Comparison between overlap and twisted mass fermions towards the chiral limit

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We compare overlap fermions, which are chirally invariant, and Wilson twisted mass fermions in the approach to the chiral limit. Our quenched simulations reveal that with both formulations of lattice fermions pion masses of O(250 MeV) can be reached in practical simulations. Our comparison is done at a fixed lattice spacing $a \simeq 0.123$ fm. Several quantities are measured, such as hadron masses and pseudoscalar decay constants.

1. INTRODUCTION

The Wilson formulation of lattice QCD exhibits various problems: the presence of unphysical small eigenvalues which give rise to exceptional configurations, the explicit breaking of chiral symmetry which complicates the pattern of operator mixing, the presence of large discretization errors which are reduced through the Symanzik improvement program. In the present study we consider two formulations of lattice QCD that are able to overcome most of these problems: overlap and twisted mass (tm) fermions. Overlap fermions have an exact chiral symmetry at finite lattice spacing $a$ and the mass is an infrared cut-off, thus allowing the approach to the chiral limit to be performed at finite $a$. For tm fermions the twisted part of the mass also provides an infrared cut-off, thus solving the practical problem of exceptional configurations which affects Wilson fermions. At maximal twist angle, moreover, one has automatic $O(a)$ improvement for various quantities like energy eigenvalues and matrix elements. The great advantages of overlap fermions have unfortunately the price of being rather expensive from the numerical point of view. On the other hand, tm fermions are rather cheap to simulate but show residual chiral symmetry breaking effects.

Our comparison is performed at a fixed value of $\beta = 5.85$ ($a^{-1} \simeq 1.605$ GeV) and no attempt of a scaling analysis is performed here. Our aim is to investigate how both formulations behave in their approach to the chiral limit for a number of quantities like hadron masses and pseudoscalar decay constants. We also provide a timing estimate, from the results in ref. 8.

2. NUMERICAL RESULTS

For overlap fermions we have 140 configurations on $12^3 \times 24$ lattices ($L_{12} \sim 1.48$ fm). The bare quark masses are $m_{ov}a = 0.01, 0.02, 0.04, 0.06, 0.08, 0.10$ and $\rho = 1.6$. The simulations for tm fermions are done at full twist so that all the quantities studied here ought to be automatically $O(a)$ improved. In the following we refer to the “twisted” basis where the action is the normal Wilson action with a bare mass term $M_{cr} + i\mu\gamma_5\tau_3$. $M_{cr}$ is the bare critical mass determined for normal Wilson fermions and, for the corresponding value of the hopping parameter, we have used $\kappa_{cr} = 0.16166(2)$. The twisted quark mass parameter $\mu a$ has been chosen to have the same values of the overlap masses plus the value 0.005 (in the plot and tables below both $m_{ov}$ and $\mu$ will be called $m_{bare}$). We collected 140 configurations on $12^3 \times 24, 140$ configurations on
14^3 \times 32 (L_{14} \sim 1.72 \text{ fm}) and 250 configurations on 16^3 \times 32 (L_{16} \sim 1.97 \text{ fm}) lattices. For both, overlap and tm fermions, a multiple mass solver (MMS) has been employed.

### 2.1. HADRON MASSES

We extract hadron masses by fitting the behaviour of suitable two point functions at large euclidean time\(^2\). We check in various ways (including the use of Jacobi smearing) that our determination is not contaminated by the presence of excited states. Pseudoscalar masses are extracted from the correlation functions \(C_P(x_0) = \sum_x \langle P^b(x)P^b(0) \rangle\) and (only for overlap) \(C_{P-S}(x_0) = \sum_x \langle P^b(x)P^b(0) - S^b(x)S^b(0) \rangle\) where \(b\) is the flavour index and, in order to avoid problems of mixing with the scalar density, in the tm case we only consider \(a = 1, 2\). In \(C_{P-S}(x_0)\) the contribution of the topological zero modes of the overlap operator cancels. Results are reported in Fig. 1 and in Tab. 1.

For tm fermions we have performed simulations on three volumes and finite volume effects turn out to be very small for all the values of the mass. In the following, we will present only results obtained on the 16^3 \times 32 lattice. For overlap fermions we extract the pion mass from \(C_{P-S}\) (Fig. 1 shows how large can be the finite volume effects due to the exact zero modes present in \(C_P\), at small quark masses). The lowest pion mass turns out to be very small (\(M_\pi^m \simeq 230 \text{ MeV}\) and \(M_\pi^m L_{12} = 1.73\)) and thus, despite the cancellation above, a finite size effect at percent level can not be excluded. In Fig. 1 results for \(O(a)\) improved Wilson fermions are also reported. In this case the simulations had to be stopped at rather large values of the quark mass to avoid exceptional configurations. With both, tm and overlap fermions, we can reach instead very low values of \(M_\pi\).

For overlap fermions, \(M_\pi^2\) has, to a very good approximation, a linear behaviour with \(m_\pi\), and a linear extrapolation to the chiral limit gives an intercept of \(-0.002(6)\). For tm fermions the behaviour is better described by a quadratic form and the fit gives an intercept of 0.0054(4). This value, non-compatible with zero, is due to the residual \(O(a)\) uncertainty in \(m_\pi\). This uncertainty also induces an \(O(a^3\mu^2)\) effect in the pion mass.

