construct $\mathcal{C}$ taking $Z$ into account. The amplitudes $A_{q,n}$ correspond to $\langle 0|\bar{q}q|n \rangle$ with $n \equiv \eta, \eta',...$ and $q = \ell, s, c.$
3.1 Flavour Content and Mixing

One might first of all be interested in the quark flavour content of a given state in order to compare to phenomenology. From the components $\eta_{0,1,2}^{(n)}$ of the eigenvectors $\eta^{(n)}$ defined above, we can reconstruct the flavour contents $c^{(n)}_{\ell,s,c}$ of the states. Since we have changed the basis according to eqs. (11) and (13), we reconstruct $c^{(n)}_{\ell,s,c}$ from

$$
c^{(n)}_{\ell} = \frac{1}{\mathcal{N}^{(n)}}(\eta_{0}^{(n)})
$$

$$
c^{(n)}_{c} = \frac{1}{\mathcal{N}^{(n)}}(-Z^{-1}\eta_{1}^{(n)} + \eta_{2}^{(n)})/\sqrt{2}
$$

$$
c^{(n)}_{s} = \frac{1}{\mathcal{N}^{(n)}}(-Z^{-1}\eta_{1}^{(n)} - \eta_{2}^{(n)})/\sqrt{2}
$$

with normalisation

$$
\mathcal{N}^{(n)} = \sqrt{(\eta_{0}^{(n)})^2 + (Z^{-1}\eta_{1}^{(n)})^2 + (\eta_{2}^{(n)})^2}.
$$

At this point the ratio $Z$ is again required. The flavour non-singlet renormalisation factors have been evaluated non-perturbatively for our situation [27]. Another way to get access to these ratios of renormalisation constants is available: we require that unphysical amplitudes (such as the connected correlator from source $\bar{s}\Gamma s$ to sink $\bar{c}\Gamma c$ in the physical basis), which are formally order $a$ contributions in the twisted mass formulation, be minimised.

For instance, for $B35$ this procedure gives $Z = 0.70$, while for $D15$ we obtain $Z = 0.75$. For comparison the preliminary RI-MOM flavour non-singlet value [28] for $\beta = 1.95$ is $0.700(8)$ and at $\beta = 2.1$ is $0.737(14)$. This close agreement indicates that we have a reliable estimate of $Z$. Moreover, it turns out that the consequence of an error in this ratio on our mixing angles is minimal, see the discussion in section 4.

The mixing between $\eta$ and $\eta'$ is usually expressed in terms of mixing angles in an appropriate basis. Here we use the quark flavour basis considering only light and strange quarks. With

$$
|\eta_\ell\rangle \equiv \frac{1}{\sqrt{2}}(|\bar{u}u\rangle + |\bar{d}d\rangle), \quad |\eta_s\rangle \equiv |\bar{s}s\rangle
$$

one arrives at

$$
\begin{pmatrix}
|\eta\rangle \\
|\eta'\rangle
\end{pmatrix} = \begin{pmatrix}
\cos \phi & -\sin \phi \\
\sin \phi & \cos \phi
\end{pmatrix} \cdot \begin{pmatrix}
|\eta_\ell\rangle \\
|\eta_s\rangle
\end{pmatrix}.
$$

For a detailed discussion including the charm quark see for instance ref. [29].

On the lattice, however, we have to work with the amplitudes $A_{q,n}$ defined above. Following refs. [2,5], we first rotate the matrix $\mathcal{C}_R(t)$ back to the original
form $C(t)$ in eq. (9) in the way prescribed above (including $Z$). The amplitudes $A_{q,n}$ in eq. (16) of a factorising fit to the rotated correlation matrix are then directly related to the mixing angles via [29]

$$
\begin{pmatrix}
A_{\ell,n} & A_{s,\eta'} \\
A_{\ell,\eta'} & A_{s,n}
\end{pmatrix} =
\begin{pmatrix}
f_\ell \cos \phi_\ell - f_s \sin \phi_s \\
f_\ell \sin \phi_\ell & f_s \cos \phi_s
\end{pmatrix},
$$

where we ignored the charm contribution. Hence, the mixing angles $\phi_\ell$ and $\phi_s$ can be extracted from

$$
\tan \phi_\ell = \frac{A_{\ell,\eta'}}{A_{\ell,\eta}}, \quad \tan \phi_s = -\frac{A_{s,\eta}}{A_{s,\eta'}},
$$

where the renormalisation constants cancel in the ratio. Following the RBC / UKQCD and the Hadron Spectrum collaborations we also define a common angle $\phi$ (representing the geometric mean of $\phi_\ell$ and $\phi_s$)

$$
\tan^2(\phi) = -\frac{A_{\ell,\eta'}A_{s,\eta}}{A_{\ell,\eta}A_{s,\eta'}},
$$

inspired by arguments that $\phi_\ell$ and $\phi_s$ should actually agree [29,30], see also ref. [5]. We do not include the charm quark in the discussion here, because it turns out that its contribution to $\eta$ and $\eta'$ is negligible.

4 Results

We have computed all contractions needed for building the correlation matrix of eq. (11). For the connected contributions, we used stochastic time-slice sources (the so called “one-end-trick” [31]). For the disconnected contributions, we used stochastic volume sources with complex Gaussian noise [31]. As discussed in ref. [6], one can estimate the light disconnected contributions very efficiently using the identity

$$
D_u^{-1} - D_d^{-1} = -2i\mu_\ell D_d^{-1} \gamma_5 D_u^{-1}.
$$

For the heavy sector such a simple relation does not exist, but we can use the so called hopping parameter variance reduction, which relies on the same equality as in the mass degenerate two flavour case (see ref. [31] and references therein)

$$
D_h^{-1} = B - BHB + B(HB)^2 - B(HB)^3 + D_h^{-1}(HB)^4
$$

with $D_h = (1 + HB)A$, $B = 1/A$ and $H$ the two flavour hopping matrix. The number of stochastic volume sources $N_v$ per gauge configuration we used for both the heavy and the light sector is given for each ensemble in table 1. In
### Table 3
Results of $aM_{\eta}$, $aM_{\eta}'$ for all ensembles and the corresponding values for the charged pion mass $M_{PS}$ and the kaon mass $M_K$. Most of the kaon and pion mass values have been published already in ref [7], however, we have recomputed the pion mass values with our statistics.

