First results of ETMC simulations with $N_f = 2+1+1$ maximally twisted mass fermions

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We present first results from runs performed with $N_f = 2+1+1$ flavours of dynamical twisted mass fermions at maximal twist: a degenerate light doublet and a mass split heavy doublet. An overview of the input parameters and tuning status of our ensembles is given, together with a comparison with results obtained with $N_f = 2$ flavours. The problem of extracting the mass of the *K*- and *D*-mesons is discussed, and the tuning of the strange and charm quark masses examined. Finally we compare two methods of extracting the lattice spacings to check the consistency of our data and we present some first results of χPT fits in the light meson sector.

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1. Introduction

The twisted mass formulation of Lattice QCD [1, 2] is being studied extensively with $N_f = 2$ dynamical flavours by the European Twisted Mass (ETM) collaboration [3 – 7]. In this formulation of QCD, the Wilson term is chirally rotated within an isospin doublet. To include a dynamical strange quark in a unitary setup, we add, in addition to the strange quark a charm quark in a heavier and mass-split doublet as discussed in [8 – 10]. We will briefly describe our action in section 2, recapitulate our procedure for tuning to maximal twist and focus on the tuning of the heavy doublet. We give an overview of the runs we have carried out and section 3 gives first results for some light-quark sector observables.

2. Lattice setup

In the gauge sector we use the Iwasaki gauge action [11]. With this gauge action we observe a smooth dependence of (possible) phase sensitive quantities on the hopping parameter κ around its critical value κ_{crit}. The fermionic action for the light doublet is given by:

$$S_l = a^4 \sum_x \left\{ \bar{\chi}_l(x) \left[D_W[U] + m_{0,l} + i \mu_l \gamma_5 \tau_3 \right] \chi_l(x) \right\}, \tag{2.1}$$

using the same notation as used in [10]. In the heavy sector, the action becomes:

$$S_h = a^4 \sum_x \left\{ \bar{\chi}_h(x) \left[D_W[U] + m_{0,h} + i \mu_\sigma \gamma_5 \tau_1 + \mu_\delta \tau_3 \right] \chi_h(x) \right\}. \tag{2.2}$$

At maximal twist, physical observables are automatically $\mathscr{O}(a)$ improved without the need to determine any action or operator specific improvement coefficients. The gauge configurations are generated with a Polynomial Hybrid Monte Carlo (PHMC) updating algorithm [12 – 14].

2.1 Tuning action parameters

Tuning to maximal twist requires to set $m_{0,l}$ and $m_{0,h}$ equal to some proper estimate of the critical mass $m_{\mathrm{crit}} = m_{\mathrm{crit}}(\beta)$ [8]. Here we set $m_{0,l} = m_{0,h} \equiv 1/(2\kappa) - 4$. As has been shown in [9], this is consistent with $\mathscr{O}(a)$ improvement defined by the maximal twist condition $a m_{\mathrm{PCAC},l} = 0$ (see also ref. [10]). The numerical precision at which the condition $m_{\mathrm{PCAC},l} = 0$ is fulfilled in order to avoid residual large $\mathscr{O}(a^2)$ effects when the pion mass is decreased is, for the present range of lattice spacings, $|\varepsilon/\mu_l| \lesssim 0.1$, where ε is the deviation of $m_{\mathrm{PCAC},l}$ from zero [4, 15]. As explained in [10], tuning to κ_{crit} was performed independently for each μ_l value. From table 1 we observe that the estimate of κ_{crit} depends weakly on μ_l. The heavy doublet mass parameters μ_σ and μ_δ should be adjusted in order to reproduce the values of the renormalized s and c quark masses. The latter are related to μ_σ and μ_δ via [8]:

$$(m_{s,c})_{\mathrm{R}} = \frac{1}{Z_P} \left(\mu_\sigma \mp \frac{Z_P}{Z_S} \mu_\delta \right), \tag{2.3}$$

where the $-$ sign corresponds to the strange and the $+$ sign to the charm. In practice we fix the values μ_σ and μ_δ by requiring the resulting K- and D-meson masses to match experimental results.