One can also notice from Fig. 1 that the pion masses obtained with tm always lay above the ones obtained with overlap fermions. This is due to the renormalization factor \(Z_m^{\text{V}}\) (needed to obtain the renormalization group invariant quark mass) that, for tm fermions, turns out to be roughly a factor 2.5 larger than the corresponding one for overlap fermions (which is close to 1).

The vector meson mass has been extracted from \(C_A^a(x_0) = \sum_k \sum_x \langle A_k^a(x)A^b_k(0) \rangle\) (\(a = 1, 2\)) and \(C_V^a(x_0) = \sum_k \sum_x \langle V_k^a(x)V^b_k(0) \rangle\) in the tm and overlap case respectively. The results are plotted in Fig. 2. In the tm case we observe (both with and without smearing) a progressive worsening of the plateaux for the effective masses as the quark mass decreases. This phenomenon is particularly evident for the lowest three masses where, due to these uncertainties, we prefer not to plot any result.

\(\begin{align*}
M_\pi a & \quad f_\pi a \\
0.005 & \quad 0.1694(24) & \quad 0.0694(17) \\
0.01 & \quad 0.140(20) & \quad 0.2276(22) & \quad 0.0934(90) & \quad 0.0904(12) \\
0.02 & \quad 0.196(14) & \quad 0.3141(20) & \quad 0.1012(53) & \quad 0.1022(12) \\
0.04 & \quad 0.280(10) & \quad 0.4468(18) & \quad 0.1060(34) & \quad 0.1170(13) \\
0.06 & \quad 0.346(8) & \quad 0.5552(15) & \quad 0.1106(25) & \quad 0.1265(12) \\
0.08 & \quad 0.401(7) & \quad 0.6505(13) & \quad 0.1157(22) & \quad 0.1411(12) \\
0.10 & \quad 0.451(6) & \quad 0.7373(14) & \quad 0.1209(21) & \quad 0.1522(13)
\end{align*}\)

Table 1

\(M_\pi a\) and \(f_\pi a\) for overlap and tm fermions.
We have also computed the proton and the $\Delta^{++}$ correlators with interpolating operators $B^\text{oct}_\alpha = \epsilon^{abc}(d^a T C \gamma_5 u^b) u^c_\alpha$ and $B^\text{dec}_{k,\alpha} = \epsilon^{abc}(u^a T C \gamma_5 b^k) u^c_\alpha$ (with $k=1,2,3$ equivalent) respectively. The results are presented in Fig. 2.

In the overlap case, due to the smaller volume, the decuplet turns out to be too noisy for a reliable estimate. In the tm case, the same phenomenon as for $M_{\rho}$ has been observed on the lowest three masses. Notice that, in order to obtain the physical two point correlators, one has to rotate those computed in the “twisted” basis according to

\[
\langle \bar{B}_{\alpha}^{\text{dec}}(x) B_{\beta}^{\text{dec}}(0) \rangle_{\text{phys}} = \frac{1}{2} (1 + i\gamma_5)_{\alpha\gamma} \times \langle \bar{B}_{\gamma}^{\text{dec}}(x) B_{\delta}^{\text{dec}}(0) \rangle_{\text{th}} (1 + i\gamma_5)_{\delta\beta}.
\]

### 2.2. DECAY CONSTANTS

By using the PCAC relation, the pseudoscalar decay constants have been computed (without need of any renormalization constant) from the ratio $f^\text{ov}_\pi = 2 m_{\text{bare}} |\langle 0 | P | \pi \rangle| / M^2_\pi$, where $m_{\text{bare}}$ stands either for $m_{\text{ov}}$ or for $\mu$. Results are reported in Tab. 1 and plotted in Fig. 3. At one loop in quenched chiral perturbation theory (qChPT), $f_\pi$ has neither chiral logarithms nor finite volume effects: $f_\pi = f (1 + (\alpha_5 M_\pi^2 / (4\pi f)^2)$ with $f$ and $\alpha_5$ low energy constants. In the overlap case $f_\pi$ nicely follows the linear behaviour predicted by qChPT. Neglecting $SU(3)$ breaking effects (which are well below our statistical uncertainty) we get $f_\pi = 155(11)$ MeV, $f_K = 173(8)$ MeV, $f_K / f_\pi = 1.11(3)$.

In the case of tm fermions, we observe a bending of $f^\text{tm}_\pi$ when the pion mass is small. It has been argued that for $O(\alpha)$ improved quantities, the condition $m_{\text{tm}} \gg a^3 \Lambda^2_{\text{QCD}}$ has to be satisfied in order for the breaking of the chiral symmetry not to be driven by the Wilson term. The puzzling fact is that, assuming a coefficient of order one, this condition seems to be satisfied by all of our data points. In Fig. 3 the vertical line shows the r.h.s of the stronger condition $m_{\text{tm}} \gg a^2 \Lambda^2_{\text{QCD}}$, which should be valid for non-improved quantities. We are thus left with the question of which inequality has to be satisfied: either the weaker one with a large coefficient or the stronger one with a coefficient of order one. This phenomenon, together with that observed for $M_\rho$ and $M_{\text{baryon}}$ at the smallest quark masses, requires further investigation at smaller values of $a$.

Finally we find that tm fermions are a factor of 20-40 faster than overlap fermions and thus have the potential for dynamical simulations at realistically small quark masses on the next generation of supercomputers.

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