Efficient Simulation of Heavy Quark Vacuum Polarization

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Abstract

We outline a simple way to include heavy quark vacuum polarization in lattice QCD simulations. The method, based on effective field theory, requires only a trivial modification of the gluon action and has no impact on simulation times. We assess the range of validity for this procedure, and the impact that it may have.

1 Introduction

The inclusion of light quark vacuum polarization in lattice QCD Monte Carlo simulations has long been a major problem. With the development of improved staggered fermions [1] it has become possible to do high-precision lattice QCD, with good control over all systematic errors [2]. One such systematic error is the continued exclusion of heavy quark vacuum polarization. State of the art lattice simulations only include the effects of light (s, u and d) quark vacuum polarization.

The exclusion of heavy quark vacuum polarization is a good approximation because, as we shall discuss, their effect on simulation results is suppressed by a factor of $\bar{q}^2/m^2$, where $\bar{q}$ is a typical lattice momentum. For many lattice calculations (hadron spectra, decay constants) $\bar{q} \approx \Lambda_{QCD} \approx 250$MeV. For a charm quark $m_c \approx 1$GeV this could be as large as a 6% effect. Today’s lattice calculations aspire to few percent (1–3%) errors [2], so for truly high-precision work, this error should be removed. It would be good to have a method for removing it without having to do full dynamical simulations of the heavy quarks. Fortunately these effects can be handled using effective field theory.

2 The Effective Lagrangian

The earliest example of an effective field theory is the Euler–Heisenberg non-linear photon theory [3]. This is an expansion of QED for low-energy photons
with average energies $\omega \ll m_e$. Euler and Heisenberg were concerned with non-linear interactions between four photons, these corrections begin at $O(\omega^4/m_e^4)$, however there is a correction to the photon propagator which is a $O(\omega^2/m_e^2)$ effect. Similar expansions apply to QCD.

It is straightforward to write down the most general effective action that will account for these effects

$$S_{EH} = \int d^4x \left[ -\frac{1}{4} F_\mu^a F_\nu^a + \sum_Q \left( \sum_n \frac{C_{O_n}}{m_Q^{n+1}} O_n \right) \right]$$  \hspace{1cm} (1)

where $O_n$ are operators of dimension $2(n+1)$ built out of $F_\mu^a$, $\tilde{F}_\mu^a$, $D_\mu$ that respect the symmetries of QCD, $C_{O_n}$ are the coefficients of these operators and the sum runs over all heavy quark flavors $Q = c, b, t$. The operators of higher dimensions are suppressed by powers of the heavy quark masses. In this note, we will be concerned with only the operators of dimension six.

At dimension six there are two operators we need to consider \[5\]

$$G_1 = g_s f_{abc} F_\mu^a F_\nu^b F_\sigma^c F^{\sigma\mu}$$ \hspace{1cm} (2)

$$G_2 = \frac{1}{2} D_\mu F_\nu^a D_\nu F_\sigma^a$$ \hspace{1cm} (3)

With these operators the effective action is

$$S_{EH} = \int d^4x \left[ -\frac{1}{4} F_\mu^a F_\nu^a + \sum_Q \left( \frac{C_{G_1}}{m_Q^2} G_1 + \frac{C_{G_2}}{m_Q^2} G_2 \right) \right]$$  \hspace{1cm} (4)

This action can be matched to full QCD order by order in perturbation theory, since a heavy quark loop is highly virtual. Matching at leading order gives the coefficients \[6\]

$$C_{G_1} = -C_F \frac{\alpha_s}{360\pi}, \quad C_{G_2} = -C_F \frac{\alpha_s}{15\pi}$$ \hspace{1cm} (5)

where $C_F = 4/3$ for $SU(3)$.

For matching to the lattice theory it is convenient to rewrite the action in terms of a different basis of operators. We introduce the operator \[5\]

$$G_3 = D_\lambda F_\mu^\lambda D_\nu F_\nu^a$$ \hspace{1cm} (6)

and make use of the relation \[5\]

$$\int d^4x G_1 = \int d^4x \left[ \frac{1}{2} G_3 - 2G_2 \right]$$ \hspace{1cm} (7)

to rewrite the action as

$$S_{EH} = \int d^4x \left[ -\frac{1}{4} F_\mu^a F_\nu^a + \sum_Q \left( \frac{C_{G_1}}{2m_Q^2} G_3 + \frac{C_{G_2} - 2C_{G_1}}{m_Q^2} G_2 \right) \right].$$  \hspace{1cm} (8)
In this brief note we are primarily concerned with the effect of heavy quark vacuum polarization on the gluon action. With this in mind we make a field transformation

$$A_\mu^a \rightarrow A_\mu^a + \frac{C}{m_Q^2} \alpha_s D^\nu F_\nu^a$$

which gives

$$F_\mu^a F_\nu^a \rightarrow F_\mu^a F_\nu^a - \frac{8C}{m_Q^2} \alpha_s G_2 + O\left(\frac{1}{m_Q^4}\right).$$

We can pick the constant $C$ to eliminate $G_2$ from the gluon action. This transformation will introduce additional four-quark operators which should be incorporated into the fermion actions used in the simulations.

