Twisted mass QCD and the FNAL heavy quark formalism.

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Abstract

At tree level, I discuss modifying the FNAL heavy quark formalism to include a twisted mass term. I find that at maximal twist the so called KLM factor is independent of the heavy mass.

1 Introduction and motivation

Although only recently developed, twisted mass QCD is already proving to be an excellent technique for producing accurate lattice QCD results. Twisted mass lattice QCD \cite{1,2} calculations have been used to test and constrain chiral perturbation theory \cite{3,4,5}, study baryons \cite{6}, heavy-light mesons \cite{7}, flavour singlet mesons \cite{8}, static-light mesons \cite{9}, and the pion form factor \cite{10}. A key theoretical advantage of the twisted mass formalism is that the action is automatically $O(a)$ improved at maximal twist \cite{2,11}. Twisted mass QCD has recently been reviewed \cite{12,13}.

An important part of the twisted mass program is that there are power counting arguments to understand the $O(a^2)$ corrections for light quarks \cite{14}. These are based on a Simmons analysis that is suitable for light quarks. As the mass of the heavy quark increases towards the mass of the charm quark and beyond, then $O((aM_Q)^2)$ effects may become sizable. One way to estimate heavy quark mass effects is to use the FNAL heavy quark mass formalism \cite{15}.

The full FNAL heavy quark formalism requires tuning the terms in the heavy quark action. For example the clover coefficient of the clover term and the coefficient of the spatial Wilson term. There have been a few numerical studies of the required tuning \cite{16,17,18,19,20,21}. However, many groups have used the FNAL formulation to estimate heavy mass corrections to decay constants and masses \cite{22,23,24} for the standard Wilson and clover actions. The prescription was to use the kinetic mass and to multiply the quark fields by the KLM factor in equation \cite{1}

$$Z_{KLM} = \sqrt{2Ke^{m_0}} \quad \text{(1)}$$

where $m_0$ is defined in

$$m_0 = \log\left(\frac{1}{2\kappa} - 3\right). \quad \text{(2)}$$
and $\kappa$ is the standard hopping parameter used in the clover and Wilson actions. The corrections to equation I that include non-perturbative $O(a)$ mass corrections are in [23].

A numerical test of the KLM factors is reported by El-Khadra et al. [16] and a test of the FNAL formalism for the charm mass reported by Dougall et al. [26]. A critical comparison of the KLM factors to renormalisation factors determined non-perturbatively is in [27]. The aim of this paper is to find the equivalent KLM factor for twisted mass fermions at tree level.

Throughout this paper I will mostly only consider tree level perturbation theory. This is in the spirit of estimating and correcting the leading $O((am_Q)^n)$ corrections to the results of twisted mass calculations. I also don’t consider the two doublet twisted mass formalism for including non-degenerate quarks in unquenched calculations [28, 29]. The results will be useful to analyse existing $n_f=2$ twisted mass calculations and twisted mass calculations that use the Osterwalder-Seiler action [30, 31] for the heavy quarks in unquenched calculations with $2+1+1$ flavours of sea quarks.

The theoretical foundations of twisted mass QCD [1, 32, 2] use a mass independent renormalisation scheme [33], but the FNAL heavy quark formalism uses mass dependent renormalisation factors. The issue of mass dependent versus mass independent renormalisation schemes is reviewed by Georgi [34] and Kronfeld [35].

## 2 A brief introduction to twisted mass QCD

I first review the twisted mass quark action in the continuum.