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Label	β	κ	$a\mu_l$	$a\mu_\sigma$	$a\mu_\delta$	L/a	T/a	$m_\pi L$	$|\varepsilon/\mu_l|$
C_1	1.90	0.1632700	0.0040	0.150	0.190	20	48	3.0	0.14(14)
C_2	1.90	0.1632700	0.0040	0.150	0.190	24	48	3.5	0.07(14)
A_1	1.90	0.1632650	0.0060	0.150	0.190	24	48	4.1	0.03(3)
A_2	1.90	0.1632600	0.0080	0.150	0.190	24	48	4.8	0.02(2)
$A_3 D_1$	1.90	0.1632550	0.0100	0.150	0.190	24	48	5.3	0.02(2)
A_4	1.90	0.1632720	0.0030	0.150	0.190	32	64	4.0	0.08(7)
$A_5 C_3$	1.90	0.1632700	0.0040	0.150	0.190	32	64	4.5	0.04(5)
A_6	1.90	0.1632670	0.0050	0.150	0.190	32	64	5.0	0.05(2)
D_2	1.90	0.1632550	0.0100	0.150	0.197	24	48	5.3	0.35(1)
B_1	1.95	0.1612400	0.0025	0.135	0.170	32	64	3.4	0.06(6)
B_2	1.95	0.1612400	0.0035	0.135	0.170	32	64	4.0	0.02(2)
B_3	1.95	0.1612360	0.0055	0.135	0.170	32	64	5.0	0.08(1)
B_4	1.95	0.1612320	0.0075	0.135	0.170	32	64	5.8	0.05(1)
B_5	1.95	0.1612312	0.0085	0.135	0.170	24	48	4.6	0.01(2)

Table 1: Input parameters, $m_\pi L$ and $|\varepsilon/\mu_l|$ for all ensembles used in this paper. Every ensemble has ~ 5000 thermalized trajectories of length $\tau = 1$. We have two main ensemble sets: *A* and *B*, at $\beta = 1.90$ and $\beta = 1.95$ respectively. Ensembles labeled *C* are used to check finite size effects. Ensembles labeled *D* are used to check/tune the strange and charm quark masses.

2.2 Determination of heavy-light meson masses

Since the twisted mass lattice Dirac operator of the non-degenerate heavy quark doublet (cf. (2.2)) contains a parity odd and flavour non-diagonal Wilson term, parity as well as flavour are not anymore quantum numbers of the theory. In contrast to parity and flavour conserving lattice formulations, it is not possible to compute correlation functions restricted to a single parity and flavour sector in this setup. While the *K*-meson will remain the lightest state and therefore relatively easy to extract, for a theoretically clean determination of the *D*-meson mass one has to consider the four sectors labeled by parity $\mathscr{P} = \pm$ and flavour $= s/c$ at the same time. And since besides the *K*-meson there are a number of $K + n \times \pi$ states and possibly also "positive parity *K* states" below the *D*-meson, this renders the *D* a highly excited state. At currently available statistics it seems extremely difficult to extract such a high lying state.

As such, we resort to a different strategy in order to extract this mass. We attempt to determine the mass of the *D*-meson without computing the full low-lying spectrum, e.g. we do not determine all low lying states below the *D*. To this end we apply smearing techniques (cf. [16], where the same setup was used) to construct highly optimized trial states with large overlap to the *K*- and *D*-meson, and make certain assumptions about these trial states, which will be motivated and detailed in an upcoming publication. To extract the *D*-meson mass, we applied three different methods: (1) solving a generalized eigenvalue problem, (2) performing a multi-exponential fit and (3) rotating the twisted basis correlators back to the physical basis (in order to do this we need to compute the light and heavy twist angle and a ratio of the appropriate renormalization constants). The values of the *D*-meson mass extracted from these three different methods are consistent with each other.

