Finite volume renormalization scheme for fermionic operators

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We propose a new finite volume renormalization scheme. Our scheme is based on the Gradient Flow applied to both fermion and gauge fields and, much like the Schrödinger functional method, allows for a nonperturbative determination of the scale dependence of operators using a step-scaling approach. We give some preliminary results for the pseudo-scalar density in the quenched approximation.

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1. Introduction

Renormalization is a major problem for calculations of moments of generalized parton distribution functions (GPDs) in lattice QCD. The lattice breaks rotational symmetry, causing operators of different mass dimension to mix. This mixing complicates the renormalization of high moments of GPDs and therefore only calculations of a few low moments exist in the literature.

Smearing has long been used as a tool to aid renormalization on the lattice [1, 2]. Recent developments of Gradient Flow (GF) methods [3, 4, 5] in both the gauge and fermion sectors offer an opportunity to improve current renormalization methods for the twist-2 operators relevant to moments of GPDs. Using smearing to alleviate the mixing of lattice twist-2 operators with lower dimensional operators was recently discussed in [6].

In this work we explore the possibility of using the Gradient Flow to define a new renormalization scheme. This nonperturbative scheme potentially provides a simple way to calculate the mixing coefficients required to subtract power divergent lower dimensional operators from lattice twist-2 matrix elements. We propose a method that extends the approach taken in [7], which uses the Gradient Flow to define a renormalized QCD coupling constant in finite volume, to compute the scale dependence of twist-2 operators as well as the mixing coefficients. Here we outline our proposal and, as a first step towards understanding the effectiveness of our approach, we compute the step-scaling function for the pseudo-scalar density.

2. The Gradient Flow

Lüscher introduced the Gradient Flow method for both fermions and gauge fields, which corresponds to smearing all degrees of freedom in a new, continuous flow time direction s [5]. The flow equations can be written as

$$\partial_s V_\mu(x,s) = -g_0^2 \partial_{V_\mu(x,s)} S_w V_\mu(x,s), \quad \partial_s \psi(x,s) = \vec{\Delta}\psi(x,s), \quad \text{and} \quad \partial_s \overline{\psi}(x,s) = \overline{\psi}(x,s)\overleftarrow{\Delta}, \quad (2.1)$$

where S_w is the Wilson gauge action and the derivative $\partial_{V_\mu(x,s)}$, taken with respect to the smeared gauge links $V_\mu(x,s)$, is defined as in [3]. We denote the smeared fermion fields $\psi(x,s)$ and $\overline{\psi}(x,s)$, and define the lattice Laplacian as $\Delta = \nabla_\mu^\dagger \nabla_\mu$, where ∇_μ is the covariant backward lattice derivative.

The smeared fields satisfy the boundary conditions

$$V_\mu(x,0) = U_\mu(x), \qquad \psi(x,0) = q(x), \quad \text{and} \quad \overline{\psi}(x,0) = \overline{q}(x). \quad (2.2)$$

Here the $U_\mu(x)$ are the unsmeared gauge fields and $\overline{q}(x)$ and $q(x)$ the unsmeared quark fields.

If the underlying theory, defined as a path integral over the unsmeared fields, is renormalized, then correlation functions of the gauge fields require no additional renormalization, as shown in [4]. At finite flow time the smeared fermion fields require one additional wave function renormalization [5]. One way to easily understand this is to notice that the effective smearing range, which is proportional to $\sqrt{s}$, acts as a regulator that eliminates additional divergences at non-zero flow time.

3. Finite Volume Renormalization Scheme

We define the renormalization constant $Z_{\mathscr{O}_\Gamma}(\mu)$ of an operator $\mathscr{O}_\Gamma$ at a scale μ as

$$Z_{\mathscr{O}_\Gamma}(g_0,\mu) = \mathscr{N}\frac{\sum_x \langle V_\nu(x,s)V_\nu(0,0)\rangle}{\sum_x \langle \mathscr{O}_\Gamma(x,s)\mathscr{O}_\Gamma(0,0)\rangle}, \quad (3.1)$$

where g_0 is the bare gauge coupling constant and

$$V_\nu(x,s) = \bar{\psi}(x,s)\gamma_\nu\psi(x,s), \qquad \text{and} \qquad \mathscr{O}_\Gamma(x,s) = \bar{\psi}(x,s)\Gamma\psi(x,s). \qquad (3.2)$$

Here Γ is some gamma matrix.

