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Finite volume renormalization schemes and the fermionic gradient flow

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We consider finite volume renormalization schemes for fermion bilinear operators in lattice QCD, with fermionic source fields defined at finite gradient flow time. In order to assess the options for boundary conditions and kinematical parameters we evaluate the relevant correlation functions at leading order in perturbation theory.

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Introduction

Non-perturbative renormalization of composite operators and their matrix elements is best performed by applying the step-scaling method to an intermediate finite volume renormalization scheme [1]. Matching to low energy physics requires that the finite volume scheme can be accurately evaluated at the bare couplings used in simulations of hadronic physics. In this regime, the gradient flow for the gauge field [2] has been essential for recent progress with the strong coupling [3], and one may hope for similar benefits when extending the flow to fermion fields [4]. A natural first application would be the renormalization of quark masses, which, due to the PCAC relation, is tantamount to the renormalization of the pseudoscalar density, $\overline{\psi}_u \gamma_5 \psi_d$. One thus requires correlation functions of the pseudoscalar density and some source field with known behaviour under renormalization. A known solution are SF boundary source fields [5] and these have been used extensively, cf. [6] for a recent reference. However, one may hope that the fermion flow provides alternative source fields which allow for better precision in the matching to hadronic physics. For a first attempt in this direction, using a finite volume scheme on a hyper-torus, cf. [7]. Here we use Schrödinger Functional (SF) and chirally rotated SF boundary conditions (χSF) [8] for the fundamental fields and consider different definitions of the fermionic flow. We present some results at leading order of perturbation theory, in particular we identify a set-up and parameter choices with reasonably small cutoff effects.

This report is organized as follows. In Sect. 1 we first recall some general properties of the gradient flow and its renormalization properties, for both gauge and quark fields. We then discuss possible set-ups for the fermion flow. In Sect. 2 we give some preliminary results at leading perturbative order, and we present tentative conclusions in Sect. 3.

1. Renormalization conditions for composite operators

1.1 Gradient flow for gauge and fermion fields

The gradient flow defines gauge and fermion fields, $B_\mu(t,x)$, $\chi(t,x)$ and $\overline{\chi}(t,x)$ as functions of the flow time $t \geq 0$, with the fundamental fields of QCD serving as initial values,

$$B_\mu(t,x)|_{t=0} = A_\mu(x)\,, \qquad \chi(t,x)|_{t=0} = \psi(x)\,, \qquad \overline{\chi}(t,x)|_{t=0} = \overline{\psi}(x)\,, \tag{1}$$

As for the gauge fields, the gradient flow differential equations take the form (in the continuum notation)[2]

$$\begin{aligned} &\partial_t B_\mu = D_\nu G_{\nu\mu}\,, \\ &G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + \left[B_\mu, B_\nu\right]\,, \qquad D_\mu = \partial_\mu + \left[B_\mu, \cdot\right]\,, \end{aligned} \tag{2}$$

while for quark fields the simplest choice is [4]

$$\partial_t \chi = \Delta\chi\,, \qquad \partial_t \overline{\chi}^\dagger = \Delta\overline{\chi}^\dagger, \qquad \Delta = D_\mu D_\mu\,, \quad D_\mu = \partial_\mu + B_\mu\,. \tag{3}$$

Here the notation $\overline{\chi}^\dagger$ indicates hermitian conjugation of the row-vector $\overline{\chi}$ in colour and spinor space. All flow equations being first order in the flow time derivative, the flowed fields are uniquely determined by their initial value at $t = 0$.

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The main interest in finite flow time observable derives from their simple renormalization properties. In particular, composite gauge invariant fields, polynomial in $B_\mu(t,x)$ and its derivatives, are renormalized once the underlying theory, defined as a path integral over the fundamental fields, is renormalized as usual [9]. If the fermion fields χ and $\overline{\chi}$ are included, the composite field receives the same (t-independent) multiplicative renormalization factor,

$$\chi = Z_\chi^{-1/2}\chi_{\rm R}\,, \qquad \overline{\chi} = Z_\chi^{-1/2}\overline{\chi}_{\rm R}\,, \tag{4}$$

for each of the fermion fields it contains [4]. Note that this renormalization factor is gauge invariant and completely unrelated to the (gauge dependent) wave function renormalization of fundamental quark fields.

The conventional fermion flow equations are based on the covariant Laplacian operator and thus are the same for all spin components of the fermion fields. Replacing the Laplacian by the square of the Dirac operator,

$$\Delta = D_\mu D_\mu \longrightarrow \gamma_\mu D_\mu \gamma_\nu D_\nu = D_\mu D_\mu + \frac{1}{4}[\gamma_\mu, \gamma_\nu] G_{\mu\nu}\,, \tag{5}$$

introduces an additional, spin-dependent Pauli term. This option was mentioned by Lüscher as a possible choice [4] but not further explored. More recently, Boers [10] extended the perturbative analysis to include this case and confirmed that the renormalization properties of flow observables remain qualitatively unchanged.

