Quark masses and decay constants in $N_f = 2 + 1 + 1$ isoQCD with Wilson clover twisted mass fermions

G. Bergner$^a$, P. Dimopoulos$^b$, J. Finkenrath$^c$, E. Fiorenza$^d$, R. Frezzotti$^e$, M. Garofalo$^f$, B. Kostrzewa$^g$, F. Sanfilippo$^h$, S. Simula$^h$, U. Wenger$^i$

$^a$ University of Jena, Institute for Theoretical Physics, Max-Wien-Platz 1, D-07743 Jena, Germany
$^b$ Dipartimento di Scienze Matematiche, Fisiche e Informatiche, Università di Parma, via Università, 12 - I 43121 Parma
$^c$ Computation-based Science and Technology Research Center, The Cyprus Institute, 20 Konstantinou Kavafi Street, 2121 Nicosia, Cyprus
$^d$ CP3 -Origins & IMADA, University of Southern Denmark, Campusvej 55, 5230 Odense, Denmark
$^e$ University of Rome Tor Vergata and INFN Roma Tor Vergata, Via della Ricerca Scientifica 1, I-00133, Rome, Italy
$^f$ Dip. di Matematica e Fisica, University of Roma Tre, Via della Vasca Navale 84, I-00146 Rome, Italy
$^g$ HISKP (Theory), Rheinische Friedrich-Wilhelms-Universität Bonn, Nussallee 14-16, 53115 Bonn, Germany
$^h$ INFN section of Roma Tre, Via della Vasca Navale 84, I-00146 Rome, Italy
$^i$ Institute for Theoretical Physics, Albert Einstein Center for Fundamental Physics, University of Bern, Sidlerstr. 5, CH-3012 Bern, Switzerland

We present a preliminary study of the pion, kaon and D-meson masses and decay constants in isosymmetric QCD, as well as a preliminary result for the light-quark renormalized mass. The analysis is based on the gauge ensembles produced by ETMC with $N_f = 2 + 1 + 1$ flavours of Wilson-clover twisted mass quarks, spanning a range of lattice spacings from $\sim 0.10$ to $0.07$ fm and include configurations at the physical pion point on lattices with linear size up to $L \sim 5.6$ fm.

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$^*$Speaker.
$^†$marco.garofalo@roma2.infn.it

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1. Action

We present a preliminary analysis based on the gauge ensembles produced by the Extended Twisted Mass Collaboration (ETMC) in isosymmetric QCD (isoQCD) with $N_f = 2 + 1 + 1$ flavours of Wilson-clover twisted mass quarks [1], i.e. in a lattice setup where physical observables can be evaluated at maximal twist with no $O(a)$ scaling violations [2]. The lattice action is given by

$$S = S_g + S_{tm}^l + S_{tm}^d,$$

where for $S_g$ we choose the Iwasaki improved gluon action (see e.g. eq. (2) of [1]). For the light (up and down) sea quark doublet $\chi_l = (u, d)^T$, the twisted mass action [3] takes the form

$$S_{tm}^l = \sum S_l(x) \left[ D_W(U) + \frac{i}{4} c_{SW} \sigma_{\mu\nu} F_{\mu\nu}(U) + m_0 + i\mu_l \tau_3 \gamma_5 \right] \chi_l(x).$$

(1.1)

where $\mu_l$ is the twisted and $m_0$ the (untwisted) Wilson bare quark mass. The Pauli matrix $\tau_3$ acts in flavour space and $D_W$ is the massless Wilson-Dirac operator. The Wilson quark mass $m_0$ and the clover term $\frac{1}{4} c_{SW} \sigma_{\mu\nu} F_{\mu\nu}(U)$ with Sheikoleslami-Wohlert improvement coefficient $c_{SW}$ [4] are trivial in flavour space.

For the strange ($s$) and charm ($c$) sea quark pair (field $\chi_h = (c, s)^T$) the action reads [5]

$$S_{tm}^h = \sum_x R_h(x) \left[ D_W(U) + \frac{i}{4} c_{SW} \sigma_{\mu\nu} F_{\mu\nu}(U) + m_{0h} - \mu_3 \tau_1 + i\mu_5 \tau_2 \gamma_5 \right] \chi_h(x).$$

(1.2)

The term $\mu_5 \tau_1$ is absent in eq. (1.2) as the $u$ and $d$ quarks are mass degenerate. By tuning the light and heavy Wilson bare quark masses $m_0$ and $m_{0h}$ to their common critical value $m_{\text{crit}}$ the maximally twisted fermion action is obtained for which all physical observables are $O(a)$-improved [2, 5].

