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

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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 ~ 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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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

$$S = S_g + S^{\ell}_{tm} + S^{h}_{tm} \,, \tag{1.1}$$

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 $\chi_\ell = (u,d)^t$, the twisted mass action [3] takes the form

$$S^{\ell}_{tm} = \sum_x \bar{\chi}_\ell(x) \left[D_W(U) + \frac{i}{4} c_{SW} \sigma_{\mu\nu} \mathscr{F}_{\mu\nu}(U) + m_0 + i\mu_\ell \tau^3 \gamma^5 \right] \chi_\ell(x) \,. \tag{1.2}$$

where μ_ℓ is the twisted and m_0 the (untwisted) Wilson bare quark mass. The Pauli matrix τ_3 acts in flavour space and D_W is the massless Wilson-Dirac operator. The Wilson quark mass m_0 and the clover term $\frac{i}{4} c_{SW} \sigma_{\mu\nu} \mathscr{F}_{\mu\nu}(U)$ 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]

$$S^{h}_{tm} = \sum_x \bar{\chi}_h(x) \left[D_W(U) + \frac{i}{4} c_{SW} \sigma_{\mu\nu} \mathscr{F}_{\mu\nu}(U) + m_{0h} - \mu_\delta \tau_1 + i\mu_\sigma \tau^3 \gamma^5 \right] \chi_h(x) \,. \tag{1.3}$$

The term $\mu_\delta \tau_1$ 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_{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 a $\sim 10\%$ accuracy, the clover term coefficient c_{SW} can be fixed through its estimate in one-loop [7] tadpole boosted perturbation theory, namely $c_{SW} \cong 1 + 0.113(3) \frac{g_0^2}{P}$ with P the plaquette expectation value. Here we follow this prescription at all values of g_0^2 (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_{crit}, as determined in the unitary setup and with action [8]

$$S^{h,val}_{tmOS} = \sum_{f=c,s} \sum_x \bar{\chi}_f(x) \left[D_W(U) + \frac{i}{4} c_{SW} \sigma_{\mu\nu} \mathscr{F}_{\mu\nu}(U) + m_{crit} + i\mu_f^{OS} \gamma^5 \right] \chi_f(x) \,. \tag{1.4}$$

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

$$m^{val,ren}_{c,s} = \frac{1}{Z_P} \left(\mu_\sigma \pm \frac{Z_P}{Z_S} \mu_\delta \right) \,, \tag{1.5}$$

name	$L^3 \cdot T/a^4$	Nconf	κ	$a\mu_\ell$	$a\mu_\sigma$	$a\mu_\delta$	β
cA211.53.24	$24 \cdot 48$	628	0.1400645	0.0053	0.1408	0.1521	1.726
cA211.40.24	$24 \cdot 48$	662	0.1400645	0.0040	0.1408	0.1521	1.726
cA211.30.32	$32 \cdot 64$	1237	0.1400645	0.0030	0.1408	0.1521	1.726
cA211.12.48	$48 \cdot 96$	322	0.1400650	0.0012	0.1408	0.1521	1.726
cB211.25.48	$48 \cdot 96$	314	0.1394267	0.0025	0.1246864	0.1315052	1.778
cB211.072.64	$64 \cdot 128$	187	0.1394265	0.00072	0.1246864	0.1315052	1.778
cC211.06.80	$80 \cdot 160$	210	0.1387510	0.0006	0.106586	0.107146	1.836

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, $\kappa = (8+2am_{crit})^{-1}$, bare twisted masses $a\mu_\ell$, $a\mu_\sigma$, $a\mu_\delta$, and β. We have set $c_{SW} = [1.74, 1.69, 1.645]$ for $\beta = [1.726, 1.778, 1.836]$, respectively.

name	$a\mu_\ell^{valence} = a\mu_\ell$	$a\mu_s$	$a\mu_c$
cA211.53.24	0.0053	0.0176, 0.0220, 0.0264	0.2596, 0.2856, 0.3115, 0.3433
cA211.40.24	0.0040	0.0176, 0.0220, 0.0264	0.2596, 0.2856, 0.3115, 0.3433
cA211.30.32	0.0030	0.0176, 0.0220, 0.0264	0.2596, 0.2856, 0.3115, 0.3433
cA211.12.48	0.0012	0.0176, 0.0220, 0.0264	0.2596, 0.2856, 0.3115, 0.3433
cB211.25.48	0.0025	0.0148, 0.0185, 0.0222	0.2181, 0.2399, 0.2617, 0.2884
cB211.072.64	0.00072	0.0148, 0.0185, 0.0222	0.2181, 0.2399, 0.2617, 0.2884
cC211.06.80	0.0006	0.0128, 0.0161, 0.0193	0.1907, 0.2098, 0.2288, 0.2522

Table 2: Values of the valence bare quark masses for each of the ensembles analysed here.

with Z_P and Z_S 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 β, 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 μ_ℓ equal to its sea counterpart, as well as at three values of quark mass (μ_s) in the strange region and four values of the quark mass (μ_c) 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 DDαAMG multi-grid algorithm optimized for twisted mass fermions [9].