$$S_F = \int d^4x \bar{\chi} (\gamma_\mu D_\mu + m_q + i\mu_q \gamma_5 \tau^3) \chi$$

where $\tau^3$ is the third Pauli spin matrix in flavour space, and $m_q$ and $\mu_q$ are mass parameters. The fields $\chi$ and $\bar{\chi}$ are in the twisted basis. The quarks fields can be transferred to what is known as the "physical basis" by the transformation:

$$\psi = \exp(i\omega \gamma_5 \tau^3/2) \chi \quad \bar{\psi} = \bar{\chi} \exp(i\omega \gamma_5 \tau^3/2)$$

where $\tan \omega = \mu_q/m_q$. After the transformation in equation 4, the twisted quark action in the physical basis is

$$S_F = \int d^4x \bar{\psi} (\gamma_\mu D_\mu + \sqrt{m_q^2 + \mu_q^2}) \psi$$

The lattice version of the twisted mass action in equation 3 is written down in the standard way. However, to prepare for applying the FNAL heavy quark formalism, I consider a twisted version ($S_{lat,F}$) of the action written down by Lin
and Christ [19]. Lin and Christ [19] have a table that summaries the choices of coefficients used by other heavy quark formulations [15, 36]. The version of the twisted Wilson action used in existing numerical calculations uses $\zeta = r_s = 1$. I only use arbitrary value of $\zeta$ and $r_s$ in section 5. The twisted QCD action in the twisted basis is

$$S_{\text{lat},F} = \sum_x \chi(x)(\gamma_0 D_0 + \zeta \gamma_i D_i - \frac{1}{2} D_0^2 - r_s \frac{1}{2} D_i^2 + m_q + i r_3 \gamma_5 \mu_q) \chi(x)$$  \hspace{1cm} (6)

The derivatives are defined by

$$D_\mu \psi(x) = \frac{1}{2} [U_\mu(x) \psi(x + \hat{\mu}) - U_\mu^\dagger(x) \psi(x - \hat{\mu})]$$  \hspace{1cm} (7)

and

$$D_\mu^2 \psi(x) = U_\mu(x) \psi(x + \hat{\mu}) + U_\mu^\dagger(x) \psi(x - \hat{\mu}) - 2 \psi(x)$$  \hspace{1cm} (8)

The special choice of $\omega = \pi/2$ is known as maximal twist, where all of the quark mass is in the $\gamma_5 \tau^3$ term. At maximal twist there are no $O(a)$ corrections to the continuum result [2, 11]. Achieving maximal twist is non-trivial, because of the additive mass renormalisation of the Wilson formulation, but achievable numerically in practise.

3 The FNAL heavy quark formalism for Wilson fermions

The FNAL formalism for heavy quarks was originally described by [15]. Further developments of the FNAL lattice heavy quark formulation are described in [36, 35, 19, 20, 37]. Here I review the free field calculation from El-Khadra et al. [15] as warm up to adding a twisted mass term.

The formalism starts with the quark propagator in momentum and time.

$$S(t, \vec{p}) = e^{-E_i \sinh E \gamma_0 \text{sign}(t) - i \gamma_i \hat{p}_i + m_q + 1 - \cosh E + \frac{1}{2} \hat{p}_i \hat{p}_i} 2 Z_2 \sinh E$$  \hspace{1cm} (9)

where $\hat{p}_i = \sin(a p_i)$ and $\hat{p}_i = 2 \sin(\frac{a p_i}{2})$. and $Z_2$ is calculated to be

$$Z_2 = 1 + m_q a + \frac{1}{2} \hat{p}^2 a^2$$  \hspace{1cm} (10)

Equation 9 is only valid for $t > 0$, because there is an additional term at $t = 0$. As $a m_q$ gets very large, $1/Z_2$ will get very small and this will cause problems with the dynamics.

In the FNAL formulation, when the quark mass gets heavy, the dispersion relation of the heavy quark gets modified to

$$E^2 = M_1^2 + \frac{M_1}{M_2} \hat{p}^2 + ...$$  \hspace{1cm} (11)
where $M_1$ is known as the rest mass and $M_2$ is called the "kinetic" mass. Another closely related way to measure the deviations of the lattice dispersion relation from the continuum one is via the "speed of light" [38].

\[ M_1 = \frac{1}{a} \ln(1 + m_q a) \] (12)

Expanding the rest mass in terms of $m_q a$ gives

\[ M_1 = m_q - \frac{1}{2} m_q^2 + \frac{1}{3} m_q^3 + O(m_q^4) \] (13)

The second term in the expansion is the leading $b_m$ improvement term in the ALPHA formulation of the clover action [39]. The connection between the ALPHA formulation of the clover fermion action with the FNAL formulation of the heavy fermion action is demonstrated at one loop by Mertens et al. [40] for the quark mass.

