Stout-link smearing in lattice fermion actions

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The properties of the momentum space quark propagator in Landau gauge are studied for the overlap quark action in quenched lattice QCD. Numerical calculations are performed over four ensembles of gauge configurations, where three are smeared using either 1, 3, or 6 sweeps of stout-link smearing. We calculate the non-perturbative wave function renormalization function \( Z(p) \) and the non-perturbative mass function \( M(p) \) for a variety of bare quark masses. We find that the wave-function renormalization function is slightly sensitive to the number of stout-link smearing sweeps. For the mass function we find the effect of the stout-link smearing algorithm to be small for moderate to light bare quark masses. For a heavy bare quark mass we find a strong dependence on the number of smearing sweeps.

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The quark propagator is one of the fundamental components of Quantum Chromodynamics (QCD). Although it is not a physical observable, many physical quantities are related to it. By studying the momentum-dependent quark mass function in the infrared region we can gain valuable insights into the mechanisms of dynamical chiral symmetry breaking and the associated dynamical generation of mass. At high momenta, one can also use the quark propagator to extract the running quark mass \( \mu \).

Lattice QCD techniques provide an avenue for the non-perturbative study of the quark propagator. There have been several lattice studies of the momentum space quark propagator \([2,3,4,5,6,7,8,9,10,11]\) using different fermion actions. Finite volume effects and discretization errors have also been extensively explored in lattice Landau gauge \([11,11]\).

The overlap fermion formalism \([12,13]\) realizes an exact chiral symmetry on the lattice and is automatically \( O(a) \) improved. There are many salient features of overlap fermions, which include no additive renormalizations to the quark masses, an index theorem linking the number of zero-modes of the Dirac operator to the topological charge \( Q \), and evading the so called “no-go theorem” etc., however they are rather computationally demanding. There are many suggestions on how to reduce the computational cost. One such proposal is the use of a more elaborate kernel, together with a fattening of the gauge links \([14,15,16]\).

The idea of any UV-filtered fermion action \([13,20,21,34,35]\) is that one will carry out the calculation on a smoothed copy of the actual gauge field and evaluate the Dirac operator on that background. This yields a new fermion action which differs from the old one by terms which are both simultaneously ultralocal and irrelevant. The term “UV-filtered” indicates that such an action is less sensitive to the UV fluctuations of the gauge background. Sometimes, one also speaks of “fat-link” actions.

There is a great amount of freedom available when generating a smoothed copy of some gauge field. One needs to decide on the smoothing recipe (APE \([17,18]\), HYP \([19]\), stout-link \([22]\), etc.), on the parameter \((\alpha, n_{\text{iter}})\), and on the number of iterations, \(n_{\text{iter}}\). In any case, with fixed \((\alpha, n_{\text{iter}})\) the filtered “fat-link” action is in the same universality class as the usual “thin-link” version \([20]\). Unfortunately, if any smoothing process is over-applied, some important properties of the theory are lost. Therefore, one needs to find a balance between the smoothing procedure, which will accelerate convergence of the quark operator inversion and improve the localization properties, at the danger of losing important physics. Recently, Stephan Durr and collaborators \([10,21,21]\) applied 1-3 sweeps stout-link smearing \([22]\) to the lattice gauge configurations and analysed how this affected various physical quantities. They claim that it is safe to use 1-3 sweeps of standard stout-link smearing on the gauge configurations. More recently, 6 sweeps of stout-link smearing was used in the Science article exploring the hadron mass spectrum \([30]\).

In this paper, we investigate the momentum space quark propagator on quenched gauge configurations. We utilise both the original lattice configurations and also the configurations which are produced by one, three, and six sweeps of standard stout-link smearing respectively. We compare results across all four cases, in order to explore the effect of smearing on the quark propagator with different quark masses, different lattice momenta, etc.

The massive overlap operator can be written as \([23]\)

\[
D(\mu) = \frac{1}{2} \left[ 1 + \mu + (1 - \mu) \gamma_5 \epsilon(H_w) \right],
\]

where \(H_w(x,y) = \gamma_5 D_w(x,y)\) is the Hermitian Wilson-Dirac operator, \(\epsilon(H_w) = H_w / \sqrt{H_w^2}\) is the matrix sign function, and the dimensionless quark mass parameter \(\mu\).
where \( m^0 \) is the bare quark mass and \( m_w \) is the Wilson quark mass which, in the free case, must lie in the range \( 0 < m_w < 2 \).