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

$$C(t) = \frac{1}{L^3} \sum_{\vec{x},\vec{z}} \langle 0 | P_{qq'}(x) P_{qq'}(z)^\dagger | 0 \rangle \, \delta_{t,(t_x - t_z)} \,, \tag{1.6}$$

where $P_{qq'}(x) = \overline{\chi}_q(x) i\gamma_5 \chi_{q'}(x)$ with single-flavour χ_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 groundstate masses (M_{PS}) and matrix elements. [1] 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 $\mathscr{Z}_{PS} = |\langle PS|P_{qq'}|0\rangle|^2$ determines the PS-meson decay constant with no need of any renormalization constant [3], namely

$$af_{PS} = a(\mu_q + \mu_{q'}) \frac{\sqrt{a^4 \mathscr{Z}_{PS}}}{aM_{PS} \sinh(aM_{PS})} \ . \quad (1.7)$$

For all ensembles the value of the bare parameter $am_{0(h)}$ is tuned towards am_{crit} so that the renormalized untwisted current quark mass $Z_A am_{PCAC}$ 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 of am_{PCAC} is observed in the MC simulation and $Z_A am_{PCAC} = -0.00015(4)$ for $a\mu_\ell = 0.0012$ is found. This small systematic error has been corrected by "reweighting" from $\kappa = 0.1400650$ to $\kappa_{crit.} = 0.1400640$.

2. Lattice calibration and determination of w_0 from f_π

We carried out fits of the dependence of f_π, written in units of the gradient flow scale w_0 [13], on the meson mass M_π^2 using the SU(2) chiral perturbation theory (ChPT) formula

$$(f_\pi w_0) = (f w_0) \left[1 - 2\xi_\ell^M \log \xi_\ell^M + P_3 \xi_\ell^M + P_4 a^2/w_0^2\right] K_f^{FSE} \ , \quad (2.1)$$

where $\xi_\ell^M = M_\pi^2/(16\pi^2 f^2)$ 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 $P_3 = 2\bar{\ell}_4 + 4\log\left(M_\pi^{phys}/(4\pi f)\right)$, with M_π^{phys} being the value of the pion mass at the physical point. The factor K_f^{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^{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 $f_\pi^{phen.} = 130.41$ 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)

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

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 Ω baryon mass rather than f_π^{phen}.

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 $Bm_s^{LO} =$

[1] As 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. $\lambda_0(t,t_0) = C\left(e^{-M_{PS}(t-t_0)} + e^{-M_{PS}(T-(t-t_0))}\right)$.

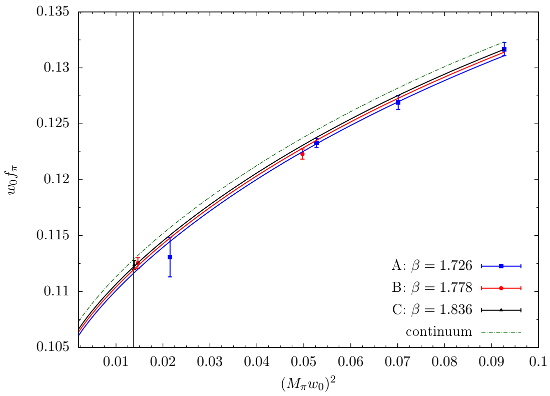

Figure 1: Preliminary chiral and continuum fit of f_π as a function of M_π in units of the gradient flow scale w_0 [13]. The fit function we employ is given in Eq. (2.1)

$M_K^2 - M_\pi^2/2 = 0.186, 0.212, 0.252$ GeV^2 which at the leading order in ChPT is proportional to the renormalised strange quark mass. Then for each value of Bm_s^{LO} we extrapolate to the continuum limit and to the physical M_π using our best fit to the data for $w_0 f_K$ according to the Ansatz

$$w_0 f_K \;=\; P_1' \left[1 - \frac{3}{4}\xi_\ell^M \log \xi_\ell^M + P_2' \xi_\ell^M + P_4' a^2\right], \tag{3.1}$$

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

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

$$f_K = 154(2)\ \text{MeV}, \qquad f_K/f_\pi = 1.182(16)\ \text{MeV}, \tag{3.2}$$

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 $M_D^{ref} = 1.61, 1.73, 1.84, 1.95$ GeV (with scale from Sect. 2). Then for each M_D^{ref} mass value we extrapolate to the continuum limit and the physical M_π using our best fit to the data according to the polynomial Ansatz

$$w_0 f_D = P_1(1 + P_2 M_\pi^2 + P_3 M_\pi^4 + P_4 a^2)\,. \tag{3.3}$$

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

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

$$f_D = 215(6)\ \text{MeV}\,. \tag{3.4}$$

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_π and the decay constant f_π to the SU(2) ChPT formula

$$(M_\pi w_0)^2 = 2(Bw_0)(m_\ell w_0)\left[1 + \xi_\ell \log \xi_\ell + P_1 \xi_\ell + P_2\, a^2/w_0^2\right] K_{M^2}^{FSE}\,, \tag{4.1}$$

$$(f_\pi w_0) = (f w_0)\left[1 - 2\xi_\ell \log \xi_\ell + P_3 \xi_\ell + P_4\, a^2/w_0^2\right] K_f^{FSE}\,, \tag{4.2}$$