On the lattice with Wilson fermions, the (unimproved) Wilson-Dirac operator takes the form

$$D_W = \sum_{\mu=0}^{3} \left\{ \gamma_\mu \left(\frac{\nabla_\mu + \nabla^*_\mu}{2} \right) - \frac{a}{2} \nabla^*_\mu \nabla_\mu \right\}\,, \tag{6}$$

with γ_μ the gamma matrices, and ∇_μ and ∇^*_μ the forward and backward lattice derivatives, respectively. On the lattice, the modified fermionic flow equations then take the form

$$\partial_t \chi = D_W^\dagger D_W \chi\,, \qquad \partial_t \overline{\chi}^\dagger = D_W D_W^\dagger \overline{\chi}^\dagger\,, \tag{7}$$

In infinitely extended, continuous space-time and to lowest perturbative order (without background gauge field), Eqs. (7) and (3) become the same. This may change in a finite volume set-up where it depends on the choice of boundary conditions.

1.2 Boundary conditions for the fields

We now consider a finite space-time volume $L^3 \times T$, with extent L in all spatial directions and Euclidean time extent T. Boundary conditions for all fields need to be specified. For the gauge fields (both fundamental and at finite flow time), we impose Schrödinger Functional (SF) boundary conditions for definiteness [5], but open or mixed SF and open boundary conditions would be options, too. Note that these differences would not affect our leading order results for the fermionic correlation functions.

For the fundamental fermion fields we use SF boundary conditions, i.e. Dirichlet boundary conditions are imposed on half of the spinor components at $x_0 = 0$ and the other half at $x_0 = T$

$$\begin{aligned} &P_+\psi(x)|_{x_0=0} = 0\,, \quad P_-\psi(x)|_{x_0=T} = 0\,, \qquad P_\pm = \frac{1}{2}(\mathbb{1} \pm \gamma_0)\,, \\ &\overline{\psi}(x)P_-|_{x_0=0} = 0\,, \quad \overline{\psi}(x)P_+|_{x_0=T} = 0\,. \end{aligned} \tag{8}$$

This is consistent with the fact that, at the classical level, the fermion fields satisfy the Dirac equation, which is first order in Euclidean time. However, the flowed fermion fields, χ and $\overline{\chi}$, satisfy equations (3) and (7) which are second order in Euclidean time. Hence Dirichlet boundary conditions for all components at the Euclidean time boundaries would then seem a natural choice,

$$\chi(t,x)|_{x_0=0} = 0 = \chi(t,x)|_{x_0=T}\,, \qquad \overline{\chi}(t,x)|_{x_0=0} = 0 = \overline{\chi}(t,x)|_{x_0=T}\,. \tag{9}$$

However, there are many other options. In particular, when defining the flow equation with the same finite volume Wilson-Dirac operator as the one for the fundamental fermions, the boundary conditions for χ and $\overline{\chi}$ become a mixture of Dirichlet and Neumann conditions, i.e. one obtains Dirichlet conditions for the same spinor components as for ψ and $\overline{\psi}$, whereas the complementary components satisfy Neumann conditions [5].

Furthermore, on the lattice with an even number N_f of Wilson fermions, there exists an alternative formulation of the Schrödinger functional, the chirally rotated SF (χSF). While its continuum limit is equivalent to the standard SF, the χSF has the technical advantage of being compatible with automatic O(a) improvement. In the following we will use the χSF, as it also simplifies the lowest order calculation of the basic 2-point function for the flowed fermion fields. Hence we consider isospin doublets ψ, $\overline{\psi}$ for up and down quark. The χSF b.c.'s read [8]

$$\begin{aligned} &\tilde{Q}_+\psi(x)|_{x_0=0} = 0\,, \quad \tilde{Q}_-\psi(x)|_{x_0=T} = 0\,, \quad \tilde{Q}_\pm = \frac{1}{2}\left(\mathbb{1} \pm i\gamma_0\gamma_5\tau^3\right)\,, \\ &\overline{\psi}(x)\tilde{Q}_-|_{x_0=0} = 0\,, \quad \overline{\psi}(x)\tilde{Q}_+|_{x_0=T} = 0\,. \end{aligned} \tag{10}$$

and the Pauli matrix τ^3 acts on the flavour indices of the doublets. Using the flow equations with the χSF Wilson-Dirac operator automatically implements the χSF boundary conditions for both ψ and χ fields, with additional Neumann conditions for the complementary components of χ and $\overline{\chi}$.