The bare quark propagator in coordinate space is given by

\[
S^{\text{bare}}(m^0) = \tilde{D}^{-1}(\mu),
\]

where

\[
\tilde{D}^{-1}(\mu) = \frac{1}{2m_w} \tilde{D}^{-1}(\mu)
\]

and

\[
\tilde{D}^{-1}(\mu) = \frac{1}{1 - \mu} \left[ D^{-1}(\mu) - 1 \right].
\]

When all interactions are turned off, the inverse bare lattice quark propagator reduces to the tree-level version, and in momentum space is given by

\[
(S^{(0)})^{-1}(p) = i \left( \sum_{\mu} C^{(0)}_{\mu}(p) \gamma_\mu \right) + B^{(0)}(p),
\]

where \( p \) is lattice momentum. One can calculate \( S^{(0)}(p) \) directly by setting all links to unity in coordinate space, doing the matrix inversion, and then taking its Fourier transform. It is then possible to identify the appropriate kinematic lattice momentum \( q \) directly from the definition

\[
q_{\mu} \equiv C^{(0)}_{\mu}(p).
\]

The form of \( q_{\mu}(p_{\mu}) \) is shown and its analytic form given in Ref. 9. Having identified the appropriate kinematical lattice momentum \( q \), we can now define the bare lattice propagator as

\[
S^{\text{bare}}(p) = \frac{Z(p)}{i\Phi + M(p)}.
\]

This ensures that the free lattice propagator is identical to the free continuum propagator. Due to asymptotic freedom the lattice propagator will also take the continuum form at large momenta. In the gauge sector, this type of analysis dramatically improves the gluon propagator.

The two Lorentz invariants can then be obtained via

\[
Z^{-1}(p) = \frac{1}{12\kappa^2} \text{Tr}(\Phi S^{-1}(p)),
\]

\[
M(p) = \frac{Z(p)}{12} \text{Tr}(S^{-1}(p)).
\]

Here \( Z(p) \) is the wave-function renormalization function and \( M(p) \) is the mass function. The above equations imply that \( Z(p) \) is directly dependent on our choice of momentum \( q \), whilst \( M(p) \) is not.

Standard stout-link smearing, using an isotropic smearing parameter \( \rho_{\text{sm}} \), involves a simultaneous update of all links on the lattice. Each link is replaced by a smeared link \( \tilde{U}_\mu(x) \)

\[
\tilde{U}_\mu(x) = \exp(iQ_\mu(x)) U_\mu(x) ,
\]

where

\[
Q_\mu(x) = i \left( \Omega^1_\mu(x) - \Omega_\mu(x) \right) - \frac{i}{6} \text{Tr}(\Omega^1_\mu(x) - \Omega_\mu(x)),
\]

with

\[
\Omega_\mu(x) = \rho_{\text{sm}} \sum \{ 1 \times 1 \text{ loops involving } U_\mu(x) \}.
\]

We work on \( 16^3 \times 32 \) lattices, with gauge configurations created using a tadpole improved, plaquette plus rectangle (Lüscher-Weisz 27) gauge action through the pseudo-heat-bath algorithm. The lattice spacing, \( a = 0.093 \text{ fm} \), is determined from the static quark potential with a string tension of \( \sqrt{s} = 440 \text{ MeV} \) 28. The number of configurations to be used for each ensemble in this study is 50. The first smeared ensemble is created by applying one sweep of stout-link smearing to the original configurations with a smearing parameter of \( \rho = 0.10 \). The second smeared ensemble is created using three sweeps of stout-smearing with the same value of \( \rho \). We work in an \( O(a^2) \)-improved Landau gauge, and fix the gauge using a Conjugate Gradient Acceleration 29 algorithm with an accuracy of \( \theta \equiv \sum |\partial_a A^\mu(x)|^2 < 10^{-12} \). The improved gauge-fixing scheme was used to minimize gauge-fixing discretization errors 30.

Our numerical calculation begins with an evaluation of the inverse of \( D(\mu) \) on the unfixed gauge configurations, where \( D(\mu) \) is defined in Eq. 11. We then calculate the quark propagator of Eq. 9 for each configuration and rotate it to the Landau gauge by using the corresponding gauge transformation matrices \( \{ G_\mu(x) \} \). We then take the ensemble average to obtain \( S^{\text{bare}}(x, y) \). The discrete Fourier transformation is then applied to \( S^{\text{bare}}(x, y) \) and the momentum-space bare quark propagator, \( S^{\text{bare}}(p) \), is finally obtained.