2.3 Status

The left panel of figure 1 shows the tuning of the strange quark mass by showing the difference, scaled with the chirally extrapolated value of r_0/a between twice the K-meson mass squared and the pion mass squared. Set *A* at $\beta = 1.90$, $a\mu_\delta = 0.190$ (green points) appears to overshoot the physical point (the black cross on the left), while set *B* (red points) extrapolates better. To improve the tuning of the strange quark mass for set *A*, we are currently applying a reweighting procedure as described in [10] in the parameters $a\mu_\delta$ and κ. The blue point with a different heavy sector splitting $a\mu_\delta = 0.197$ is a run to check this procedure. Though this run is not tuned to maximal twist yet, the K-meson mass appears to be much closer to its physical value. The right panel of figure 1 shows the mass of the D-meson (obtained in this case by method (3)) as a function of the pion mass squared for various simulation points as well as the experimental value from the Particle Data Group [17] . The plot demonstrates that we have tuned the charm (sea) quark mass in our simulations to a physically realistic value. As a final check, we also use an estimate of Z_P/Z_S to verify that $m_c \sim 10 m_s$.
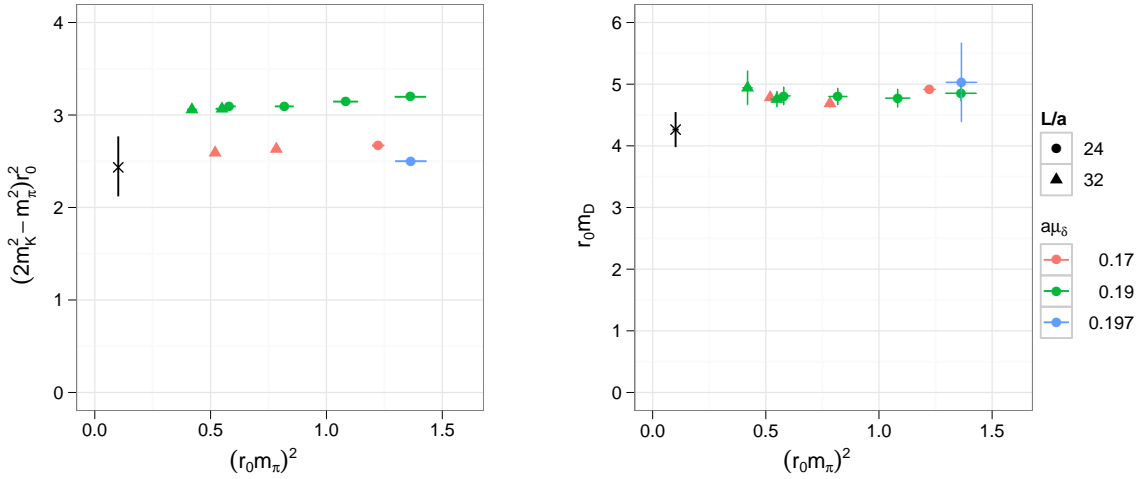

Figure 1: $r_0^2(2m_K^2 - m_\pi^2)$ and $r_0 m_D$ as functions of $(r_0 m_\pi)^2$, showing the status of the tuning of the strange and charm quark mass respectively. The experimental value from PDG is added as the black cross ($r_0 = 0.45(3)$ fm was used). Red points label the $\beta = 1.95$ runs, green points label the $\beta = 1.90$ runs, where the single blue point corresponds to $\beta = 1.90$ with a different heavy sector splitting $a\mu_\delta$. Circles denote runs with $L/a = 24$, triangles indicate a volume with $L/a = 32$.