Finally, we rescale the fields $A \rightarrow A/g_s$, and express the action as

$$S_{EH} = -\frac{1}{2g_s^2} \int d^4x \left\{ \sum_{\mu\nu} \text{Tr} [F_\mu^{\nu} F_\nu^{\mu}] + \sum_Q \frac{1}{m_Q^2} \left( C_F \frac{\alpha_s}{180\pi} \sum_{\mu\nu\lambda} \text{Tr} [D_\lambda F_\mu^{\nu} D_\lambda F_\nu^{\mu}] \right) \right\}.$$  \hspace{1cm} (11)

Our goal is to construct a lattice gluon action that reproduces this action. Before we do this, it is useful to consider how large the mass $m_Q$ should be in order that the expansion in $m_Q^{-2}$ is sensible.

### 3 Limits on $m_Q$

In order to set limits on the expansion in $m_Q^{-2}$ we look at one part of the matching calculation for $G_2$. To match the coefficient $C_{G_2}$ one can consider (light) quark-quark scattering at one loop order in continuum QCD. The only effect of virtual heavy quarks at this order will be their contribution to the gluon vacuum polarization. Therefore, we can get a check on the validity of the expansion by investigating the one-loop gluon propagator in continuum QCD.

In full QCD the renormalized gluon propagator is given (in Feynman gauge) by

$$D_{\mu\nu}(q^2) = \frac{-ig_{\mu\nu}}{q^2 \left[ 1 - \Pi(q^2) \right]}.$$  \hspace{1cm} (12)

We separate the contribution of heavy quark loops out of the self energy

$$\Pi(q^2) = \sum_Q \Pi_Q(q^2) + \Pi_{QCD}(q^2).$$  \hspace{1cm} (13)

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1This technique is used to eliminate the same operator in the lattice theory, with $m^{-2} \rightarrow a^{-2}$. 

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The light quark and gluonic parts of the self energy will be described by the standard QCD action, so we’ll just retain the heavy quark contribution. Therefore, we will consider the propagator

$$D_{\mu\nu}(q^2) = \frac{-ig_{\mu\nu}}{q^2 \left[ 1 - \sum_Q \hat{\Pi}_Q(q^2) \right]}.$$  (14)

The contribution to the self energy can be found in any textbook (for example [7]) it’s just the QED contribution times the color factor $C_F$.

$$\hat{\Pi}_Q(q^2) = -C_F \frac{2\alpha_s}{\pi} \int_0^1 dx x(1-x) \log \left[ \frac{1}{1 - \frac{q^2}{m_Q^2}x(1-x)} \right].$$  (15)

Expanding in $q^2/m_Q^2$ we find

$$\hat{\Pi}_Q(q^2) = -C_F \frac{\alpha_s}{15\pi} \frac{q^2}{m_Q^2}.$$  (16)

The range of validity for the expansion in $1/m_Q^2$ is set by the radius of convergence of the logarithm in (15),

$$|q| < 2m_Q.$$  (17)

Since our goal is to use this expansion in lattice simulations it is useful to express this in lattice units, multiplying both sides by $a$, and taking the momentum $|q| = \Lambda_{QCD}$

$$m_Q a > 0.5\Lambda_{QCD} a$$

For a 0.1 fm lattice $\Lambda_{QCD} a \approx 0.1 - 0.3$, so we get a very loose limit, $m_Q a > 0.05 - 0.15$. At this lattice spacing, $m_c a = 0.5$, so this bound is satisfied. Notice that for low momentum processes it is not necessary for $m_Q a$ to be greater than one, fundamentally this is an expansion in $|q|/m_Q$ not $1/(m_Q a)$. For processes that involve larger internal momenta this limit is more strict. For example, the semileptonic form factor for $B \to \pi + \ell + \nu$ can involve internal momenta as high as

$$\sqrt{\frac{\Lambda_{QCD} m_b}{2}} \approx 1\text{GeV}.$$  (19)

With $|q| = 1\text{GeV}$ (19) is still satisfied for a charm quark, but for lighter quarks it wouldn’t be. When we match to the lattice theory we will find another bound on $m_Q a$.