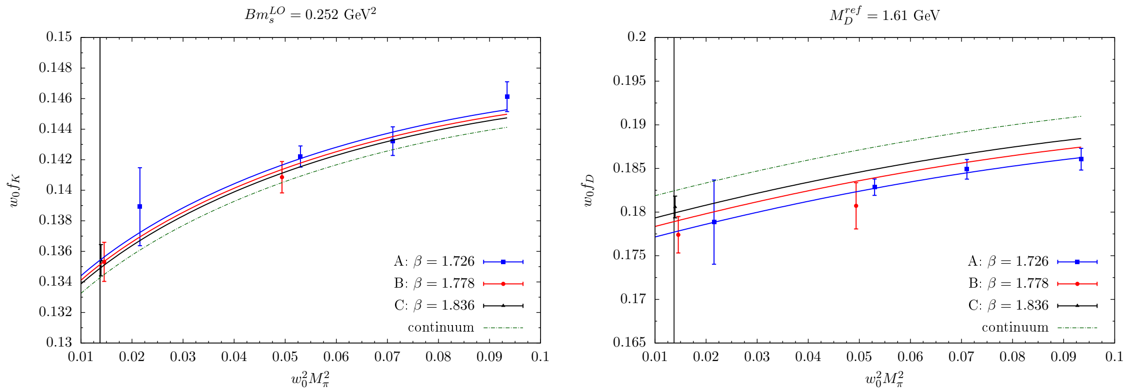

Figure 2: Preliminary chiral and continuum fit of f_K (left) and f_D (right) as a function of M_π in units of the gradient flow scale w_0 [13]. f_K is plotted at a fixed $Bm_s^{LO} = 0.252$ GeV^2. f_D is plotted at a fixed $M_D^{ref} = 1.61$ GeV. The fit functions we employ are given in Eq. (3.1) for f_K and Eq. (3.3) for f_D.

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

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

and $m_\ell = \mu_\ell / Z_P$ the renormalized mass. The renormalization factors Z_P 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 $\overline{MS}$ 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 $K^{FSE}_{M^2/f}$ represents the correction for FSE as computed in Ref. [14].
In Fig. 3 we show our chiral and continuum fits. Imposing as above $M_\pi = 134.80$ MeV and $f_\pi^{phen} = 130.41$ MeV we find the preliminary results

$$m_{ud}(\overline{MS},\, 2\text{ GeV}) = 3.66(11)\text{ MeV}\,, \qquad w_0 = 0.1703(18)\text{ fm}\,, \quad \bar{\ell}_3 = 2.9(2)\,, \tag{4.3}$$

$$\bar{\ell}_4 = 4.3(1)\,, \qquad B = 2539(78)\text{ MeV}\,, \quad f = 122.1(2)\text{ MeV}\,. \tag{4.4}$$

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

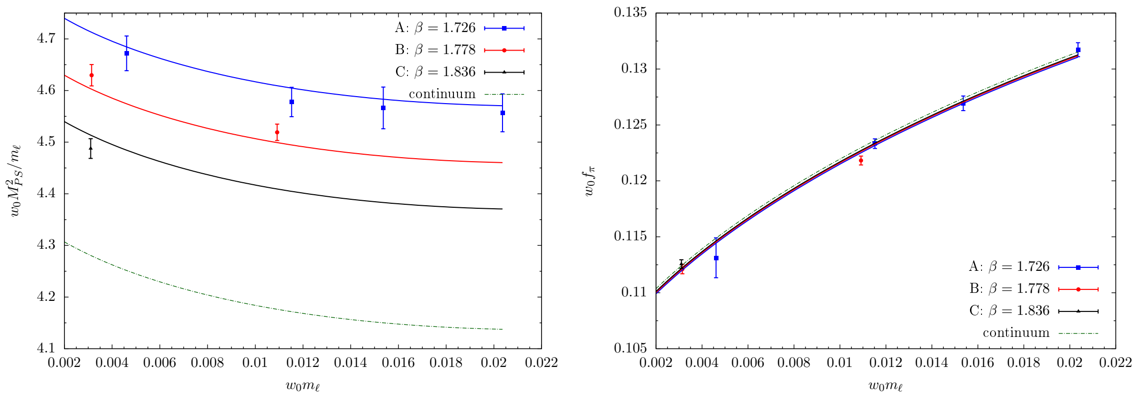

Figure 3: Preliminary chiral and continuum fits of M_π (left) and f_π (right) as a function of the renormalized quark mass m_ℓ in units of the gradient flow scale w_0 [13].

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. 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.

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