In this framework isospin breaking lattice artifacts affect significantly the unitary neutral pion mass making it typically smaller than its charged counterpart, which in turn may render unquenched Monte Carlo simulations numerically unstable. This phenomenon here is substantially suppressed by introducing a clover term in the action [6, 1], which proves crucial for simulations close to the physical pion point with lattice spacings in the range $(0.10, 0.07)$ fm [1], where topological freezing is not a problem. Within $\sim 10\%$ accuracy, the clover term coefficient $c_{SW}$ can be fixed through its estimate in one-loop [7] tadpole boosted perturbation theory, namely $c_{SW} \approx 1 + 0.113(3) \frac{\delta^2}{P}$ with $P$ the plaquetto expectation value. Here we follow this prescription at all values of $\delta^2$ (corresponding to lattice spacings $a \sim 0.10, 0.08, 0.07$ fm - see Sect. 2). The parameters of the various simulation ensembles are shown in Table 1.

For the ($c, s$) quark sector we adopt a mixed action setup using Osterwalder-Seiler fermions in the valence, with the same critical mass, $m_{\text{crit}}$, as determined in the unitary setup and with action [8]

$$S_{tmOS}^{h, val} = \sum f = c, s \sum_{x} R_f(x) \left[ D_W(U) + \frac{i}{4} c_{SW} \sigma_{\mu\nu} F_{\mu\nu}(U) + m_{\text{crit}} + i\mu_5^{OS} \right] \chi_f(x).$$

(1.4)

Reflection positivity of renormalized correlation functions in the continuum limit is guaranteed because the renormalized $c$ and $s$ valence masses are matched to their sea counterparts through

$$m_{\text{ren}}^{val, ren} = \frac{1}{Z_P} \left( \mu_\sigma \pm \frac{Z_P}{Z_S} \mu_\delta \right),$$

(1.5)
Table 1: Simulations details for the ETMC gauge ensembles with \( N_f = 2 + 1 + 1 \) Wilson-clover twisted mass quarks: volume, number of gauge configurations analyzed, \( \kappa = (8 + 2am_{\text{crit}})^{-1} \), bare twisted masses \( a\mu_l, a\mu_s, a\mu_\delta \), and \( \beta \). We have set \( c_{SW} = [1.74, 1.69, 1.645] \) for \( \beta = [1.726, 1.778, 1.836] \), respectively.

<table>
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<tr>
<th>name</th>
<th>( L^3 \cdot T/a^4 )</th>
<th>Nconf</th>
<th>( \kappa )</th>
<th>( a\mu_l )</th>
<th>( a\mu_s )</th>
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<td>24 \cdot 48</td>
<td>628</td>
<td>0.1400645</td>
<td>0.0053</td>
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<td>0.1521</td>
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<tr>
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<td>322</td>
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<td>0.0012</td>
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<td>0.1521</td>
<td>1.726</td>
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<td>0.0025</td>
<td>0.1246864</td>
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<td>1.778</td>
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<td>210</td>
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Table 2: Values of the valence bare quark masses for each of the ensembles analysed here.

<table>
<thead>
<tr>
<th>name</th>
<th>( a\mu_{l,s,c}^{\text{valence}} )</th>
<th>( a\mu_l )</th>
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<tr>
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<td>0.0148</td>
<td>0.0185</td>
<td>0.0222</td>
</tr>
<tr>
<td>cB211.072.64</td>
<td>0.00072</td>
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<td>0.0185</td>
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<td>0.0128</td>
<td>0.0161</td>
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</table>

with \( Z_P \) and \( Z_\delta \) denoting the non-singlet pseudoscalar and scalar Wilson fermion quark bilinear renormalization constants. In this way we avoid any undesired \( s-c \) quark mixing (through cutoff effects) in the valence and preserve the automatic \( O(a) \) improvement of physical observables [8].