3. Results

As a first check of our data, we have compared it to the extensively analysed data set that exists for our $N_f = 2$ data. To compare the two sets, we plot dimensionless physical ratios in figure 2. The figure shows no evidence of disagreement between all our results, suggesting small discretisation effects and small effects of dynamical *s*- and *c*-quarks for these observables.
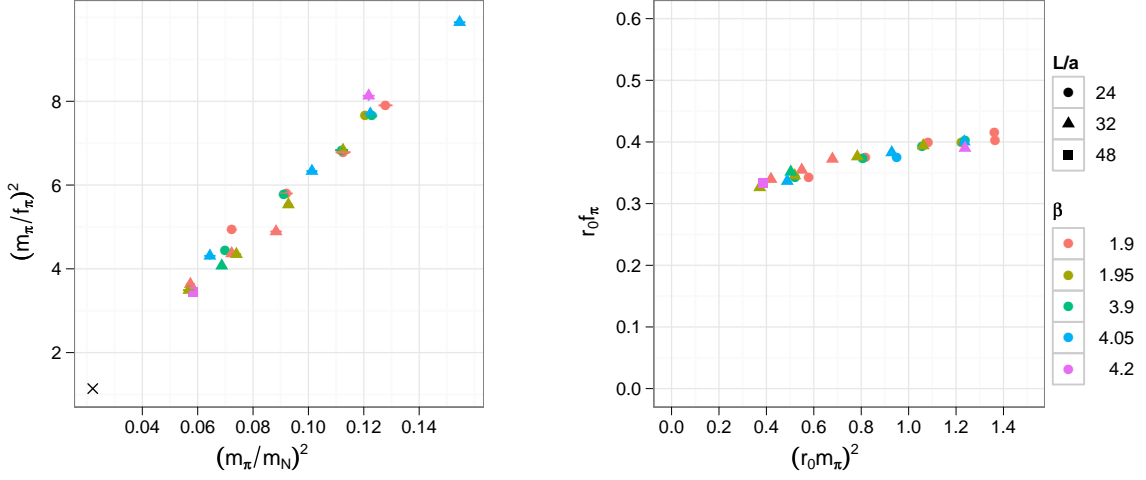
Figure 2: $(m_\pi/f_\pi)^2$ vs $(m_\pi/m_N)^2$ (left) and $r_0 f_\pi$ vs $(r_0 m_\pi)^2$ (right) for both $N_f = 2+1+1$ data (with $\beta = 1.90, 1.95$) and $N_f = 2$ data (with $\beta = 3.9, 4.05, 4.2$ and using a different gauge action). In the left plot, m_N is the nucleon mass, and the physical point is included as the black cross. In both plots finite size corrections are not applied, and in the right plot the chirally extrapolated values for r_0/a were used.

3.1 Light meson chiral perturbation theory fits

In order to extract the lattice spacing and light quark mass from our data-sets, we perform a next to leading order $SU(2)$ chiral perturbation theory fit of the m_π and f_π data. We use continuum formulae and correct for finite size effects either without any new low energy constants à la Gasser and Leutwyler [18], or with $\bar{l}_1$ and $\bar{l}_2$ added in, as described in [19]. The results are listed in table 2. We have performed these fits for ensemble sets A and B separately, and also combined them in a single fit. In table 2, we include a systematic error, estimated at $2-5\%$, coming from the dispersion of the values of the fitted parameters between NLO and NNLO. Note that since the quark mass enters the χPT expression, in order to combine the two sets at different lattice spacings, we need to know the renormalization factor of the quark mass $Z_\mu = 1/Z_P$, a computation which is not yet complete. Assuming that Z_P is effectively a function of β in the range of parameters we are considering, we can fit the ratio of those Z_P-values and lattice spacings and extract lattice spacings from the combined fit. In every fit we use as inputs the physical f_π and m_π, and extract f_0, $\bar{l}_3$ and $\bar{l}_4$. A complete analysis (analogous to [20]) of the systematic effects is in progress.

set	pts	f_0(MeV)	$\bar{l}_3$	$\bar{l}_4$	$a_{\beta=1.90}$(fm)	$a_{\beta=1.95}$(fm)
A & B	11	121(4)	3.5(2)	4.7(2)	0.086(6)	0.078(6)
A	6	121(4)	3.4(2)	4.8(2)	0.086(7)	
B	5	121(4)	3.7(2)	4.7(2)		0.078(7)

Table 2: Results from the NLO $SU(2)$ χPT fits for combined, only set A and only set B respectively. Errors are dominated by a systematic error of $2-5\%$ due to performing an NLO fit. The column "pts" refers to the number of ensembles used in that fit.

