We present a new (and general) algorithm for deriving lattice Feynman rules which is capable of handling actions as complex as the Highly Improved Staggered Quark (HISQ) action. This enables us to perform a perturbative calculation of the influence of dynamical HISQ fermions on the perturbative improvement of the gluonic action in the same way as we have previously done for asqtad fermions. We find the fermionic contributions to the radiative corrections in the Lüscher-Weisz gauge action to be somewhat larger for HISQ fermions than for asqtad.
1. Introduction

Continuing rapid advances in parallel computing, along with theoretical progress in the formulation of lattice field theories with fermions, have led to lattice QCD simulations with dynamical light quarks becoming the norm rather than the exception.

The Fermilab Lattice, MILC and HPQCD collaborations have an ambitious program which to date has made several high-precision predictions from unquenched lattice QCD simulations [1]. This body of work is based on the Symanzik-improved staggered-quark formalism, specifically the use of the asqtad [2] action. More recently, the Highly Improved Staggered Quark (HISQ) action has been used to further suppress taste-changing interactions and to allow the use of heavier quarks at the same lattice spacing by removing tree-level $O((ma)^4)$ artifacts from the quark action [4]. In order to consistently use the HISQ action for the sea quarks as well [5], the calculation of HISQ quark loops on the Symanzik-improvement of the gluon action is also needed. Having previously carried out that calculation for the asqtad action [6], we update our calculation here to apply to the case of dynamical HISQ fermions.

2. Perturbation Theory for the HISQ action

The HISQ action is defined by an iterated smearing procedure with reunitarisation:

$$U_{\text{HISQ}} = (F_{\text{asq}} \circ P_{U(3)} \circ F_{\text{Fat7}})[U] \tag{2.1}$$

where $U = \exp(gA)$ is the unsmeared gauge field, $P_{U(3)}$ denotes the polar projection onto $U(3)$ (as used in simulations, and not $SU(3)$), and the Fat7 and modified asq smearings are defined in [4]. Straightforward application of the methods from [7] to this action is unfeasible, since the memory requirements for expanding the action directly into monomials quickly become excessive. We therefore take advantage of the two-level structure inherent in the definition of the action and split the derivation and application of the Feynman rules into two steps.

In the first step, the Feynman rules for the outer layer (the modified asqtad action) are derived in the same way as previously. We use our HiPPy python code [7] to expand the asq’ action in terms of the Fat7R smeared link

$$U_{\mu}^{\text{Fat7R}}(x) = (P_{U(3)} \circ F_{\text{Fat7}})[U_{\mu}] = e^{B_{\mu}(x + \frac{1}{2} \hat{\mu})} \tag{2.2}$$

with a Lie-algebra–valued field $B_{\mu}$, giving the usual monomials

$$V_r = \frac{g_f}{r!} \sum f_{r,i}^{\text{asq}} \bar{\psi}(x_{r,i}) B_{\mu_1}(v_{r,i,1}) \cdots B_{\mu_r}(v_{r,i,r}) \Gamma_{r,i} \psi(y_{r,i}) \tag{2.3}$$

To derive the full HISQ Feynman rules, we also need to know the expansion of $B_{\mu}$ in terms of the original gauge potential $A_{\mu}$. To obtain this, we write the Fat7-smeared link as \footnote{In the following, we will suppress Lorentz and lattice site indices.} $F_{\text{Fat7}}[U] = M = HV$, where $H^\dagger = H$ and $V \in U(3)$. We can now use our HiPPy expansion routines [7] to obtain an expansion

$$M = e[1 + a_{\mu} * A_{\mu} + a_{\mu\nu} * (A_{\mu} * A_{\nu}) + \ldots] \tag{2.4}$$
where, e.g. \( a_{\mu\nu} (A_{\mu} A_{\nu}) = \sum_{x,y} a_{\mu\nu}(x,y) A_{\mu}(x+\frac{1}{2}\hat{\mu}) A_{\nu}(y+\frac{1}{2}\hat{\nu}) \). Then unitarity of \( V \) implies that \( R \equiv MM^\dagger = H^2 \) and hence \( V = R^{-1/2}M \) using the expansion

\[
R^{-1/2} = (1 + (R - 1))^{-1/2} = 1 - \frac{1}{2} (R - 1) + \frac{3}{8} (R - 1)^2 + \ldots \tag{2.5}
\]

Rearranging the result as

\[
B = \log(V) = (V - 1) - \frac{1}{2} (V - 1)^2 + \ldots \tag{2.6}
\]

finally yields the desired expansion of \( B \).