| ensemble | $aM_{PS}$ | $aM_K$ | $aM_{\eta}$ | $aM_{\eta}'$ |
|----------|-----------|---------|-------------|-------------|
| A30.32   | 0.12374(27)| 0.25150(29)| 0.286(15) | 0.49(6)     |
| A40.24   | 0.14517(39)| 0.25884(43)| 0.281(18) | 0.39(6)     |
| A40.32   | 0.14174(26)| 0.25666(23)| 0.281(11) | 0.49(9)     |
| A60.24   | 0.17340(39)| 0.26695(52)| 0.290(7)  | 0.59(9)     |
| A80.24   | 0.19888(37)| 0.27706(61)| 0.302(8)  | 0.60(8)     |
| A100.24  | 0.22097(40)| 0.28807(34)| 0.315(11)| 0.50(7)     |
| A80.24s  | 0.19870(50)| 0.25503(33)| 0.270(9)  | 0.54(9)     |
| A100.24s | 0.22149(39)| 0.26490(74)| 0.280(5)  | 0.66(12)    |
| B25.32   | 0.10768(30)| 0.21240(50)| 0.234(10)| 0.50(8)     |
| B35.32   | 0.12445(29)| 0.21840(28)| 0.237(9)  | 0.59(9)     |
| B55.32   | 0.15503(48)| 0.22799(34)| 0.249(14)| 0.60(10)    |
| B75.32   | 0.18121(24)| 0.23753(32)| 0.253(13)| 0.44(7)     |
| B85.24   | 0.19373(58)| 0.24392(59)| 0.260(12)| 0.51(12)    |
| D15.48   | 0.07004(19)| 0.16897(85)| 0.201(9)  | 0.38(8)     |
| D45.32sc | 0.07981(30)| 0.17570(84)| 0.192(15)| 0.30(4)     |

### Table 4
Results for the mixing angles in eqs. (19) and (20) from a $4 \times 4$-correlation function matrix using local (L) and fuzzed (F) operators for all ensembles.

| ensemble | $\phi_\ell^L$ | $\phi_s^L$ | $\phi_s^F$ | $\phi_\ell^F$ | $\phi_s^F$ |
|----------|---------------|------------|-----------|---------------|------------|
| A30.32   | 57(15)        | 49(13)     | 56(15)    | 36(9)         | 53(13)     |
| A40.24   | 39(16)        | 41(11)     | 39(16)    | 43(11)        | 40(12)     |
| A40.32   | 56(18)        | 33(11)     | 54(18)    | 33(11)        | 44(11)     |
| A60.24   | 66(15)        | 29(13)     | 66(15)    | 30(13)        | 49(8)      |
| A80.24   | 73(7)         | 20(10)     | 73(7)     | 24(10)        | 48(6)      |
| A100.24  | 62(10)        | 37(10)     | 62(10)    | 39(9)         | 50(5)      |
| A80.24s  | 59(16)        | 36(16)     | 59(16)    | 41(16)        | 48(12)     |
| A100.24s | 75(13)        | 20(16)     | 76(12)    | 25(16)        | 50(7)      |
| B25.32   | 74(13)        | 25(10)     | 73(13)    | 28(10)        | 52(6)      |
| B35.32   | 67(14)        | 19(7)      | 63(15)    | 22(8)         | 42(6)      |
| B55.32   | 74(11)        | 14(6)      | 73(11)    | 18(7)         | 43(6)      |
| B75.32   | 50(14)        | 52(15)     | 50(14)    | 52(15)        | 51(11)     |
| B85.24   | 60(16)        | 47(20)     | 61(16)    | 46(19)        | 54(13)     |
| D15.48   | 59(14)        | 25(9)      | 57(14)    | 29(9)         | 41(10)     |
| D45.32sc | 60(19)        | 57(15)     | 59(19)    | 58(15)        | 59(15)     |

order to check that the stochastic noise introduced by our method is smaller than the gauge noise we have increased $N_s$ from 24 to 64 for ensemble $B25.32$. This increase in $N_s$ did not reduce the error on the extracted masses.
Also, we use both local and fuzzed operators to enlarge our correlation matrix by a factor two. In addition to the interpolating operator quoted in eqs. (6) and (7), one could also consider the $\gamma$-matrix combination $i\gamma_0\gamma_5$, which would increase the correlation matrix by another factor of two. However, the corresponding correlation functions turn out to be too noisy to give any further improvement at this stage. The values for the number of gauge configurations $N_{\text{conf}}$ investigated per ensemble are summarised in table 1.

Errors are always computed using a bootstrap procedure with 1000 bootstrap samples. To account for autocorrelation we block the data in blocks of length $N_b$. The values of $N_b$, see table 1, have been chosen such that the blocks are statistically independent. As autocorrelation appears to be significant – in particular for $M_{\eta'}$ – we have computed the integrated autocorrelation time $\tau_{\text{int}}$ in units of HMC trajectories of length 1 using the $\Gamma$-method [32] for the elements of the correlation matrix $C_R$ at fixed time $t/a = 3$ for several ensembles. Most affected by autocorrelation are the matrix elements with light quark content. All other elements of $C_R$ are only mildly affected. For instance, for ensemble $D15.48$ the matrix element with only light quark content has integrated autocorrelation time of $\tau_{\text{int}} = 9(2)$, while the elements without light quark content have at most $\tau_{\text{int}} = 1.3(2)$. Note that our normalisation is such that $\tau_{\text{int}} = 0.5$ corresponds to no autocorrelation. Alternatively to the $\Gamma$-method we have varied the blocklength of the bootstrap method and found that for a blocklength of $N_b = 10$ or larger the error for all matrix elements for ensemble $D15.48$ stays constant within error. From the latter method we obtain $\tau_{\text{int}} = 7(2)$ for the matrix elements with light quark content consistent with the result from the $\Gamma$-method. $N_b = 10$ corresponds for $D15.48$ to 20 HMC trajectories of length 1 (see ref. [33] for a description of the HMC algorithm used).