We use the mean-field improved Wilson action in the overlap fermion kernel. The value \( \kappa = 0.19163 \) is used in the Wilson action, which provides \( m_w a = 1.391 \) for the Wilson regulator mass in the interacting case 9. We calculate the overlap quark propagator for 15 bare quark masses on each ensemble by using a shifted Conjugate Gradient solver. The bare quark mass \( m^0 \) is defined by Eq. 2. In the calculation, we choose the mass parameter \( \mu = 0.009, 0.010, 0.012, 0.014, 0.016, 0.018, 0.021, 0.024, 0.030, 0.036, 0.045, 0.060, 0.075, 0.090, \) and 0.105. This choice of \( \mu \) corresponds to bare quark masses, in physical
units, of $m^0 = 53, 59, 71, 82, 94, 106, 124, 142, 177, 212, 266, 354, 442, 531,$ and 620 MeV respectively.

The partial results for the mass function $M(p)$ and the wave-function renormalization function $Z^{(R)}(p) = Z(\zeta;p)$ on a $16^3 \times 32$ lattice without any smearing in Landau gauge were reported in Ref. [11]. Here we focus on a comparison of the behavior of the overlap fermion propagator when using different numbers of stout-link smearing sweeps. All data is cylinder cut [24]. Statistical uncertainties are estimated via a second-order, single-elimination jackknife.

In a standard lattice simulation, one begins by tuning the value of the input bare quark mass $m^0$ to give the desired renormalized quark mass, which is usually realized through the calculation of a physical observable. However, smearing a lattice configuration filters out the ultraviolet physics and the renormalization of the mass will be different. To some extent, the effect is similar to that of an increase in the lattice spacing $a$. After smearing, the same input $m^0$ will therefore give a different renormalized quark mass. The input bare quark mass must then be re-tuned in order to reproduce the same physical behavior as on the unsmeared configuration.

We wish to directly study how the quark propagator $S(p)$ is affected by smearing, through a calculation of the mass $M(p)$ and wave-renormalization $Z(p)$ functions. In order to replicate the re-tuning procedure described above, we begin by first calculating $M(p)$ and $Z(p)$ for all values of $m^0$ listed previously, over all four types of configurations. We then select a value of the bare quark mass $m^0$ to investigate, and force the mass functions $M(p)$ to agree at a given reference momentum, $\zeta$. This is achieved by interpolating $M(p)$, for the smeared configurations, between neighboring values of the bare quark masses, in order to determine the required effective bare quark mass. Any reasonable choice of $\zeta$ should suffice. By reasonable, we mean any point out of the far infrared (IR) or ultraviolet (UV) momentum regions, where lattice artifacts will spoil the results.

In comparing the renormalization function, we first interpolate $Z(p)$ to the effective bare quark mass, obtaining $Z^{(I)}(p)$. We then multiplicatively renormalize $Z^{(I)}(p)$ to $Z^{(R)}(p) \equiv Z(\zeta, p)$, subject to $Z(\zeta, \zeta) = 1$.

We begin with a comparison of the functions $M(p)$ and $Z^{(R)}(p)$ for a small bare quark mass, with three choices of the reference momentum $\zeta = 2.0, 3.9$ and 6.0 GeV. The interpolated mass functions for the smallest bare quark mass $m^0 = 53$ MeV are given in Fig. 1. We note the significant reduction in the statistical error, even after a single sweep of smearing. For all choices of $\zeta$, the mass functions display strong agreement over all four levels of smearing, with the only differences occurring in the most infrared points. For the function $Z^{(R)}(p)$ the effect of smearing is also subtle, however the link smearing does introduce a minor splitting in the UV region. This splitting leads to small differences in the lower momentum regions of $Z^{(R)}(p)$ when we select $\zeta = 6.0$ GeV.

Next we consider a moderate bare quark mass of 177 MeV, for which the functions $M(p)$ and $Z^{(R)}(p)$ are shown in Fig. 2. As in the case of a small bare quark mass, we find that the mass function appears independent of the choice of reference momentum, however the discrepancy at the most infrared point is no longer apparent. The renormalization function displays the same splitting in the UV region. The effect of smearing on the quark propagator still appears to be relatively minor at this value of $m^0$.

Finally we consider a larger choice of the bare quark mass, $m^0 = 531$ MeV. A consideration of the mass functions $M(p)$ given in Fig. 3 reveals a strong dependence on the choice of reference momentum $\zeta$. We see that a choice of either $\zeta = 3.9$, or 6.0 GeV leads to large discrepancies in both the low and moderate momentum regions. With a choice of $\zeta = 2.0$ GeV we are able to obtain agreement in the low momentum region.