We choose a novel normalization factor, $\mathscr{N}$, that is given by

$$\mathscr{N} = \frac{\sum_x \langle \mathscr{O}_\Gamma(x,s)\mathscr{O}_\Gamma(0,0)\rangle_{\text{cg}}}{\sum_x \langle V_\nu(x,s)V_\nu(0,0)\rangle_{\text{cg}}}, \qquad (3.3)$$

where the subscript cg signifies that we evaluate the expectation value of the matrix element over an ensemble of constant gauge fields. Our choice of normalization removes the need to account for gauge zero modes, which would otherwise require a nonperturbative treatment when matching perturbatively to the $\overline{MS}$ scheme.

We calculate the correlation functions in finite volume of size L^4 and set $\mu = 1/L$. Following [7] we set the flow time to

$$s = c^2 \frac{L^2}{8}, \qquad (3.4)$$

where c is a constant that defines the renormalization scheme. In this work we investigate a range of values for the constant c. The optimum value is $c \simeq 0.3$, as discussed in [7], and is determined by the interplay of statistical errors and systematic uncertainties from cut-off effects. On the one hand, large values of c increase statistical errors in the determination of the renormalization factor. On the other hand, small values of c lead to renormalized couplings that have large discretization errors and are only weakly dependent on the bare coupling (see Figure 1), which entails a prohibitively large spread of bare coupling values for the step-scaling procedure.

We would like to highlight the four following features of our definition of the renormalization factor, $Z_{\mathscr{O}_\Gamma}(g_0,\mu)$, in Equation (3.1).

Mixed smeared and unsmeared fields   The denominator in Equation (3.1) is a correlation function between the local (un-smeared) quark bilinear operator, $\mathscr{O}_\Gamma(0,0)$, and the smeared operator at some non-zero flow time, $\mathscr{O}_\Gamma(x,s)$.

Wave function renormalization cancellation   This correlation function only requires a renormalization factor for the local quark bilinear. In principle the smeared quark bilinear requires an additional wave function renormalization, as discussed in [5]. We have, however, chosen the numerator of Equation (3.1) so that the wave function renormalization parameters at both zero and non-zero flow time cancel.

Constant field normalization   We adopt the renormalization condition of Equation (3.3) so that the perturbative expansion of the renormalization constant receives no contributions at tree level from insertions of the gauge zero modes. This simplifies the perturbative expansion in finite volume at one loop level, at the cost of having to evaluate the contributions from zero modes nonperturbatively. The authors of [7] treat these zero mode contributions analytically. We evaluate Equation (3.3) numerically. We work in a finite volume with anti-periodic boundary conditions for fermions, so there are no fermionic zero modes and correlation functions can be evaluated with massless fermions. For this exploratory work we use Wilson fermions and fix the bare quark mass to the critical mass.

Local vector current We use the local vector current in Equations (3.1) and (3.3). We intend to use the conserved vector current in the future, because this simplifies the renormalization condition. This work is a proof of principle calculation, so it is sufficient to study our renormalization scheme using the simpler local vector current.

4. Coupling constant and operator scale dependence

Following the approach taken in [7], we examine the discrete β-function, defined as

$$\mathscr{B}(\mu) = \frac{\overline{g}^2(\mu/2) - \overline{g}^2(\mu)}{2\log 2}$$

for a step size of two. Here $\overline{g}^2(\mu)$ is the renormalized coupling defined in [7]. Our numerical results can be compared to the universal β-function at one loop in perturbation theory: $\mathscr{B}(\mu) = 11\overline{g}^4(\mu)/(16\pi^2)$. The relation between $\overline{g}^2(\mu)$ and, for example, the $\overline{MS}$ coupling, contains odd powers of $\overline{g}(\mu)$. Therefore, as noted in [7], only the one loop coefficient is scheme independent. Higher order corrections to the perturbative β-function have not been calculated yet, so direct comparison with analytic results is not possible.