The autocorrelation depends on the lattice spacing. With increasing value of the lattice spacing the autocorrelation becomes less. For instance, the light-only matrix element has $\tau_{\text{int}} = 6(1)$ for $B25.32$ and $\tau_{\text{int}} = 4(1)$ for $A30.32$, compared to the aforementioned $\tau_{\text{int}} = 9(2)$ for $D15.48$. The quark mass dependence is not significant.

The details of our GEVP and fitting procedures to extract $\eta$ and $\eta'$ masses are explained in appendix A, together with fit ranges and $\chi^2$ values. For the masses we used only the blocked bootstrap method to analyse autocorrelation and found that the $\eta'$ state (in agreement to what we found in the $N_f = 2$ case [6]) shows significant autocorrelation, whereas the $\eta$ is less affected. Again, for ensemble $D15.48$ a blocksize of $N_b = 10$ seems to yield statistically independent blocks. We emphasise that with our values of $N_{\text{conf}}$ we can hardly use $N_b > 20$, because the number of blocks becomes too small. Therefore, we cannot exclude that there is autocorrelation on longer scales.
Fig. 1. (a) Effective masses in lattice units determined from solving the GEVP for a $3 \times 3$ matrix with $t_0/a = 1$ for ensemble B25.32. (b) the same, but for a $6 \times 6$ matrix. For comparison also the fit results (see text) for the two lowest states are shown (cf. table 3).

4.1 Extraction of Masses

In the left panel of figure 1, we show the effective masses determined from solving the GEVP for ensemble $B25.32$ from a $3 \times 3$ matrix with local operators only. For the purpose of this plot, we kept $t_0/a = 1$ fixed. One observes that the ground state is very well determined and it can be extracted from a plateau fit. The second state, i.e. the $\eta'$, is much more noisy and a mass determination is questionable, at least from a $3 \times 3$ matrix. Enlarging the matrix size significantly reduces the contributions of excited states to the lowest states and, due to smaller statistical errors at smaller $t$ values, a determination becomes possible. This can be seen for a $6 \times 6$ (including fuzzing) matrix in the right panel of figure 1. Our final results and errors for the masses are indicated in figure 1 by the horizontal bands. We do not determine them from a constant fit to the plateau, but by a three state cosh fit to the eigenvalues, possibly with larger $t_0$ values, see appendix A. As shown, the procedure gives very good agreement with a plateau fit for the $\eta$, but slightly lower values for the $\eta'$. This indicates non-negligible systematic uncertainties in the extraction of the $\eta'$ mass value.

The third state appears to be in the region where one would expect the $\eta_c$ mass value, however, the signal is lost at $t/a = 5$, which makes a reliable determination unfeasible. Note that the two plots in figure 1 are rather independent of the particular ensemble chosen.

To gain further confidence in our identification of the $\eta$ and $\eta'$ states, we
also determine the flavour content of the two states as explained above. As an example we show in the left panel of figure 2 the flavour content of the \( \eta \) for ensemble \( B25.32 \). It becomes evident that – as one would expect from phenomenology – the \( \eta \) has a dominant strange quark content, while the \( \eta' \), shown in the right panel of figure 2 is dominated by light quarks. Note that we do not include a gluonic operator in our analysis, so we only discuss the relative quark content. For both, the charm contribution is compatible with zero.

In figure 3 we show the masses of the \( \eta \) (filled symbols) and \( \eta' \) (open symbols) mesons for the various ensembles we used as a function of the squared pion mass, everything in units of \( r_0 \). All the masses have been determined from solving the GEVP for a 6 \( \times \) 6 matrix, the details are described in appendix A. The results have been independently cross-checked using a factorising fit, and corroborated. We have collected all the values for \( aM_\eta \) and \( aM_\eta' \) together with kaon and pion mass values in table 3 with statistical errors only. Note that the values for \( aM_K \) and \( aM_{PS} \) are published for most of the ensembles already in ref. [7]. But we have recomputed the pion mass values with our statistics, and added ensembles as compared to ref. [7]. The methods for computing the kaon mass in \( N_f = 2 + 1 + 1 \) Wilson twisted mass lattice QCD are described in ref. [17].

It is clear from the figure that the \( \eta \) meson mass can be extracted with high precision, while the \( \eta' \) meson mass is more noisy. The former can be understood, because in the SU(3) symmetric limit the \( \eta \) meson is a flavour octet with all disconnected contributions vanishing, while the \( \eta' \) is the flavour singlet.

Fig. 2. (a) Squared flavour content of \( \eta \) for B25.32 from 3 \( \times \) 3-matrix using local operators only. (b) Squared flavour content of \( \eta' \) for B25.32.
Fig. 3. (a) $\eta$ (filled symbols) and $\eta'$ (open symbols) masses in units of chirally extrapolated $r_0$ (listed in table 2) as a function of $(r_0 M_{PS})^2$.

with non-vanishing disconnected contributions[1].

The results displayed in figure 3 have been obtained using the bare values of $a\mu_\sigma$ and $a\mu_\delta$ as used for the production of the ensembles. Those values, however, did not lead to the physical values of, e.g., the kaon and D-meson masses [7,17]. We show the kaon mass as a function of the squared pion mass, in the left panel of figure 4, for all $A$ ensembles. It is clearly evident that the re-tuned ensembles ($A80.24s$ and $A100.24s$) have values for the kaon mass closer to the physical one (see also e.g. ref. [7,20]). In the right panel of figure 4 we show $r_0 M_\eta$ also for all $A$ ensembles (including $A80.24s$ and $A100.24s$), and the same pattern as for the kaon mass is observed. Furthermore, the physical strange and charm quark mass values differ among the $A$, $B$ and $D$ ensembles. Hence, figure 3 is not yet conclusive with regards to the size of lattice artifacts and the extrapolation to the physical point. What we can recognise is that the light quark mass dependence in the $\eta$ appears to be rather weak.