The $M_2$ kinetic mass is extracted using [15]

\[ \frac{1}{M_2} = \frac{\partial^2 E}{\partial p_1 \partial p_1} \bigg|_{p_1=0} \] (14)

For Wilson fermions the standard result is

\[ \frac{1}{M_2} = \frac{2}{m_q a(2 + m_q a)} + \frac{1}{1 + m_q a} \] (15)

with an expansion in the quark mass:

\[ M_2 = a m_q - \frac{1}{2} (a m_q)^2 + (a m_q)^3 - \frac{7}{4} (a m_q)^4 + O((a m_q)^5) \] (16)

The KLM factor is defined [22] via equation (17)

\[ Z_{KLM}^2 \sum_x \langle 0 \mid \psi(x) \bar{\psi}(0) \mid 0 \rangle^{\text{latt}} = \int d^3 x \langle 0 \mid \psi(x) \bar{\psi}(0) \mid 0 \rangle^{\text{cont}} \] (17)

hence

\[ Z_{KLM} = \sqrt{Z_2(p^2 = 0)} = \sqrt{1 + m_q} \] (18)

There is a prescription for constructing amplitude factors for operators that are extended in space and time, such as conserved currents [41, 27] that I do not discuss.

4 The FNAL heavy quark formalism for twisted mass QCD

For the twisted mass formulation I first match the twisted heavy action onto a twisted continuum fermion action in equation [4] then rotate back to the standard
continuum action in the physical basis. This two step procedure seems more natural than trying to match the action in the twisted basis back to the continuum Dirac action in one step. I add the superscript $T$ to show that the quantities are for the twisted action.

The quark propagator in time and spatial momentum for Wilson twisted mass fermions has been written down by Cichy et al. [42] in the twisted basis, as part of their study of the pion and nucleon correlators in free field theory for the twisted mass action and a variety of actions that obeyed the Ginsparg-Wilson relation.

\[
S(\vec{p},t) = \frac{1}{2Z_T^2 \sinh E_T}(1_f(\text{sgn}(t) \sinh E_T \gamma_4 - i\gamma_5 \hat{p}_4)) + [(1 - \cosh E) + am_q + \frac{1}{2} \hat{p}_i \hat{p}_i)] - ia\mu_q \gamma_5 \tau^3 e^{-E_T t}
\]  

(19)

The rest mass ($M_1$) is obtained [32, 12] from the energy ($E_T$) at zero three momentum:

\[
cosh M_T^1 = 1 + \frac{a^2 m_q^2 + a^2 \mu_q^2}{2(1 + am_q)}
\]

(20)

At maximal twist, equation 20 shows the pole mass $M_T^1$ is a function of the $(a\mu_q)^2$ so there will be no dependence on odd powers of the lattice spacing, consistent with the general symmetry arguments [12]. The corrections to the continuum $M_1 = a\mu_q$ are much smaller than for the Wilson action in equation 13.

\[
M_T^1 = a\mu_q - \frac{1}{24} (a\mu_q)^3 + \frac{3}{640} (a\mu_q)^5 + O((a\mu_q)^7)
\]

(21)

The kinetic mass ($M_T^2$) is

\[
M_T^2 = a\mu_q \sqrt{4 + (a\mu_q)^2}
\]

(22)

The expansion of $M_T^2$ in terms of $\mu_q$

\[
M_T^2 = a\mu_q + \frac{5}{8} (a\mu_q)^3 + \frac{39}{128} (a\mu_q)^5 + O((a\mu_q)^7)
\]

(23)

The mass dependent amplitude is

\[
Z_T^{KLM} = \sqrt{Z_T^2(\vec{p} = 0)} = \sqrt{1 + m_q}
\]