Given this, we can now numerically reconstruct the HISQ Feynman rules for any given set of momenta from eqn. (2.3) by a convolution of the asqtad Feynman rules of eqn. (2.3) with the expansion of \( B_\mu \) in terms of \( A_\mu \), summing up all the different ways in which the gluons \( A_\mu \) going into the vertex could have come from the fields \( B_\mu \) appearing in eqn. (2.3). Compared to a simple-minded expansion of the HISQ action, this not only save enough memory to enable the derivation to be performed in practice, but also leads to a considerable speed-up in many cases. In particular, we can take advantage of the (anti-)symmetries that the expansion of \( B_\mu \) in terms of \( A_\mu \) possesses, allowing us to reduce the number of contributions we need to take into account when evaluating Feynman diagrams. In the calculation of the three-gluon vertex for the “octopus” diagram (a fermion tadpole with three gluon legs) entering the three-point function, we are able to omit the contribution from the expansion of a single \( B_\mu \) into three gluons on symmetry grounds.

### 3. On-shell improvement

The Lüscher-Weisz action is given by \([8]\)

\[
S = \sum_x \left\{ (1 - 8(c_1 + c_2)) \sum_{\mu \neq \nu} \langle 1 - P_{\mu\nu} \rangle + 2c_1 \sum_{\mu \neq \nu} \langle 1 - R_{\mu\nu} \rangle + \frac{4}{3} c_2 \sum_{\mu \neq \nu \neq \rho} \langle 1 - T_{\mu\nu\rho} \rangle \right\}, \tag{3.1}
\]

where \( P, R \) and \( T \) are the plaquette, rectangle and “twisted” parallelogram loops, respectively. The coefficients \( c_1 \) and \( c_2 \) need to be determined in order to eliminate the \( O(a^2) \) lattice artifacts.

Given two independent quantities \( Q_1 \) and \( Q_2 \) with expansions

\[
Q_i = \tilde{Q}_i + w_i (\mu a)^2 + d_{ij} e_j (\mu a)^2 + O((\mu a)^4), \tag{3.2}
\]

in powers of \( (\mu a) \), where \( \mu \) is some energy scale, we obtain the \( O(a^2) \) matching condition

\[
d_{ij} e_j = -w_i. \tag{3.3}
\]

Since this equation is linear, both sides can be decomposed into a gluonic and a fermionic part; the known gluonic part \([9, 10]\) being independent of the fermion action, we will here focus only on the fermionic part.

At tree-level, there are no fermion loops to consider, and hence the tree-level coefficients remain unchanged compared to the quenched case \([9]\). To compute to one-loop fermionic corrections to the gluon action, we will follow the same procedure as in the case of the asqtad action \([6]\).
4. Twisted boundary conditions

We work on a four-dimensional Euclidean lattice of length $La$ in the $x$ and $y$ directions and lengths $L_z, L_t$ in the $z$ and $t$ directions, respectively, where $a$ is the lattice spacing and $L, L_z, L_t$ are even integers. In the following, we will employ twisted boundary conditions in much the same way as in [9, 10]. The twisted boundary conditions we use for gluons and quarks are applied to the $(x,y)$ directions and are given by ($v = x,y$)

$$U_\mu(x + LV) = \Omega_v U_\mu(x) \Omega_v^{-1}, \quad \Psi(x + LV) = \Omega_v \Psi(x) \Omega_v^{-1},$$

(4.1)

where the quark field $\Psi_{sc}(x)$ becomes a matrix in smell-colour space [11] by the introduction of a new SU(N) quantum number “smell” in addition to the quark colour. We apply periodic boundary conditions in the $(z,t)$ directions.