While the results for the $\eta$ mass in figure 3 show a consistent picture over all lattice spacings and light quark mass values – keeping the differences in the strange and charm quark masses in mind – the $\eta'$ mass shows large fluctuations and no consistent picture. We attribute this to two observations: firstly, due to the large noise in the $\eta'$ state, the extracted masses are for most of the ensembles only an upper bound for $M_{\eta'}$, because a plateau is hardly visible.

[1] We thank Martin Savage for a useful discussion on this point.
Fig. 4. (a) The kaon mass in units of \( r_0 \) and (b) \( r_0 M_\eta \) as a function of \( (r_0 M_{PS})^2 \) also for all \( A \) ensembles. The dotted and solid curves in (a) represent the fitted \( g_K \) in eq. (23) and the shifted \( \tilde{g}_K \) (see text), respectively.

Therefore, we think the values of the \( \eta' \) mass very likely have a non-negligible systematic uncertainty stemming from the fact that the signal for the \( \eta' \) is lost in noise at rather small \( t \)-values. We are currently investigating a solver for the GEVP using a singular value decomposition, which is better suited to deal with the noise. First results are encouraging.

Secondly, the strange (and charm) quark mass values are different among the three values of the lattice spacing. The strange quark mass value has a strong influence on the \( \eta' \) meson mass, as we learn from \( A80.24, A80s, A100.24 \) and \( A100.24s \), see figure 3.

Finally, as some of our ensembles have a value of \( M_{PS} \cdot L < 3.5 \) it is interesting to estimate finite size corrections to \( M_\eta \) and \( M_{\eta'} \). We have two ensembles which differ only in \( L/a \), namely \( A40.24 \) and \( A40.32 \) with \( M_{PS} \cdot L = 3.5 \) and \( M_{PS} \cdot L = 4.5 \), respectively. For these two ensembles both masses agree within errors. In particular, \( M_\eta \) agrees precisely, as can be seen from table 3. On the same ensembles we measure a finite-size effect for the kaon of below 1%. Therefore, we conclude that at our current level of precision finite size corrections to \( M_\eta \) and \( M_{\eta'} \) are not significant. Of course, for a definite conclusion more ensembles with different \( L/a \)-values are needed.

4.2 Scaling Artifacts and Strange Quark Mass Dependence of \( M_\eta \)

For \( M_\eta \) the statistical uncertainty is sufficiently small to allow for a meaningful scaling test. For this we need to compare \( M_\eta \) at the three different values of
the lattice spacing for fixed values of for instance \(r_0 M_K, r_0 M_D, r_0 M_{PS}\) and the physical volume. From volume and the charm quark mass value we expect only little influence given our uncertainties and hence, we are going to disregard effects from slightly different physical volumes at the different \(\beta\)-values and the differences in the charm quark mass in the following.

As we do not have simulations at the three values of the lattice spacing with matched values of \(r_0 M_K\), we have to perform an interpolation in \(M_K\). For this procedure we have to rely on two pairs of ensembles, namely \((A80.24, A80.24s)\) and \((A100.24, A100.24s)\). The two ensembles within a pair differ in the values of \(a\mu_{\sigma}\) and \(a\mu_\delta\), whereas \(a\mu_\ell\) is identical. We can use these ensembles to estimate the derivative \(D_\eta\) of \(M_\eta^2\) with respect to \(M_K^2\) and use this estimate to correct for the mismatch in \(r_0 M_K\). By using this estimate of the derivative for all ensembles – not only \(A80.24\) and \(A100.24\) – we neglect the dependence of \(D_\eta\) on the lattice spacing and the light and charm quark masses.

In more detail, we treat the masses of the \(\eta\)-meson and the kaon like in chiral perturbation theory as functions \(M^2 = M^2[M_{PS}^2, M_K^2]\) and define the dimensionless quantity

\[
D_\eta(\mu_\ell, \mu_{\sigma}, \mu_\delta, \beta) \equiv \left[ \frac{d(aM_\eta)^2}{d(aM_K)^2} \right].
\]  

Next we make the approximation that \(D_\eta\) is independent of the quark mass values \(\mu_\ell, \mu_{\sigma}, \mu_\delta\) and \(\beta\). Its value is actually equal within errors when estimated from \(A80.24\) and \(A80.24s\) or from \(A100.24\) and \(A100.24s\) and on average we obtain \(D_\eta = 1.60(18)\).
Now we use this value of \( D_\eta \) to correct the three ensembles \( A60, B55 \) and \( D45 \) – which have approximately equal values of \( r_0 M_\text{PS} \approx 0.9 \) – to a common value of \( r_0 M_K \approx 1.34 \) using

\[
(r_0 \bar{M}_\eta)^2 = (r_0 M_\eta)^2 + D_\eta \cdot \Delta_K,
\]

where \( \Delta_K \) is the difference in the squared kaon mass values (in units of \( r_0 \)). We plot the resulting \( r_0 \bar{M}_\eta \) values for the three ensembles \( A60, B55 \) and \( D45 \) as a function of \( (a/r_0)^2 \) in the left panel of figure 5. The data are compatible with a constant continuum extrapolation \( r_0 M_\eta^{a \to 0, \text{const}} = 1.480(34) \), which we indicate by the horizontal line. We can also attempt a linear extrapolation, which is also shown in the figure, leading to \( r_0 M_\eta^{a \to 0, \text{lin}} = 1.61(14) \). The difference in between the two extrapolated values

\[
r_0 \Delta M_\eta^{a \to 0} = 0.13(13)
\]  

(22)
gives us an estimate on the systematic uncertainty to be expected from the continuum extrapolation. We cannot repeat this analysis for more values of \( r_0 M_\text{PS} \), as we have currently only two \( D \) ensembles analysed. We will therefore quote a 8% relative error from \( \Delta M_\eta^{a \to 0}/M_\eta^{a \to 0, \text{const}} \) for our mass estimates, which we believe is a conservative figure.