In common with other finite volume renormalization schemes, such as the Schrödinger functional method, we study the scale dependence of the renormalization parameter $Z_{\mathscr{O}_\Gamma}(\mu)$ via the continuum step-scaling function σ. We use a step factor of two for an operator $\mathscr{O}$ and first define the discrete step-scaling function, Σ, as:

$$\Sigma(\overline{g}^2(\mu), a/L) = \frac{Z_{\mathscr{O}}(g_0, \mu/2, a/L)}{Z_{\mathscr{O}}(g_0, \mu, a/L)}. \tag{4.1}$$

Then the continuum step-scaling function σ is

$$\sigma(\overline{g}^2(\mu)) = \lim_{a/L \to 0} \Sigma(\overline{g}^2(\mu), a/L). \tag{4.2}$$

5. Numerical tests

We calculated the discrete β-function and the step-scaling function for the pseudoscalar density using the Wilson gauge and fermion actions in the quenched approximation. We generated ensembles for eight lattice sizes, from $L/a = 6$ to $L/a = 24$, with a range of bare couplings, from $\beta = 6/g_0^2 = 6.6$ to $\beta = 12$. Our analysis uses ensembles with 100 configurations for each lattice volume, generated with 500 updates of one heat bath step followed by three steps of over-relaxation.

We determined the renormalized coupling in the gradient flow finite volume scheme of [7]. We present our results as a function of the bare coupling, β, in Figure 1 for different choices of the constant c (left-hand plot). In the right-hand plot of Figure 1 we plot the discrete β-function for this coupling constant, with the one loop prediction shown for comparison. Deviations from this prediction at small coupling represent discretization effects.

We determine the continuum step-scaling function of Equation (4.2) as follows:

1. Calculate $\overline{g}^2(\mu)$ and the pseudoscalar renormalization parameter, $Z_p(g_0, \mu, a/L)$, at a fixed choice of bare coupling, say $\beta = 6.6$, for a specific lattice, say, $L/a = 6$. This sets the physical scale, $\mu = 1/L$.
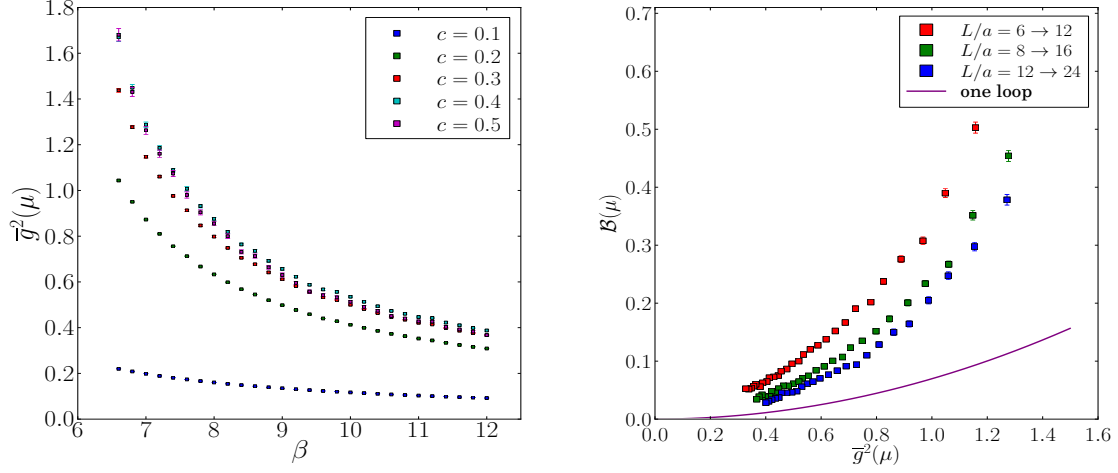
Figure 1: (Left) Dependence of the renormalized gauge coupling on the choice of the c parameter at fixed lattice extent $L/a = 8$. (Right) The discrete β-function, $\mathscr{B}(\mu)$, as a function of the renormalized coupling. Here the step size is two and we plot three different pairs of lattice extents with constant $c = 0.3$. We include the one loop prediction for comparison (solid purple line).