4 Matching to the Lattice Theory

The leading correction in (11) is trivially included in the widely used improved gluon action

$$S_L = \frac{2}{g_0^2} \sum_x \left\{ \beta_P \frac{1}{3} \text{ReTr} [1 - U_P] + \beta_R \frac{1}{3} \text{ReTr} [1 - U_R] + \beta_6 \frac{1}{3} \text{ReTr} [1 - U_6] \right\}.$$  (20)
where $U_P$ is the plaquette, $U_R$ is the rectangle, and $U_6$ is the parallelogram term. We define the operators

\[
\mathcal{F}_0 = \sum_{\mu\nu} \text{Tr} (F_{\mu\nu} F_{\mu\nu})
\]

\[
\mathcal{F}_1 = \sum_{\mu\nu} \text{Tr} (D_{\mu} F_{\mu\nu} D_{\mu} F_{\mu\nu})
\]

\[
\mathcal{F}_2 = \sum_{\mu\nu\sigma} \text{Tr} (D_{\sigma} F_{\mu\nu} D_{\sigma} F_{\mu\nu})
\]

in terms of which we have

\[
\frac{1}{3} \text{Re} \text{Tr} [1 - U_P] = -\frac{a^4}{4} \mathcal{F}_0 + \frac{a^6}{24} \mathcal{F}_1 + \mathcal{O} (a^8)
\]

\[
\frac{1}{3} \text{Re} \text{Tr} [1 - U_R] = -2a^4 \mathcal{F}_0 + 5a^6 \mathcal{F}_1 + \mathcal{O} (a^8)
\]

\[
\frac{1}{3} \text{Re} \text{Tr} [1 - U_6] = -2a^4 \mathcal{F}_0 + \frac{a^6}{3} \mathcal{F}_1 + \frac{a^6}{6} \mathcal{F}_2 + \mathcal{O} (a^8).
\]

The choice

\[
\beta_6 = 0
\]

\[
\beta_R = -\frac{1}{20u_0^2} \beta_P
\]

\[
\beta_P = \frac{5}{3}
\]

gives

\[
S_L = \frac{1}{2g_0} \int d^4 x \mathcal{F}_0 + \mathcal{O} (\alpha_s a^2, a^4, \alpha_s/(m_c a^2)) .
\]

In order to reproduce this we need to have a non-zero value for $\beta_6$. When we do this, we are forced to include an additional correction to $\beta_R$ in order to cancel any potential contribution from $\mathcal{F}_1$. We take

\[
\beta_6 = \frac{\beta_P}{u_0^2} \frac{\alpha_s}{(am_Q)^2} C^{[1]}
\]

\[
\beta_R = -\frac{1}{20u_0^2} \beta_P \left( 1 + \frac{\alpha_s}{(am_Q)^2} R^{[1]} \right)
\]

\[
\beta_P = \frac{5}{3}
\]

\[2\text{Corrections to the standard Wilson plaquette action due to heavy quark vacuum polarization have been investigated in [8,9].}\]

\[3\text{The factor of } u_0 \text{ is a tadpole improvement factor, it plays no role in our discussion.}\]
which gives

\[
S_L = -\frac{1}{2g_0^2} a^4 \sum_x \left\{ \left( 1 - \frac{\alpha_s}{(am_Q)^2} \left[ \frac{40}{3} C^{[1]} - \frac{2}{3} R^{[1]} \right] \right) F_0 \\
+ a^2 \frac{\alpha_s}{(am_Q)^2} \left[ \frac{5}{18} R^{[1]} - \frac{10}{3} C^{[1]} \right] F_1 \\
- a^2 \frac{10 \alpha_s}{9(am_Q)^2} C^{[1]} F_2 \right\},
\]

(26)

where for simplicity we just include only one flavor of heavy quark. Setting

\[
C^{[1]} = -C_F \frac{1}{200\pi} = -\frac{1}{150\pi}
\]

(27)

produces the correct coefficient for the \( F_2 \) term. The additional contribution to the coefficient of the \( F_0 \) term produces an unobservable shift in the wavefunction renormalization for the gluons, so we are free to drop it. This leaves only the \( F_1 \) term. We tune \( R^{[1]} \) to insure that its coefficient remains zero. This is easily accomplished with

\[
R^{[1]} = 12 C^{[1]} = -\frac{2}{25\pi}.
\]

(28)

With these values the lattice action correctly reproduces \( \beta \) with

\[
O (a^4, \alpha_s a^2, \alpha_s / (am_c)^4, \alpha_s^2 / (am_c)^2)
\]

(29)

errors.