Nevertheless, in order to obtain a more complete picture, we now attempt to correct all our ensembles for the slightly miss-tuned value of \( M_K \). For this we adopt the following procedure: first we perform a linear fit

\[
g_K[(r_0 M_\text{PS})^2, a, b] = a + b \cdot (r_0 M_\text{PS})^2
\]

(23)
to the values of \( (r_0 M_K)^2 \) for the \( A \)-ensembles (without \( A80.24s \) and \( A100.24s \)). We obtain \( a = 1.492(6) \) and \( b = 0.571(8) \). This curve is then shifted to a value \( \tilde{a} = 1.238(6) \) such that \( (r_0 M_K^{\text{exp}})^2 = g_K[(r_0 M_\pi)^2, \tilde{a}, b] \). We denote this new function by \( \tilde{g}_K = g_K[(r_0 M_\text{PS})^2, \tilde{a}, b] \). The two curves corresponding to \( g_K \) and \( \tilde{g}_K \) are shown in the left panel of figure 4. As it turns out, the kaon masses for the two tuned ensembles \( A80.24s \) and \( A100.24s \) are already very close to \( \tilde{g}_K \). Now we can correct the remaining \( A \) ensembles as well as the \( B \) and \( D \) ensembles to the same line of \( \tilde{g} \) by computing the difference of the squared kaon mass values to \( \tilde{g} \)

\[
\delta_K[(r_0 M_\text{PS})^2] = (r_0 M_K)^2[(r_0 M_\text{PS})^2] - \tilde{g}_K[(r_0 M_\text{PS})^2],
\]

which we can use to correct the measured \( M_\eta^2[(r_0 M_\text{PS})^2] \) corresponding to

\[
(r_0 \bar{M}_\eta)^2[(r_0 M_\text{PS})^2] = (r_0 M_\eta)^2[(r_0 M_\text{PS})^2] + D_\eta \cdot \delta_K[(r_0 M_\text{PS})^2].
\]

(24)
The result of this procedure is shown in the right panel of figure 5: we show values of \( r_0 \bar{M}_\eta \) for all our ensembles as a function of \( (r_0 M_\text{PS})^2 \). It is evident that all the data fall on a single curve within statistical uncertainties. Figure 5
Fig. 6. (a) $M_\eta/M_K$ as a function of $(r_0 M_{\pi})^2$ for all available ensembles. (b) GMO ratio (see text) as a function of $(r_0 M_{\pi})^2$ for all available ensembles. Experimental values are horizontally displaced for legibility. Confirms that $M_\eta$ is not affected by large cut-off effects. Note again that we ignored the $\mu_\ell$, $\mu_\sigma$, $\mu_\delta$ and $\beta$ dependence of $D_\eta$ and that we cannot fully estimate the systematics stemming from this approximation.

4.3 Extrapolation to the Physical Point

As $\bar{g}[(r_0 M_\pi)^2] = (r_0 M_{K}^{\text{exp}})^2$ – and the strange quark mass was fixed to its physical value using $M_{K}^{\text{exp}}$ – we can next attempt a linear fit to all corrected (by the procedure discussed above) data points for $(r_0 M_{\eta})^2[(r_0 M_{\pi})^2]$. Using $r_0 = 0.45(2)$ as discussed in section 2, the fit yields $r_0 M_\eta [r_0^2 M_{\pi}^2] = 1.252(58)_{\text{stat}}(100)_{\text{sys}}$ and in physical units

$$M_\eta(M_\pi) = 549(33)_{\text{stat}}(44)_{\text{sys}} \text{ MeV},$$

where the experimental mass-value of the neutral pion $M_{\pi^0} = 135$ MeV has been used for $M_\pi$. In the $SU(2)$ chiral limit we obtain $r_0 M_\eta^0 = 1.230(65)_{\text{stat}}(98)_{\text{sys}}$ or

$$M_\eta^0 = 539(35)_{\text{stat}}(43)_{\text{sys}} \text{ MeV}.$$  

For estimating the systematic error we used the ratio $\Delta M_\eta^{a\to0}/M_\eta^{a\to0}$ as discussed above. Note that the error on $r_0 = 0.45(2)$ significantly contributes to the statistical errors for the results in physical units.

As the procedure presented above relies on the assumption that $D_\eta$ is independent on $\mu_\ell$, $\mu_\sigma$, $\mu_\delta$ and $\beta$, it would be desirable to have a cross-check. Inspecting figure 4 once more, one observes that $M_\eta$ and $M_K$ appear to have a similar strange quark mass dependence. This motivates to search for an
appropriate ratio of quantities in which the strange quark mass dependence cancels approximately. One option is to study the ratio \( M_\eta/M_K \), which is shown in the left panel of figure 6 as a function of \((r_0 M_{PS})^2\) for all available ensembles. Strikingly, within errors all data points fall on the same curve, and in particular the points for A80.24s and A80.24s and A100.24 and A100.24s agree within errors, respectively. This confirms in particular that most of the strange quark mass dependence cancels in the ratio. Extrapolating all the data for \((M_\eta/M_K)^2\) linear in \((r_0 M_{PS})^2\) to the physical pion mass point we obtain

\[
(M_\eta/M_K)_{M_\pi} = 1.121(26) ,
\]

which is in good agreement with the experimental value \((M_\eta/M_K)_{exp} = 1.100\). Using the experimental value of \(M_K^0 = 498\) MeV we obtain

\[
M_\eta = 558(13)_{stat}(45)_{sys} \text{ MeV} ,
\]

where the first error is statistical and the second systematical as estimated from the scaling violations discussed above. The latter represents a rather conservative estimate since some of the scale dependence might cancel in the ratio \(M_\eta/M_K\). Note that in this procedure the scale \(r_0 = 0.45(2)\) fm enters only for determining the physical pion mass point. As the slope of the extrapolation is rather small, the statistical uncertainty in \(M_\eta\) is smaller than for the direct extrapolation of \((r_0 M_\eta)^2\).