(24)

At maximal twist $Z_T^{KLM}$ is 1, because $m_q$ is tuned to zero. Is is surprising that $Z_T^{KLM}$ is independent of $\mu_q$, because I would have naively expected an expression that depended on the twisted mass $\mu_q$, but with no $O(a)$ errors. In the calculation $Z_{KLM}$ is independent of $\mu_q$, because as Shindler [12] notes, the $\mu_q$ term and the Wilson terms ”point in different directions” so don’t interfere. However it would
be "cooler" to have a deeper more theoretical argument. The results for the $M_1$ and $M_2$ masses do show a dependence on $\mu a$, beyond the continuum result, but with no $O(a)$ terms as expected.

The KLM factor was originally obtained as part of deriving the transfer matrix for Wilson fermions [43, 15]. The derivation of the transfer matrix was extended to twisted mass QCD by Frezzotti et al. [32]. The normalisation of the fields in the derivation of the transfer matrix depended on a matrix called "B" in equation 13 in [43]. The equivalent "B" matrix for twisted mass QCD is the same as for Wilson fermions and independent of the $\mu q$ mass [32], and so is consistent with the KLM factor being independent of $\mu q$ at tree level.

Although this analysis is focused towards twisted mass fermions, it is interesting to try and understand the $\mu q$ independence of the KLM factor. One way of getting some insight it to look at lattice actions with more symmetry such as those with Ginsparg-Wilson symmetry [44, 45, 46], or those with a remnant of chiral symmetry such as improved staggered actions [47].

Liu and Dong have studied $O((am_Q^2)$ and $O((a^2m_Q\Lambda_{QCD})$ effects in renormalisation constants and the dispersion relation in numerical data [48, 49]. They found that the variant of the overlap action they used had lattice errors under control if they kept $am_Q < 0.5$. This numerical work suggests that a KLM factor for overlap fermions does depend on the heavy quark mass, although there are no $O(am_Q)$ corrections as expected. The work by the TWQCD collaboration uses the overlap action with much larger masses to study mesons containing the bottom quark [50].

Aarts and Foley [51] have studied an overlap operator [45, 46] in free field theory. They [51] find an overall mass dependent renormalisation factor for the quark propagator that suggests a mass dependent KLM factor. However, there are a wide variety of different solutions to the Ginsparg-Wilson relation, some of which will have a different mass dependence. Liu and Dong [48] discuss one choice that may have good properties in the heavy mass limit. It would be interesting to see if a KLM factor could parameterise the numerical data of [48, 49] using methods in [51, 52].

The tree level mass corrections to the improved staggered action called HISQ were considered by the HPQCD collaboration [17]. The coefficient of the Naik term was tuned at tree level to obtain a speed of light of one, up to errors of order $O((am_q)^{12})$. The wave function renormalisation at tree level reported by HPQCD [17] for the HISQ action with the Naik term corrected with a mass dependent factor, had an explicit but weak dependence on the quark mass.

From considering the HISQ and overlap actions above, it is unusual to have a wave function factor that does not depend on the physical quark mass.
5 Automatic O(a) improvement and the FNAL formalism

One very clever proof for the automatic O(a) improvement \[11\], used that the action in the physical basis (\(S_{\text{lat,F}}\) in equation 25 with \(\zeta=1\) and \(r_s=1\)) was invariant under the symmetry \(\mathcal{P} \times D_d \times (\mu_q \rightarrow -\mu_q)\) where \((x_P = (-x, t))\). The automatic O(a) improvement of the twisted mass Wilson action, based on the above symmetry, has been tested numerically in quenched QCD \[53, 54, 55\] and \(n_f = 2\) unquenched QCD \[14\].