2. Keep the bare coupling (and therefore the lattice spacing) fixed, double the number of lattice points, *e.g.* set $L'/a = 2L/a = 12$, and calculate $Z_p(g_0, \mu/2, a/L)$.

3. Determine the discrete step-scaling function using Equation (4.1), *i.e.* calculate the ratio $Z_p(g_0, \mu/2, a/L)/Z_p(g_0, \mu, a/L)$.

4. Now fix the renormalized coupling. For the example of $L/a = 6$ with $\beta = 6.6$, this is $\overline{g}^2(\mu) = 1.158(7)$. Choose a new lattice extent, say $L/a' = 8$ and tune the bare coupling such that the renormalized coupling is constant, $\overline{g}^2(\mu) = 1.158(7)$. This adjusts the lattice spacing on the new lattice so that the physical extent remains constant.

5. Repeat steps one to four.

6. Extract the continuum step-scaling function, Equation (4.2), from a linear fit to a/L using the results of steps one to give.

7. Repeat steps one to six with a different initial choice of bare coupling, say $\beta = 7.0$, which sets another initial physical scale μ'. Repeated application of this algorithm gives the continuum step-scaling function at a range of physical scales.

We plot the discrete step-scaling function, with the continuum limit at $a/L = 0$, in the left-hand plot of Figure 2. We include only systematic uncertainties in the plotted errorbars and in the fit. The red data points correspond to the lowest physical scale, the green to an intermediate scale and the blue to the highest physical scale. On the right-hand side of Figure 2 we illustrate our estimate for the systematic uncertainty from the continuum extrapolation and the critical mass mis-tuning.

The spread of data points at each scale demonstrates that at higher scales the continuum extrapolation is better controlled. This is largely caused by the improved tuning of the critical mass at higher values of the bare coupling. The red data points correspond to bare coupling values between $\beta = 6.6$ and $\beta = 7.4$. As we discuss in the next section, these data suffer from systematic
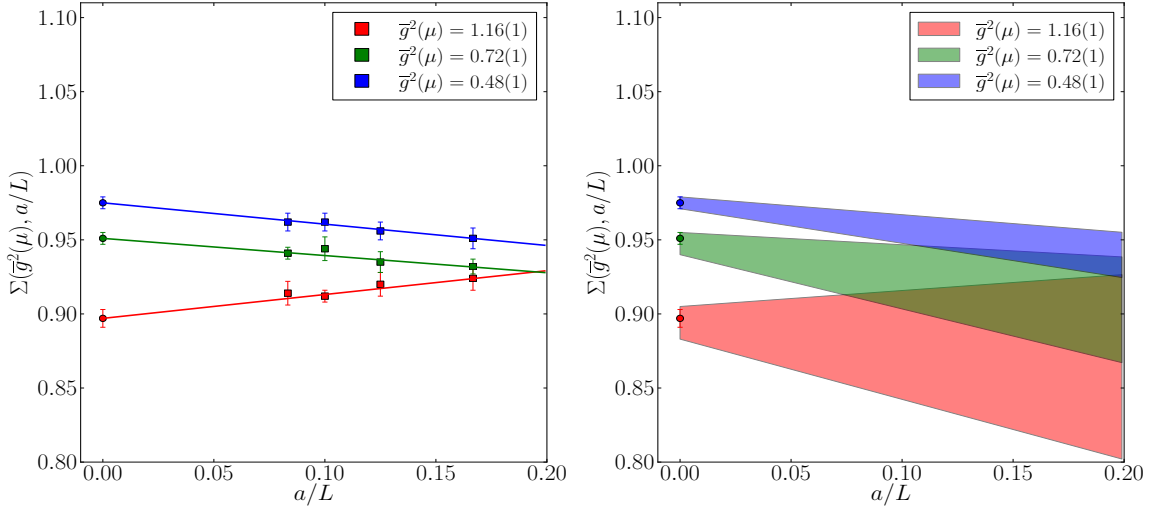
Figure 2: Continuum extrapolation of the step-scaling function of the pseudo scalar density at several values of the renormalized gauge coupling with $c = 0.3$. (Left) We plot the numerical data, with statistical uncertainties only, and include the continuum values as circular points. The lines are fits linear in a/L. (Right) Estimated systematic uncertainties. Estimates include both uncertainties from the continuum extrapolation and the critical mass mis-tuning, which are approximately 5-10% for the lowest scale (in red), decreasing to less than 1% for the highest scale (in blue).

uncertainties due to mis-tuning of the critical mass that are approximately $5 - 10\%$. In contrast, the blue data have bare couplings in the range $\beta = 9.6$ to $\beta = 10.8$, with corresponding critical mass tuning uncertainties of less than 1%.