The masses of the sea strange and charm quarks are set, at each \( \beta \), to values close to the physical ones (with a few percent tolerance) through the tuning procedure described in Ref. [1]. As for valence mass parameters, we evaluated correlators at light valence quark mass \( \mu_l \), equal to its sea counterpart, as well as at three values of quark mass (\( \mu_s \)) in the strange region and four values of the quark mass (\( \mu_\delta \)) in the charm region (see Table 2), which allows for a precise interpolation to the physical \( s \) and \( c \) point as determined by the \( K \)- and \( D \)-meson masses. Quark propagators with light and strange-like valence masses are obtained from inversions of the Dirac Matrix using the DD\( \alpha \)AMG multi-grid algorithm optimized for twisted mass fermions [9].

For each ensemble we computed the two-point pseudo-scalar (PS) correlators defined as

\[
C(t) = \frac{1}{L^3} \sum_{x,z} \langle 0 | P_{qq}(x)P_{qq}(z)^\dagger | 0 \rangle \delta_{t,(t_{x} - t_{z})} ,
\]

where \( P_{qq}(x) = \bar{\chi}_q(x)\gamma_5\chi_q(x) \) with single-flavour \( \chi_q \) and \( q \) in \( \{ l, s, c \} \). In this work for all mesons the twisted mass of the two valence quarks \( q, q' \) are always taken with opposite signs (or equivalently in the physical quark basis of Ref. [2] the Wilson parameters of the two valence quarks take opposite values), as this choice is known to suppress \( O(a^2) \) errors. These two-point correlators are evaluated for the four combinations resulting from smeared or local interpolating fields at the sink and/or the source and analysed through the GEVP method [10] for the extraction of the ground-
state masses ($M_{PS}$) and matrix elements. We employ a Jacobi smearing of the quark fields [11] combined with APE smearing of the gauge links [12].

For maximally twisted quarks the value of the matrix elements $Z_{PS} = |\langle PS | P_{\mu} | 0 \rangle|^2$ determines the PS-meson decay constant with no need of any renormalization constant [3], namely

$$af_{PS} = a(\mu_\mu + \mu_\ell) \frac{\sqrt{a^4 Z_{PS}}}{aM_{PS}\sinh(aM_{PS})}.$$  (1.7)

For all ensembles the value of the bare parameter $a_\mu(\kappa)$ is tuned towards $am_{crit}$ so that the renormalized untwisted current quark mass $Z_{Aam\text{PCAC}}$ is well below $0.1a\mu_\ell$, which is enough to make negligible the $O(a)$ errors due to small numerical deviations from maximal twist. A marginal exception occurs only for the ensemble $cA211.12.48$, where a longer autocorrelation to make negligible the $O(a)$ of the pion mass at the physical point. The factor $Z_{PS}$ is tuned towards $am_{\text{PCAC}}$ observed in the MC simulation and $Z_{Aam\text{PCAC}} = -0.00015(4)$ for $a\mu_\ell = 0.0012$ is found. This small systematic error has been corrected by “reweighting” from $\kappa = 0.1400650$ to $\kappa_{\text{crit}} = 0.1400640$.

2. Lattice calibration and determination of $w_0$ from $f_\pi$

We carried out fits of the dependence of $f_\pi$, written in units of the gradient flow scale $w_0$ [13], on the meson mass $M_{\pi}^2$ using the SU(2) chiral perturbation theory (ChPT) formula

$$(f_\pi w_0) = (f_{w_0}) \left[ 1 - 2\epsilon_\mu^M \log \xi_\mu^M + P_3 \xi_\mu^M + \frac{a^2}{w_0^4} P_4 \right] K_{f_{\text{FSE}}}^{FSE},$$  (2.1)