These boundary conditions lead to a change in the Fourier expansion of the fields: in the twisted $(x,y)$ directions the momentum sums are now over

$$p_v = mn_v, \quad -\frac{NL}{2} < n_v \leq \frac{NL}{2}, \quad v = (x,y),$$

(4.2)

where $m = \frac{2\pi}{NL}$. The modes with $(n_x = n_y = 0 \mod N)$ are omitted from the sum in the case of the gluons. The momentum sums for quark loops need to be divided by $N$ to remove the redundant smell factor.

The twisted theory can be viewed as a two-dimensional Kaluza-Klein theory in the $(z,t)$ plane. Denoting $n = (n_x, n_y)$, the stable particles in the $(z,t)$ continuum limit of this effective theory are called the A mesons ($n = (1,0)$ or $n = (0,1)$) with mass $m$ and the B mesons ($n = (1,1)$) with mass $\sqrt{2}m$ [10].

5. Small-mass expansions

Although we ultimately wish to extrapolate to the chiral limit, we cannot set $m_qa = 0$ straight away, since the correct chiral limit is $m_qa \rightarrow 0$, $ma \rightarrow 0$, $m_q/m > C$, where $C$ is a constant determined by the requirement that a Wick rotation can be performed without encountering a pinch singularity.

Therefore, we first expand some observable quantity $Q$ in powers of $ma$ at fixed $m_qa$:

$$Q(ma, m_qa) = a^{(Q)}_0(m_qa) + a^{(Q)}_2(m_qa)(ma)^2 + o((ma)^4, (ma)^4 \log(ma))$$

(5.1)

where the coefficients in the expansion are all functions of $m_qa$. There is no term at $o((ma)^2 \log(ma))$ since the gluon action is improved at tree-level to $O(a^2)$ [10]. Then, we expand the coefficients $a^{(Q)}_0(m_qa)$ in power of $m_qa$.

For $a^{(Q)}_0(m_qa)$ we have

$$a^{(Q)}_0(m_qa) = b^{(Q)}_{0,0} \log(m_qa) + a^{(Q)}_{0,0}.$$  

(5.2)

Since we expect a well-defined continuum limit, $a^{(Q)}_0(m_qa)$ cannot contain any negative powers of $m_qa$, but may contain logarithms; $b^{(Q)}_{0,0}$ is the anomalous dimension associated with $Q$, and can be determined by a continuum calculation.
Figure 1: A plot of the fermionic contributions to the one-loop A meson self-energy $m_A^{(1)}/m$ against $(ma)^2$. The vanishing of $m_A^{(1)}/m$ in the infinite-volume limit can be seen clearly.

For $a_2^{(Q)}(ma)$ we find

$$a_2^{(Q)}(ma) = \frac{a_2^{(Q)} - a_0^{(Q)}}{(ma)^2} + (a_2^{(Q)} + b_2^{(Q)} \log(ma)) (ma)^2 \Theta((ma)^4).$$

After multiplication by $(ma)^2$, the $(ma)^{-2}$ contribution gives rise to a continuum contribution to $Q$, and $a_2^{(Q)}$ is calculable in continuum perturbation theory. There can be no term in $(ma)^{-2} \log(ma)$ since this would be a volume-dependent further contribution to the anomalous dimension of $Q$, and there can be no term in $\log(ma)$ since the action is tree-level $O(a^2)$ improved.

After the chiral limit $m_q \to 0$, the term $w_i$ that appears on the right-hand side of Eqn. (3.3) is $a_2^{(Q)}$.

6. Twisted spectral quantities

The simplest spectral quantity that can be chosen within the framework of the twisted boundary conditions outlined above is the (renormalised) mass of the A meson. The one-loop correction the the A meson mass is given by

$$m_A^{(1)} = -Z_0(k) \left. \pi_1^{(1)}(k) \right|_{k=(ma,0,m,0)}$$

(6.1)

where $Z_0(k) = 1 + \Theta((ma)^4)$ is the residue of the pole of the tree-level gluon propagator at spatial momentum $k$, and $m_A^{(0)}$ is defined so that the momentum $k$ is on-shell.