3.2 Chiral extrapolation of the nucleon mass

In this section, we present preliminary results for the light quark mass dependence of the nucleon mass. We consider the one-loop result from heavy baryon chiral perturbation theory (HBχPT)

$$m_N = m_N^0 - 4c_1 m_\pi^2 - \frac{3g_A^2}{16\pi f_\pi^2}m_\pi^3 \tag{3.1}$$

and fix the scale and light quark mass to the point where the ratio m_N/m_π attains its physical value. We fix f_π and g_A to their physical values (130.7 MeV and 1.27 respectively) as has also been performed in [7]. Using this procedure, we find a lattice spacing of 0.089(2) fm and 0.077(3) fm for $\beta = 1.90$ and 1.95 respectively. The $\chi^2/(d.o.f.)$ of these fits is not very good, and fitting a linear extrapolation appears to be consistent with the data. This is not unique to our data, and has been observed by various collaborations. We therefore perform the linear fit here as well, and absorb the difference between the two extrapolations in the systematic error. A more detailed analysis of the chiral extrapolation of the nucleon mass will be presented in an upcoming study. The lattice spacings that we obtain from the chiral extrapolation of the nucleon mass are 0.089(9) fm and 0.077(4) fm for set A at $\beta = 1.90$ and set B at $\beta = 1.95$ respectively.

3.3 r_0/a extrapolation

Since r_0/a is very sensitive to κ in the vicinity of $\kappa_{\rm crit}$, the fact that we now tune to maximal twist at every value of μ_l, might, with respect to what was done for the $N_f = 2$ case, in part provide an explanation for the observed change of slope in the mass dependence of r_0/a between $N_f = 2$ and $N_f = 2 + 1 + 1$. Note however that these differences tend to diminish when increasing the value in β in the $N_f = 2 + 1 + 1$ case. We extrapolate r_0/a using a simple quadratic fit $r_0/a = c_1 + c_2 a^2 \mu_l^2$, where c_1 is the value of r_0/a in the chiral limit. We perform both a polynomial fit $r_0/a = c_1 + c_2 \mu_l + c_3 a^2 \mu_l^2$ and a linear fit $r_0/a = c_1 + c_2 a\mu_l$ to help estimate systematic errors. We find that based on the $\chi^2/$d.o.f. the quadratic fit is for both values of β the best fit. The polynomial fit gives nearly identical results for c_1, while c_1 from the linear fit is 1 to 3σ higher. Using the lattice spacings from the combined light meson chiral perturbation theory fit, we extract two predictions for r_0, which seem to agree well at $r_0 = 0.45(3)$ fm.

β	c_1(quadratic fit)	a(fm)	r_0(fm)
1.90	5.24(2)	0.086(6)	0.45(3)
1.95	5.71(4)	0.078(6)	0.45(3)

Table 3: r_0 determination for both ensembles separately. c_1(qua) is the value of a quadratic r_0/a extrapolation in the chiral limit with the statistical error in brackets. The lattice spacings a are taken from the combined light meson chiral perturbation theory fit. The obtained values for r_0 from the two ensembles seem to agree well with each other.

4. Conclusions

We have presented first results from runs performed with $N_f = 2 + 1 + 1$ flavours of dynamical twisted mass fermions. No evidence of disagreement between these results and those with $N_f = 2$

twisted mass fermions is shown through dimensionless ratio plots (of m_π, f_π, m_N and r_0/a), suggesting small discretisation effects and small effects of dynamical *s*- and *c*-quarks for these observables. We have extracted the lattice spacings of our two ensemble sets using two different methods, which agree within errors with each other. We have measured r_0 on both ensembles and found consistent results. We are in the process of performing a more detailed combined analysis in order to improve our understanding of the systematic errors.

Acknowledgments

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