The dependence of $M(p)$ on $\zeta$ indicates that the suppression of ultraviolet fluctuations by the smearing algorithm has spoiled the physics of the theory above $\sim 2 – 3$ GeV, for this value of $m^0$. These effects are clearly visible after just a single sweep of smearing at this heavy bare quark mass. We further note that in the case of 6 sweeps and $\zeta = 6.0$ GeV, the mass function drops to the bare quark mass. This is a clear indication that the Compton wavelength of the quark is small enough to reveal the void of short-distance interactions following 6 stout-link smearing sweeps.

The renormalization functions $Z^{(R)}(p)$ for a heavy bare quark mass of $m^0 = 531$ MeV are also provided in Fig. 3. Apart from the small splitting in the UV region, $Z^{(R)}(p)$ still appears to be mostly unaffected by the smearing algorithm. In Fig. 4 we show the differences in $Z^{(R)}(p)$ between the smallest and largest bare quark masses, where in order to examine the UV splitting we choose $\zeta = 2.0$ GeV. Figure 4 shows that the magnitude of the splitting in $Z^{(R)}(p)$ introduced by the smearing algorithm is unaffected of the input bare quark mass.

The stout-link smearing procedure can save a large amount of compute time in the calculation of hadronic physics. Not only is the Dirac operator easier to invert but statistical errors are reduced significantly. The conclusion drawn from this study is that up to six sweeps of stout-link smearing sweeps induces rather small effects on the quark propagator for small and moderate bare quark masses, as claimed by Durr, et al. [19, 20, 21]. After an appropriate rescaling of the bare quark mass, the renormalized quark propagator displays the same physics as the untouched configuration. The only notable exceptions are order 2% discrepancies in the renormalization function for all quark masses and the most infrared point of the lightest quark mass function. There an effect approaching $2\sigma$ is revealed.

These subtle effects provide some evidence of a link between small topologically nontrivial gauge field configurations linked to dynamical chiral symmetry breaking through their production of approximate zero-modes in
FIG. 1: The interpolated mass $M(p)$ and renormalization $Z^{(R)}(p)$ functions for the small bare quark mass, $m^0 = 53$ MeV, with three choices of $\zeta$. The effective bare quark masses are given in square brackets. There is good agreement in $M(p)$ for all choices of $\zeta$ with up to six sweeps of stout-link smearing. A small splitting in the UV region of $Z^{(R)}(p)$ is apparent after three sweeps of smearing. This leads to a disagreement in $Z^{(R)}(p)$ for a large choice of $\zeta = 6.0$ GeV.

the Dirac operator. Upon smearing this short distance physics is modified.

Certainly the effects are subtle. However, they may require further investigation in the event that fermion actions, in which all links of the action are smeared, become the action of choice for calculating the physics beyond the standard model.

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FIG. 2: The interpolated mass $M(p)$ and renormalization $Z^{(R)}(p)$ functions for the moderate bare quark mass, $m^0 = 177$ MeV, with the three choices of $\zeta$. The effective bare quark masses are given in square brackets. As with the small bare quark mass, the mass function displays good agreement for all choices of $\zeta$, and there is also a small splitting apparent in the UV region of $Z^{(R)}(p)$. We note that the differences in $Z^{(R)}(p)$ appear to be independent of the bare quark mass.

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FIG. 3: The interpolated mass $M(p)$ and renormalization $Z^{(R)}(p)$ functions for the heavy bare quark mass, $m^0 = 531$ MeV, for the three choices of $\zeta$. The effective bare quark masses are given in square brackets. We see that for this value of $m^0$, the choices $\zeta = 3.9$, and 6.0 GeV lead to large differences in the moderate and infrared momentum regions of $M(p)$. This indicates that the physics above approximately 3 GeV has been spoiled by the smearing algorithm. In $Z^{(R)}(p)$ we again find that the stout-link smearing algorithm introduces a small splitting in the infrared region.
FIG. 4: The difference $\chi(p) \equiv |Z^{(R)}_{\text{light}}(p) - Z^{(R)}_{\text{heavy}}(p)|$ between the renormalization functions $Z^{(R)}(p)$ for the heavy and small bare quark masses considered previously, with $\zeta = 2.0$ GeV. We see that the difference rapidly approaches zero, indicating that the magnitude of the splitting introduced by the smearing algorithm is independent of the input bare quark mass. The differences at lower momenta are due to a flattening of $Z(p)$ as $m^0$ is increased.
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