5.1 Tuning the critical mass

We determined the critical mass for each value of the bare coupling constant using the two-loop cactus improved critical mass of [8]. We estimate that the resulting value of the critical mass is mis-tuned by approximately 18% at $\beta = 6.0$, 15% at $\beta = 6.1$ and 12% at $\beta = 6.3$, by comparing the perturbative predictions to the nonperturbative results quoted in [9]. The smallest β value we use is 6.6, for which we estimate a critical mass mis-tuning of approximately 10%. Ref. [8] suggests that this mis-tuning is reduced to $\ll 1\%$ for the highest values of β in this work, $11 < \beta < 12$.

To estimate the resulting error in the renormalization parameter we determined Z_p at $\beta = 6.1$ and 6.3, using both the perturbative and nonperturbative values of the critical mass. We find that the resulting uncertainty is approximately 18% and 13% for $\beta = 6.1$ and 6.3 respectively, Uncertainties for the $\beta = 6.0$ ensemble were too large to use for this analysis.

Nonperturbatively tuned values of the critical mass are not available at larger values of the bare coupling. We therefore estimated the uncertainties in the renormalization factor by varying the critical mass by around 10% at higher beta values (8.0 to 12.0). This resulted in variations of Z_p of around 1%. Since the mis-tuning of the critical mass is likely to be significantly less than 10% at these values of the bare coupling, we conclude that the systematic effects of the critical mass tuning are much less than 1% for the high β range. At $\beta = 6.6$, we estimate the systematic uncertainty to be around 10%.

5.2 Other sources of uncertainty

The systematic uncertainties due to the critical mass tuning dominate the uncertainties in Z_p and consequently in $\sigma(\overline{g}^2(\mu))$, particularly at low scales. The continuum extrapolation, which is linear in the lattice spacing, because we use unimproved Wilson fermions, is the next most significant source of systematic error and the corresponding uncertainties are approximately 1-2%. Statistical errors in $Z_p(g_0, \mu, a/L)$ were calculated from jackknife estimates to include correlations between the correlation functions of the pseudoscalar and vector currents and were $\sim 0.5\%$. We determined that the bias in these uncertainties from the jackknife procedure was negligible. We estimated that uncertainties due to mis-tuning of the renormalized coupling were $\sim 0.5\%$.

6. Conclusions

We have introduced a new finite volume renormalization scheme. We define this scheme through two point correlation functions of smeared and local operators, using the Gradient Flow to smear both fermion and gauge fields. We remove any dependence on the wave function renormalization for smeared fermions by considering an appropriate ratio of correlation functions. Thus the renormalization parameter of this ratio includes only the renormalization factor of the local operator. Our scheme therefore provides a simple way to compute the renormalization parameters of lattice operators.

We adopt a normalization condition that restricts the path integral to constant gauge fields. We compute these constant gauge field correlation functions numerically. This condition simplifies the matching to the $\overline{MS}$ scheme. Furthermore, with our scheme one can nonperturbatively determine the scale dependence of the local operator using a step-scaling procedure.

Here we have demonstrated the basic features of our scheme using Wilson fermions in the quenched approximation and concentrating on the pseudo-scalar quark bilinear operator. In the future we will pursue unquenched, $O(a)$ improved calculations.

The ultimate goal of this work is to calculate nonperturbatively the renormalization constants, mixing coefficients and scale dependence of twist-2 matrix elements relevant to hadron structure calculations. Extracting phenomenologically relevant results requires matching to the $\overline{MS}$ scheme and work to carry out these matching calculations is underway.

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