Alternatively, motivated from chiral perturbation theory, we also study the GMO relation

\[
3M_\eta^2 = 4M_K^2 - M_\pi^2 .
\]

It is valid in the SU(3) symmetric case, but violated only by a few percent with physical values of the corresponding meson masses. Therefore, the strange quark mass dependence of \(3M_\eta^2/(4M_K^2 - M_\pi^2)\) should be weak. We show the dimensionless ratio \(3M_\eta^2/(4M_K^2 - M_\pi^2)\) as a function of \((r_0 M_{PS})^2\) in the right panel of figure 6. The first interesting remark on this figure is that again the data points for the ratio from A80.24 and A80.24s (A100.24 and A100.24s) – which differ in the bare strange quark mass – agree within errors, confirming that a large part of the strange quark mass dependence cancels in the ratio (like for \(M_\eta/M_K\)). Again, all the data points fall onto one single line within errors, independent of the value of the lattice spacing, the strange and the charm quark mass. If we fit a linear function in \((r_0 M_{PS})^2\) to the data we obtain

\[
\left(3M_\eta^2/(4M_K^2 - M_\pi^2)\right)_{M_\pi} = 0.966(48)
\]

at the physical pion mass, which is in agreement with experiment, \((3M_\eta^2/(4M_K^2 - M_\pi^2))_{exp} = 0.925\). Using the experimental values of \(M_\pi^0\) and \(M_K^0\) we now obtain

\[
M_\eta = 559(14)_{stat}(45)_{sys} \text{ MeV} ,
\]

18
Fig. 7. Comparison of our results for $M_\eta$ (filled symbols) (corrected for the mismatch in $M_K$ as discussed in the text) and $M_{\eta'}$ (open symbols) in physical units for all three values of the lattice spacing to results from the literature (RBC/UKQCD [2], HSC [4], UKQCD [5]. The scale for our points was set using $r_0 = 0.45(2)$ fm.

where the first error is statistical and the second systematical estimated from the scaling violations discussed above.

We remark that our value for $D_\eta = 1.60(18)$ is in rather good agreement to the value $4/3$ one would obtain naively from eq. (26).

In the results we quoted for the physical value of $M_\eta$ we specified a systematic uncertainty of 8% stemming from the continuum extrapolation. As we have some ensembles with small values of $M_{PS} \cdot L$, one might wonder how finite size corrections to $M_K$ and $M_{PS}$ influence our extrapolations. This influence is smaller than our statistical uncertainty for the following reasons: firstly, the pion mass dependence of $M_\eta$ is very weak. Secondly, corrections to $M_K$ appear to be small, as discussed earlier. And thirdly, only a few ensembles have small $M_{PS} \cdot L$, and hence, a small change in these does not affect the fit result significantly. As soon as the results for $M_\eta$ get even more precise the analysis should include finite size corrections to $M_{PS}$ and $M_K$.

In figure 7 we show a compilation of our results for $\eta$ masses (corrected for the mismatch in $M_K$, cf. figure 5) and $\eta'$ masses and those available in the literature for $N_f = 2+1$ flavour lattice QCD: in Ref. [3] $\eta$ and $\eta'$ meson masses have been computed using $N_f = 2+1$ flavours of overlap quarks at one value of the lattice spacing and large values of the pion mass. In this reference not enough details are given to be included in our comparison figure 7. In Ref. [2]
these masses have been determined using $N_f = 2 + 1$ flavours of domain wall fermions, again at a single value of the lattice spacing $a \approx 0.1$ fm and three values of the pion mass ranging from about 400 MeV to about 700 MeV. The corresponding data points are labeled RBC/UKQCD in figure 7. In Ref. [4] the Hadron Spectrum Collaboration (HSC) – also at a single value of the lattice spacing – and one value of the pion mass used Wilson fermions. Finally, in Ref. [5] data is presented for two values of the pion mass, each at a different value of the lattice spacing with staggered fermions, labeled as UKQCD in our plot. As discussed previously, we used a value of $r_0 = 0.45(2)$ fm to set the scale for our data.

Firstly, from figure 7 it is clear that the results presented in this paper significantly increase the available data for $\eta$ and $\eta'$ masses from lattice QCD. In particular, our results extend to significantly lower values of the pion mass than available before. And, within the statistical uncertainties, all the results from the different lattice formulations agree, despite the fact that the systematic uncertainties are not taken into account, and that we used $N_f = 2 + 1 + 1$ dynamical quark flavours.

Secondly, figure 7 allows to compare the statistical uncertainties quoted by the different collaborations. The figure shows that our error on the $\eta'$ masses are by far larger than what is quoted by the other collaborations. RBC/UKQCD [2] have investigated 300 configurations separated by 20 HMC trajectories, and they did not find autocorrelation among these configurations for the investigated quantities. The HSC [4] used 479 configurations also separated by 20 HMC trajectories. Both collaborations use a lattice spacing around 0.12 fm, i.e. significantly larger than our coarsest value. Compared to these two collaborations we have hence a similar number of independent configurations per ensemble, but smaller values of the lattice spacing. Our method to compute disconnected contributions involves stochastic noise, which is not the case for these two collaborations. However, we have tested that the stochastic noise is not dominantly affecting our results; the gauge noise is dominant in our data. Compared to RBC/UKQCD we have a similar number of inversions per independent gauge configuration, while HSC has many more. Clearly, the large operator basis used by HSC will help to extract the states with higher precision. An explanation for the smaller errors found by RBC/UKQCD might be the better chiral properties of their formulation, the larger value of the lattice spacing and the smaller volume in lattice units. In the staggered investigation by UKQCD [5] a similar method to ours was used, but with a larger number of independent configurations.

We would like to point out again that the large error on $M_{\eta'}$ also reflects the systematic uncertainty in identifying a plateau in its effective mass, as discussed earlier.
Fig. 8. (a) mixing angle $\phi^L$ from local amplitudes of a $4 \times 4$-matrix (no charm quark).
(b) mixing angle $\phi^F$ from fuzzed amplitudes of $6 \times 6$-matrix (including charm quark)

4.4 $\eta$ and $\eta'$ Mixing

As mentioned previously, the determination of the $\eta$ and $\eta'$ mixing angles requires the knowledge of the ratio of renormalisation constants $Z$ as discussed above.