where $\xi_\mu^M = M_{\pi}^2 \epsilon_\mu^2$ and $f$, which has been left free to vary in the fit, is the SU(2) low-energy-constant entering the leading order chiral effective Lagrangian. The parameter $P_3$ is related to the next-to-leading low-energy-constant $\bar{\ell}_4$ with $P_3 = 2\bar{\ell}_4 + 2\log \left( \frac{M_{\pi}^{\text{phys}}}{4\pi T} \right)^2$, with $M_{\pi}^{\text{phys}}$ being the value of the pion mass at the physical point. The factor $K_{f_{\text{FSE}}}^{FSE}$ represents the correction for finite size effects (FSE), as computed in Ref [14] with ChPT at NLO using a resummed asymptotic formula. To further check the values of $K_{f_{\text{FSE}}}^{FSE}$ the ETM Collaboration is generating further ensembles with the bare parameters equal to those of the ensemble $cB211.25.48$ (see Tab. 1) except for the volume. Using data from these ensembles we will be able to fix higher order details and cross-check reliability of the chiral PT FSE correction formulae we employ. The result of the fit (2.1) is plotted in Fig. 1. Imposing in the continuum limit at pion point that $M_{\pi} = 134.80$ MeV [15] and $f_{\pi}^{\text{phen}} = 130.41$ MeV [16] we find our preliminary estimate of the gradient flow scale $w_0$ and the other fit parameters (the coefficient describing lattice artefacts is compatible with zero)

$$w_0 = 0.1706(18) \text{ fm}, \quad f = 122.31(18) \text{ MeV}, \quad \bar{\ell}_4 = 4.3(1), \quad P_4 = -0.04(5).$$  (2.2)

The error quoted here and below in Eqs. (3.2), (3.4) and (4.3) are only statistical. Our value of the parameter $w_0$ is compatible with a previous estimate in the $N_f = 2 + 1 + 1$ theory [17]. In future studies we plan to set the scale using the $\Omega$ baryon mass rather than $f_{\pi}^{\text{phen}}$.

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1As discussed in [10] the mass of the lightest state is estimated through a $t$-plateau average of the smallest eigenvalue obtained (for a suitable choice of $t_0$) from the GEVP method, viz. $\lambda_0(t, t_0) = C \left( e^{-M_{\pi}(t-t_0)} + e^{-M_{\pi}(T-(t-t_0))} \right)$.
3. $f_K$ and $f_D$

In order to extract the decay constant $f_K$ at the physical point we first perform a small linear interpolation of our lattice data for each ensemble to three reference values of the quantity $B_{m_s}^{LO} = M_K^2 - M_\pi^2/2 = 0.186, 0.212, 0.252 \text{ GeV}^2$ which at the leading order in ChPT is proportional to the renormalised strange quark mass. Then for each value of $B_{m_s}^{LO}$ we extrapolate to the continuum limit and to the physical $M_\pi$ using our best fit to the data for $w_0 f_K$ according to the Ansatz

$$w_0 f_K = P_1 \left[ 1 - \frac{3}{4} \xi^M \log \xi^M + P_2^M \xi^M + P_4^M a^2 \right],$$

where $P_1^M, P_2^M$ and $P_4^M$ depend on the specific value of $B_{m_s}^{LO}$. In Fig. 2 (left panel) we show the chiral and continuum extrapolation for the largest $B_{m_s}^{LO}$.

Finally we interpolate linearly the three values of $f_K$ obtained in the continuum and chiral fit to the physical $B_{m_s}^{LO} = M_K^2 - M_\pi^2/2 = 0.233 \text{ GeV}^2$, i.e. $M_K = 494.2(4) \text{ MeV}$ [15], obtaining preliminary estimates of $f_K$ (for the scale set as in Sect. 2) and the ratio $f_K/f_\pi$.

$$f_K = 154(2) \text{ MeV}, \quad f_K/f_\pi = 1.182(16) \text{ MeV},$$

in nice agreement with previous ETMC result [18].

A similar analysis is performed to determine the decay constant of the $D$ meson. We first interpolate the data of each ensemble to certain reference masses $M_{D_s}^{ref} = 1.61, 1.73, 1.84, 1.95 \text{ GeV}$ (with scale from Sect. 2). Then for each $M_{D_s}^{ref}$ mass value we extrapolate to the continuum limit and the physical $M_\pi$ using our best fit to the data according to the polynomial Ansatz

$$w_0 f_D = P_1 \left( 1 + P_2 M_\pi^2 + P_3 M_\pi^4 + P_4 a^2 \right).$$

In Fig. 2 (right panel) we show the chiral and continuum extrapolation for one typical reference $M_{D_s}^{ref}$ value.