5 Impact on One-Loop Corrections

We combine our results with the known one loop corrections to \( \beta_R \) and \( \beta_6 \),

\[
\beta_R = -\frac{\beta_P}{16u_0^2} \left[ 1 + \alpha_s (\pi/a) \left( 0.4805 + X_R N_f - \frac{2}{25\pi} \sum_Q \frac{1}{(am_Q)^2} \right) \right]
\]

(30)

\[
\beta_6 = -\frac{\beta_P}{u_0^2} \alpha_s (\pi/a) \left( 0.03325 + X_6 N_f + \frac{1}{150\pi} \sum_Q \frac{1}{(am_Q)^2} \right).
\]

(31)

The one loop terms due to the gluons are well known [11, 12], those due to dynamical light fermions are being computed [13]. With \( am_c \approx 1 \) these corrections to the one-loop terms are 0.025 for \( \beta_R \) and 0.0021 for \( \beta_6 \).

These expressions also limit how small one can take \( a \). The coupling constant \( \alpha_s (\pi/a) \) goes to zero logarithmically as \( a \to 0 \), whereas the correction from the heavy quark vacuum polarization is growing as \( 1/a^2 \). Clearly, if we take \( a \) too small the correction term will end up larger than the tree level term. For
example, on an ultra-fine lattice, with \( a = 0.01 \) fm, we have \( m_c a = 0.05 \), which gives (setting \( N_f = 0 \))

\[
\beta_R = -\frac{\beta_P}{20u_0^2} [1 - 9.7\alpha_s(\pi/a)], \quad \beta_6 = \frac{\beta_P}{u_0^2} 0.88\alpha_s(\pi/a). \tag{32}
\]

In this case, the “correction” to \( \beta_R \) is larger than the leading order term. With \( m_c a = 0.13 \) the coefficient of the correction term becomes one, so we take this as a rough lower limit, \( a = 0.025 \) fm.

A more realistic lattice spacing is \( a = 0.09 \) fm, which gives \( m_c a = 0.45 \) and

\[
\beta_R = -\frac{\beta_P}{20u_0^2} [1 + (0.481 - 0.126)\alpha_s(\pi/a)] = -\frac{\beta_P}{20u_0^2} [1 + 0.355\alpha_s(\pi/a)], \\
\beta_6 = -\frac{\beta_P}{u_0^2} (0.0333 + 0.0105)\alpha_s(\pi/a) = -\frac{\beta_P}{u_0^2} 0.0437\alpha_s(\pi/a). \tag{33}
\]

In the this case, the corrections due to heavy quark vacuum polarization are significant but do not cause convergence problems.

## 6 Conclusion

In this note we have demonstrated that heavy quark vacuum polarization can be included in Monte Carlo lattice simulations with no additional computational cost. The action is the standard Symanzik improved gluon action

\[
S_L = \frac{2}{g_0} \sum_i \left\{ \beta_R \frac{1}{3} \text{ReTr} [1 - U_P] + \beta_R \frac{1}{3} \text{ReTr} [1 - U_R] + \beta_6 \frac{1}{3} \text{ReTr} [1 - U_6] \right\} \tag{34}
\]

with modified coefficients

\[
\beta_R = -\frac{\beta_P}{20u_0^2} \left[ 1 + \alpha_s(\pi/a) \left( 0.4805 + X_R N_f - \frac{2}{25\pi} \sum_Q \frac{1}{(am_Q)^2} \right) \right] \\
\beta_6 = -\frac{\beta_P}{u_0^2} \alpha_s(\pi/a) \left( 0.03325 + X_6 N_f + \frac{1}{150\pi} \sum_Q \frac{1}{(am_Q)^2} \right) \tag{35} \\
\beta_P = \frac{5}{3}.
\]

This action reproduces continuum QCD up to corrections of order \( a^4, (\alpha_s a)^2, \alpha_s/(am_c)^4 \) and \( \alpha_s^2/(am_c)^2 \). In order to insure reasonable behaviour of the perturbation series \( m_c a > 0.13 \) is required. With this constraint, this action should simulate processes with average internal momentum \( |q| \ll 2m_c \). Ideally, the charm quark would be treated dynamically, then these constraints would apply \( m_c a \) instead.
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