From gauge invariance we find $a_2^{(m_A,1)} = 0$ and $a_0^{(m_A,1)}(ma) = 0$. The $\Theta(\alpha_s(ma)^2)$ contribution from improvement of the action is given by [10]

$$\Delta_{imp} m_A^{(1)}/m = -(c_1^{(1)} - c_2^{(1)})(ma)^2 + \Theta((ma)^4).$$

(6.2)
The next simplest independent spectral quantity is the scattering amplitude for A mesons at B meson threshold, which can be described by an effective AAB meson coupling constant $\lambda$ [12]:

$$\lambda = g_0 \sqrt{Z(k)Z(p)Z(q)} e_j \Gamma^{1,2,j}(k, p, q)$$  \hspace{1cm} (6.3)

with a twist factor of $\frac{1}{N} \text{Tr}([\Gamma_k, \Gamma_p][\Gamma_q])$ factored out from both sides, and the momenta and polarisations of the incoming particles are (where $r > 0$ is defined such that $E(q) = 0$)

$$k = (iE(k), k) \quad p = (-iE(p), p) \quad q = (0, q) \quad e = (0, 1, -1, 0)$$

$$k = (0, m, ir) \quad p = (m, 0, ir) \quad q = (-m, -m, -2ir)$$  \hspace{1cm} (6.4)

We expand Eqn. (6.3) perturbatively to one-loop order and find (up to $O((ma)^4)$ corrections)

$$\frac{\lambda^{(1)}}{m} = \left(1 - \frac{1}{24} m^2 \right) \frac{\Gamma^{(1)}}{m} - \frac{d}{dk} \left. \pi_1^{(1)}(k) \right|_{k=0} - \frac{1}{12} \frac{d^2}{dq^0} \left. \left( e^i e^j \pi^{(1)}_{ij}(q) \right) \right|_{q=0}$$  \hspace{1cm} (6.5)

The derivatives of Feynman diagrams are computed using automatic differentiation [13]. Continuum calculations of the anomalous dimension and infrared divergence give

$$b^{(\lambda, 1)}_{0,0} = - \frac{N_f}{3\pi G^2}, \quad c^{(\lambda, 1)}_{2,-2} = - \frac{N_f}{120\pi G^2}.$$  \hspace{1cm} (6.6)

The improvement contribution to $\lambda$ is [10]

$$\Delta_{imp} \frac{\lambda^{(1)}}{m} = 4(9c_1^{(1)} - 7c_2^{(1)})(ma)^2 + O((ma)^4).$$  \hspace{1cm} (6.7)

7. Results

To extract the improvement coefficients from our diagrammatic calculations, we compute the diagrams for a number of different values of both $L$ and $m_q$ with $N_f = 1$, $N = 3$. At each value of $m_q$, we then perform a fit in $ma$ of the form given in Eqn. (5.1) to extract the coefficients $a_n^{(Q, 1)}(m_q a)$, $n = 0, 2$. Our fits confirm that $a_0^{(ma, 1)}(m_q a) = 0$.
Performing a fit of the form (5.2) and (5.3), respectively, on these coefficients, we are able to extract the analytically-known coefficients with high accuracy, along with the required $(ma)^2$ contributions.

Solving equation (3.3) for $c_i^{(1)}$ given the fitted values for $\alpha_2^{Q,0}$, our results can be summarised as

$$c_1^{(1)} = -0.025218(4) + 0.0110(3)N_f$$
$$c_2^{(1)} = -0.004418(4) + 0.0016(3)N_f$$

where the quenched ($N_f = 0$) results are taken from [10]. The shift from the unquenched values is surprisingly large, even compared to the coefficients for asqtad fermions [6]. At first sight, this may seem like a surprise, since HISQ is supposed to be the more highly-improved action. However, HISQ is designed to suppress taste-changing interactions (low momentum quark/high momentum gluon couplings), but these coefficients come from high momentum quark/low momentum gluon couplings, for whose suppression the HISQ action is not tuned.

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