Finally the four values of $f_D$ obtained for different $M_{D_s}^{ref}$ in the continuum and physical pion mass limits, are interpolated linearly to the physical (isospin averaged) $M_D^{iso} = 1.867 \text{ GeV}$ [16], obtaining the preliminary (with scale set as in Sect. 2)

$$f_D = 215(6) \text{ MeV}.$$
We show our chiral and continuum fits. Imposing as above

\[ f_K \text{ is plotted at a fixed } B_m^{LO} = 0.252 \text{ GeV} \text{. } f_D \text{ is plotted at a fixed } M_D^{ref} = 1.61 \text{ GeV. } \]

The fit functions we employ are given in Eq. (3.1) for \( f_K \) and Eq. (3.3) for \( f_D \).

4. Renormalized light quark mass \( m_{ud} \)

In this section we present our preliminary result for the average light quark renormalized mass \( m_{ud} \). We fit the pion mass \( M_\pi \) and the decay constant \( f_\pi \) to the SU(2) ChPT formula

\[
(M_\pi w_0)^2 = 2(B w_0)(m_\ell w_0) \left[ 1 + \xi_\ell \log \xi_\ell + P_1 \xi_\ell + \frac{a^2}{w_0^2} P_2 \right] K_{FSE}^{FSE},
\]

\[
(f_\pi w_0) = (f w_0) \left[ 1 - 2 \xi_\ell \log \xi_\ell + P_3 \xi_\ell + \frac{a^2}{w_0^2} P_4 \right] K_{FSE}^{FSE},
\]

with the terms \( \propto P_2 \) and \( \propto P_4 \) describing the dominating lattice artifacts,

\[
\xi_\ell = 2 B_0 m_\ell / (16 \pi^2 f^2), \quad P_1 = -\bar{\ell}_3 - 2 \log \left( \frac{M_\pi^{phys}}{4 \pi f} \right), \quad P_3 = 2 \bar{\ell}_4 + 4 \log \left( \frac{M_\pi^{phys}}{4 \pi f} \right)
\]

and \( m_\ell = \mu_\ell / Z_\rho \) the renormalized mass. The renormalization factors \( Z_\rho \) have been calculated at each \( g_0^2 \) with \( \sim 1\% \) percent accuracy in the RI’-MOM scheme and then converted (with N3LO accuracy) to the \( \overline{\text{MS}} \) scheme using \( N_f = 4 \) gauge ensembles generated for the purpose of evaluating renormalization constants in mass-independent schemes. The quantity \( B, f, \bar{\ell}_3, \bar{\ell}_4, P_2, P_4 \) are left as fit parameters and the factor \( K_{FSE}^{FSE} \) represents the correction for FSE as computed in Ref. [14].

In Fig. 3 we show our chiral and continuum fits. Imposing as above \( M_\pi = 134.80 \text{ MeV and } f_\pi^{phys} = 130.41 \text{ MeV we find the preliminary results} \]

\[
m_{ud}(\overline{\text{MS}}, 2 \text{ GeV}) = 3.66(11) \text{ MeV}, \quad w_0 = 0.1703(18) \text{ fm, } \quad \bar{\ell}_3 = 2.9(2),
\]

\[
\bar{\ell}_4 = 4.3(1), \quad B = 2539(78) \text{ MeV, } \quad f = 122.1(2) \text{ MeV.}
\]

The values found for \( w_0, \bar{\ell}_4 \) and \( f \) are compatible with those in Eq. (2.2).

5. Outlook and Acknowledgements

We have discussed a first analysis of the gauge ensembles produced by ETMC with \( N_f = 2 + 1 + 1 \) flavours of Wilson-clover twisted mass quarks. The results are preliminary because a thorough study of the systematic uncertainties in finite size corrections, in the chiral and continuum extrapolations and in the computation of \( m_{ud} \) renormalization constant is not included here.
Figure 3: Preliminary chiral and continuum fits of $M_\pi$ (left) and $f_\pi$ (right) as a function of the renormalized quark mass $m_\ell$ in units of the gradient flow scale $w_0$ [13].

However already at this stage it is apparent that the physical pion mass point is safely reached and quite small lattice artifacts are found even for charmed observables.

The computation of the correlators was carried out on the Marconi-KNL supercomputer at CINECA within the PRACE project Pra17-4394. We thank all of ETMC for collaboration.

References