The \(\mathcal{P}\) symmetry transformation is defined by

\[
\begin{align*}
U_0(x) & \rightarrow U_0(x_P) \\
U_k(x) & \rightarrow U_k^\dagger(x_P - a\hat{k}) \\
\psi(x) & \rightarrow \gamma_0 \psi(x_P) \\
\bar{\psi}(x) & \rightarrow \bar{\psi}(x_P) \gamma_0
\end{align*}
\]

and the \(D_d\) symmetry is defined by

\[
\begin{align*}
U_\mu(x) & \rightarrow U_\mu^\dagger(-x - a\hat{\mu}) \\
\psi(x) & \rightarrow e^{3\pi i/2} \psi(-x) \\
\bar{\psi}(x) & \rightarrow e^{3\pi i/2} \bar{\psi}(-x)
\end{align*}
\]

The argument in \[11\] only required that the action was invariant under the group \(\mathcal{P} \times D_d \times (\mu_q \rightarrow -\mu_q)\) and not that the action is also invariant under the full hypercubic group. To connect with the proof in \[11\], I consider the twisted mass action in equation 6 at maximal twist rotated into the physical basis in equation 25

\[
S_{\text{lat,F}} = \sum_x \bar{\psi}(x)(\gamma_0 D_0 + \zeta \gamma_i D_i + \mu_q - i\tau_3 \gamma_5(-\frac{1}{2}D_0^2 - r_s \frac{1}{2}D_i^2 + m_{cr})\psi(x) \quad (25)
\]

where \(m_{cr}\) is \(m_q\) tuned to the critical mass from setting the PCAC mass to zero.

The action \(S_{\text{lat,F}}\) in equation 25 with arbitrary \(\zeta\) and \(r_s\) parameters is also invariant under \(\mathcal{P} \times D_d \times (\mu_q \rightarrow -\mu_q)\), hence it should be automatically O(a) improved. The clover term should have a coefficient that is an odd power of the quark mass. The two parameters: \(\zeta\) and \(r_s\), need to be tuned for the twisted version of the heavy quark action, but should only be an even power of the quark mass. The recent work on an improved Fermilab heavy quark action included dimension 7 operators \[37\], so adding a twisted mass term, may help with the design of more highly improved heavy quark actions.

I don’t see any simple connection between the symmetry \(\mathcal{P} \times D_d \times (\mu_q \rightarrow -\mu_q)\) and getting a mass independent KLM factor in equation 24.
6 Conclusions

I have discussed the inclusion of a twisted mass term with the FNAL heavy fermion action at tree level. This is useful for the analysis of existing $n_f = 2$ twisted mass lattice QCD calculations with heavy masses, and heavy quark calculations using the Osterwalder-Seiler action [30, 31] on configurations with 2+1+1 flavours of sea quarks. One surprising thing about the KLM factor for twisted mass QCD was that it was independent of the twisted mass at tree level. To estimate the order of magnitude of the various improvements terms I use the numerical values $\alpha_s \sim 0.24$ and $am_Q \sim 0.26$ for the $\beta = 3.9$ data set, with a lattice spacing of 0.0855 fm, from the ETM Collaboration [7]. For the twisted quark action with heavy mass $m_Q$, automatic $O(a)$ improvement means that the leading error should be $O((am_Q)^2)$ which is approximately 7%. The mass independence of the KLM factor for twisted mass fermions implies that the leading corrections are $O((\alpha_s am_Q)^2)$ and numerically about 2%. The preliminary numerical results from lattice QCD calculations with heavy quark from twisted mass QCD seem to have larger errors than the above estimates.

I showed that the symmetry that protects the twisted Wilson action from $O(a)$ corrections, should also protect an action where the hyper-cubic invariance is broken, as used in the FNAL heavy quark action. Some quantities such as the hyperfine splitting in charmonium are known to be sensitive to the value of the clover coefficient and lattice spacing errors [57, 58, 59, 60] so automatic $O(a)$ improvement should be useful.

Since twisted mass QCD has no $O(a)$ errors, it is in principle possible to use lattice calculations at three different lattice spacings and take a consistent continuum limit for calculations that include heavy quarks. It may be useful to supplement the ”brute force approach” with an estimate of systematic errors from the FNAL heavy quark formalism.

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