We determine the amplitudes $A_{\ell,\eta}$, $A_{\ell,\eta'}$, $A_{s,\eta}$ and $A_{s,\eta'}$ from a factorising fit to the correlation matrix $C(t)$ rotated to its original form. For the factorising fit we consider only light and strange degrees of freedom (both, local and fuzzed), as the charm does not contribute within errors. We then determine $\phi_{\ell}$ and $\phi_s$ from eq. (19) and $\phi$ from eq. (20). The errors are again determined using a bootstrap procedure with 1000 bootstrap samples. All results from a $4 \times 4$ matrix fit are collected in tab. 4. Results from a $6 \times 6$ matrix can be found in the appendix.

The results for $\phi$ are shown in figure 8. In the left panel we show $\phi$ in degrees determined from local amplitudes (L), and in the right panel from fuzzed amplitudes (F), both as a function of $(r_0M_{PS})^2$. Both agree nicely and we do not observe a dependence on the lattice spacing and $(r_0M_K)^2$, at least within the relatively large errors. The dependence on $(r_0M_{PS})^2$ is weak, the data is compatible with a linear extrapolation to the physical pion mass point, which leads to a value of

$$\phi = 44(5)^\circ,$$

using a combined fit to local and fuzzed data. In the octet basis this would correspond to a $\eta_8, \eta_1$ mixing angle $\theta = \phi - 54.7^\circ = -10(5)^\circ$. For this extrapolation we ignored a possible strange and charm quark mass dependence of $\phi$. Our result for $\phi$ is in agreement with the results from RBC/UKQCD [2], HSC [4] and an old UKQCD work [34], which all quote something in between
40° and 50°. In the recent UKQCD staggered investigation [5] a value of 34(3)° is favoured. Comparing to experimental and phenomenological results [29,35,5] we find excellent agreement to results from radiative decays and glueball mixing (∼ 42°). Results from photon fusion and charm-η production favour a value of ∼ 33°. Note that one has to keep in mind that our determination of the mixing angle is likely to be affected by systematic uncertainties.

We have checked that this determination is not affected by our uncertainty on the ratio of renormalisation constants $Z$. For this we varied $Z$ in a large range from 0.4 to 1.0, and we found that this does not affect the extraction of the mixing angles. As an example we show the dependence of $\phi^L$ for ensemble D15.48 in figure 9 on $Z$. The variation introduced by $Z$ is by far smaller than the statistical uncertainty. We observe the same for the other ensembles and conclude that our evaluation of the angles is not affected by systematic uncertainties stemming from the $Z$ ratio within our statistical uncertainties.

While figure 8 indicates that the angle $\phi$ behaves regularly and the linear extrapolation to the physical pion mass appears to be reasonable, the results for $\phi_t$ and $\phi_s$ are diverse, see table 4. We attribute this to large statistical and systematic uncertainties in these quantities. We hope to be able to investigate $\phi_t$ and $\phi_s$ further once we have improved our determination of the $\eta'$ state.

5 Summary and Discussion

We presented the first computation of $\eta$ and $\eta'$ meson masses from lattice QCD with degenerate up/down, heavier strange and even heavier charm dynamical quarks in the Wilson twisted mass formulation. Our results based on ETMC
gauge configurations cover three values of the lattice spacing from $\sim 0.09$ fm down to $\sim 0.06$ fm and a range of pion masses from 230 MeV to 500 MeV. The results presented here are therefore the first covering three values of the lattice spacing and a range of pion masses down to 230 MeV. Kaon and D-meson masses are close to their physical values. We observe in both, $\eta$ and $\eta'$ masses, only a mild dependence on the light quark mass. The $\eta$ meson mass can be determined with high statistical accuracy, while the $\eta'$ suffers from noise and large autocorrelation times.

In our simulations, the bare strange and charm quark masses were kept fixed for each value of the lattice spacing separately, apart from two additional $A$-ensembles. As the kaon mass values deviate from the experimental values by up to 10%, we applied three methods to correct for this mismatch: firstly, by estimating the strange quark mass dependence from the aforementioned additional $A$-ensembles, secondly by considering the ratio $M_{\eta}/M_K$ and thirdly, by using the GMO relation eq. 26. All three methods seem to indicate that lattice artifacts are only weakly affecting the $\eta$ mass. As our best estimate we extract

$$M_\eta = 557(15)_{\text{stat}}(45)_{\text{sys}} \text{ MeV}$$

by a weighted average over the three methods. The first error is statistical and the second systematic from the continuum extrapolation. The result is in good agreement with the experimental value for $M_\eta$.

We also determine the $\eta$ and $\eta'$ mixing angle $\phi$ using amplitudes from a factorising fit model. Again, we observe little light quark mass and lattice spacing dependence within errors. But this time also the strange quark mass dependence is smaller than our (large) statistical uncertainty. Our best estimate for the mixing angle $\phi$ is

$$\phi = 44(5)$$

with statistical error only. In an octet basis this corresponds to $\theta = -10(5)^\circ$. The agreement of our estimate for $\phi$ with most experimental and phenomenological [29,35] and most other lattice determinations [2,4,34] is excellent. The value is also very close to the quadratic GMO estimate of 44.7°. But results from photon fusion and charm-$\eta$ production, as well as the lattice determination from ref. [5] find a value of $\sim 34^\circ$. Estimating the systematics for the angle becomes difficult, because the statistical uncertainties for each ensemble are large.

It is evident that the $\eta'$ mass is affected by large statistical and systematical uncertainties. It also shows a large autocorrelation time. Hence, we currently cannot make a reliable estimate of the physical $\eta'$ mass value. We therefore plan in the future to apply additional noise reduction techniques to get a better signal also for the $\eta'$ state. There are actually two promising approaches, the point-to-point method described in ref. [6] and an extension of the noise reduction trick used here only for estimating the light disconnected contribu-
tions. Also, investigating the SVD solver further might be a promising way forward.

Finally, determining the flavour singlet decay constants is of large phenomenological interest. We are currently investigating our signals for \( \langle 0 | A_\mu | \eta \rangle \) and \( \langle 0 | A_\mu | \eta' \rangle \).

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A.1 Generalised Eigenvalue Problem (GEVP)

For the determination of masses and identification of flavour contents of the states we employ the variational approach in eq. (14). We extract the eigenvalues $\lambda^{(n)}(t, t_0)$ from the GEVP and determine then the masses from a fit to $\lambda$. The errors of $\lambda$ are determined using a bootstrap procedure with 1000 bootstrap samples, after the data is blocked in order to account for autocorrelation. An overview of the remaining GEVP and fitting parameters is listed in table A.1. Due to the rather large difference in the signal-to-noise ratio between the two lowest lying states we use two different approaches for $\eta$ and $\eta'$:

1. For the ground-state ($\eta$) we fit a single $\cosh$ in $t$ in a region $[t^\eta_1, t^\eta_2]$ to our data for $\lambda^{\eta}(t, t_0)$. The lower bound of the fit-range $t^\eta_1$ is chosen by visual inspection of the effective mass plot to lie at the beginning of the plateau and also such that further increasing $t^\eta_1$ does not change the value of the resulting mass within errors. The latter is also true for the choice of the starting value $t^\eta_0$ in eq. (14). In principal choosing $t_0$ larger leads

| ensemble | $t^\eta_0$ | $t^\eta_1$ | $t^\eta_2$ | $(\chi^2)^\eta$/dof | $t^{\eta'}_0$ | $t^{\eta'}_1$ | $t^{\eta'}_2$ | $(\chi^2)^{\eta'}$/dof |
|----------|------------|------------|------------|---------------------|------------|------------|------------|---------------------|
| A30.32   | 2          | 7          | 17         | 0.205               | 1          | 2          | 11         | 0.277               |
| A40.24   | 2          | 7          | 16         | 0.135               | 1          | 2          | 10         | 0.185               |
| A40.32   | 2          | 7          | 15         | 0.092               | 1          | 2          | 10         | 0.130               |
| A60.24   | 2          | 7          | 15         | 0.137               | 1          | 2          | 10         | 0.296               |
| A80.24   | 2          | 7          | 16         | 0.108               | 1          | 2          | 10         | 0.137               |
| A100.24  | 2          | 7          | 15         | 0.214               | 1          | 2          | 11         | 0.137               |
| A80.24s  | 2          | 7          | 17         | 0.230               | 1          | 2          | 11         | 0.440               |
| A100.24s | 2          | 7          | 16         | 0.086               | 1          | 2          | 10         | 0.116               |
| B25.32   | 3          | 6          | 11         | 0.222               | 1          | 2          | 11         | 0.463               |
| B35.32   | 2          | 8          | 17         | 0.110               | 1          | 2          | 10         | 0.433               |
| B55.32   | 2          | 8          | 18         | 0.167               | 1          | 2          | 11         | 0.366               |
| B75.32   | 2          | 8          | 14         | 0.301               | 1          | 2          | 10         | 0.338               |
| B85.24   | 2          | 8          | 16         | 0.106               | 1          | 2          | 10         | 0.127               |
| D15.48   | 3          | 8          | 16         | 0.190               | 2          | 3          | 12         | 0.114               |
| D45.32sc | 3          | 8          | 19         | 0.1743              | 2          | 3          | 18         | 0.105               |

Table A.1
Parameters of the GEVP applied to the 6×6-matrix from local and fuzzed operators.

In this appendix we summarise the technical details of our numerical methods for extracting masses and angles.
| $\beta$ | 1.90 | 1.95 | 2.10 |
|---|---|---|---|
| $Z$ | 0.6703(8) | 0.6859(9) | 0.7493(11) |

Table A.2
Values for $Z$ from matching mixed action (Osterwalder-Seiler) to unitary approach.

to smaller masses, though due to noise we are only able to moderately increase $t_0$ before the error gets too large.

(2) For the first excited state ($\eta'$) we perform a three state cosh-fit to the data of $\lambda^{\eta'}(t, t_0)$, starting from the lowest $t_1^{\eta'}$ possible, i.e. $t_1^{\eta'} = t_0^{\eta'} + 1$ in order to use as many points as possible. This is necessary because for many ensembles there is no clear plateau in the effective masses reached before the signal is lost in noise. Therefore, this procedure is a major source of systematic error for the determination of $\eta'$ masses, at least for those cases where only few points are available. Only for the $D$-Ensembles it turns out to be possible to choose $t_0^{\eta'} > 1$, for all other ensembles we had to use $t_0^{\eta'} = 1$.

The upper bound of the fit range $t_2^n$ is independently determined for every state $n$ by the last eigenvalue $\lambda^{(n)}(t_2, t_0)$ distinguishable from noise. Note that the value of $t_2$ is not very important for the fit, as eigenvalues at large $t$ have typically large errors and therefore do not contribute much to the fit.

\textit{A.2 Factorising fit model}

For the extraction of amplitudes which are required to calculate mixing angles we employ the factorising fit model as detailed in eq. (16) to the matrix in the original twisted basis in eq. (9). We limit ourselves to $n = 2$ in eq. (16), i.e. a two state fit. As discussed before the ratio of renormalisation constant $Z = Z_P/Z_S$ does not affect masses and angles, but only amplitudes. For the results of the angles we used the values summarised in table A.2. They have been obtained by matching a mixed action to the unitary action and extrapolating to the chiral limit, see ref. [39]. These values agree well with the RI-MOM determination of ETMC [28,27], and the method we discussed in the text.

As we have already determined the masses from the GEVP, we use those together with their errors (see table 3) as priors to our factorising fit. This stabilises the fit procedure, but we have checked that it does not affect the result. We always use an uncorrelated $\chi^2$ function, because the correlation matrix is too noisy. Table A.3 lists the input parameters and the resulting uncorrelated $\chi^2$/dof for the fits to the $4 \times 4$ (light and strange degrees of freedom, local and fuzzed) and $6 \times 6$ (light, strange charm, and local and fuzzed) correlator matrix. The results quoted in the main text for the angles
Table A.3
Parameters for the factorising fit.

were determined using the $4 \times 4$ matrix, because the charm does not contribute. However, with the $6 \times 6$ matrix we obtain almost identical results.

The value of the lower bound of the fit range $t_1$ is chosen to be constant for every value of the lattice spacing, whereas the choice of the upper bound $t_2$ is determined by the requirement that $\chi^2$/dof < 1, and that it is close to the $t^\eta_2$ used for GEVP.