1.3 Definition of renormalization factors

We now define correlation functions of quark bilinear fields

$$O^{ij}_\Gamma(x) = \overline{\psi}_i(x)\Gamma\psi_j(x)\,, \tag{11}$$

where Γ is a product of γ-matrices, with $\Gamma = \gamma_5$ corresponding to the pseudoscalar density. The flavour assignments $i \neq j$ correspond to flavour non-singlet operators. In order to define a non-trivial correlation function the source field needs to match the flavour structure. We define

$$Q^{ij}_\Gamma(t,x) = \overline{\chi}_i(t,x)\Gamma\chi_j(t,x)\,, \tag{12}$$

which allows us to define the (unrenormalized) correlation functions

$$C[\Gamma](x,t;y) = \langle Q^{ij}_\Gamma(t,x)O^{ji}_\Gamma(y)\rangle\,, \tag{13}$$

and similar ones with both fields at finite flow time

$$D[\Gamma](x,s;y,t) = \langle Q^{ij}_\Gamma(s,x)Q^{ji}_\Gamma(t,y)\rangle\,, \tag{14}$$

In order to obtain renormalized correlation functions we introduce the renormalized composite fields

$$\left(O_{\Gamma}^{ij}(x)\right)_{\mathrm{R}} = Z_{O_\Gamma} O_{\Gamma}^{ij}(x)\,, \tag{15}$$

The source fields at non zero flow time renormalize with the square of $Z_\chi^{1/2}$ as they contain two fermion fields ($\chi_{\mathrm{R}} = Z_\chi^{1/2}\chi$ and analogously for $\overline{\chi}$) [4]. Hence, renormalized correlation functions take the form,

$$C_{\mathrm{R}}[\Gamma](x,t;y) = Z_{O_\Gamma} Z_\chi C[\Gamma](x,t;y)\,, \qquad D_{\mathrm{R}}[\Gamma](x,s;y,t) = Z_\chi^2 D[\Gamma](x,s;y,t)\,, \tag{16}$$

and renormalization conditions are typically obtained by equating such renormalized correlation functions with their tree-level expression. Obviously, there are now various options to obtain Z_{O_Γ} by taking appropriate ratios of correlation functions.

Before doing this, we make some further choices. First, we use translation invariance in the spatial directions and sum over $\mathbf{x}$. Second we set $s = t$ and render the correlation function dimensionless by multiplying with the appropriate power of the flow time t, viz.

$$g_\Gamma(x_0,y_0;t) = t^{3/2}a^3 \sum_{\mathbf{x}} C[\Gamma](x,t;y)\,, \qquad d_\Gamma(x_0,y_0;t) = t^{3/2}a^3 \sum_{\mathbf{x}} D[\Gamma](x,t;y,t)\,, \tag{17}$$

Now ratios of the type $g/\sqrt{d}$ renormalize with just the single renormalization factor, Z_{O_Γ}. Similarly, ratios like $g_{\Gamma_1}/g_{\Gamma_2}$ renormalize with the corresponding ratio of Z-factors. This also determines the desired Z-factor provided the other is either trivial or known. This is the case for those quark bilinears which are Noether currents of chiral and flavour symmetry. With Wilson fermions, the point-split vector current is exactly conserved and has $Z_{\tilde{\mathrm{V}}} = 1$, and both, the axial and the vector current renormalization constants for local currents can be very accurately measured e.g. within the χSF framework [11].

In order to define a renormalization scheme it remains to fix any remaining parameters. In particular, all dimensionful parameters must be taken in a fixed proportion to a single scale, taken to be L, the extent of the space-time volume. The dimensionful parameters to be fixed are then T, x_0, y_0 and the flow time t. We thus consider two types of renormalization conditions for a quark bilinear O_Γ,

$$\begin{aligned}
&i) \qquad Z_{O_\Gamma} \times \left[\frac{g_\Gamma}{\sqrt{d_{\Gamma'}}}\right]_{T=L,x_0=y_0=T/2,\sqrt{8t}=cL} = \left[\frac{g_\Gamma}{\sqrt{d_{\Gamma'}}}\right]^{\text{tree level}}_{T/L=1,x_0=y_0=T/2,\sqrt{8t}=cL}\,,\\
&ii) \qquad \frac{Z_{O_\Gamma}}{Z_{O_{\Gamma'}}} \times \left[\frac{g_\Gamma}{g_{\Gamma'}}\right]_{T=L,x_0=y_0=T/2,\sqrt{8t}=cL} = \left[\frac{g_\Gamma}{g_{\Gamma'}}\right]^{\text{tree level}}_{T/L=1,x_0=y_0=T/2,\sqrt{8t}=cL}\,.
\end{aligned} \tag{18}$$

Note that the right hand sides are the corresponding tree-level expression, obtained at $g_0^2 = 0$. In the second type of conditions it is understood that one of the operators at $t = 0$ is either the isovector current ($\Gamma' = \gamma_k$) or the axial vector current ($\Gamma' = \gamma_k\gamma_5$), such that their Z-factor is known. The Z-factors determined from these renormalization conditions still depend on the parameter $c = \sqrt{8t}/L$, and thus define a 1-parameter family of renormalziation schemes for the quark bilinear O_Γ.

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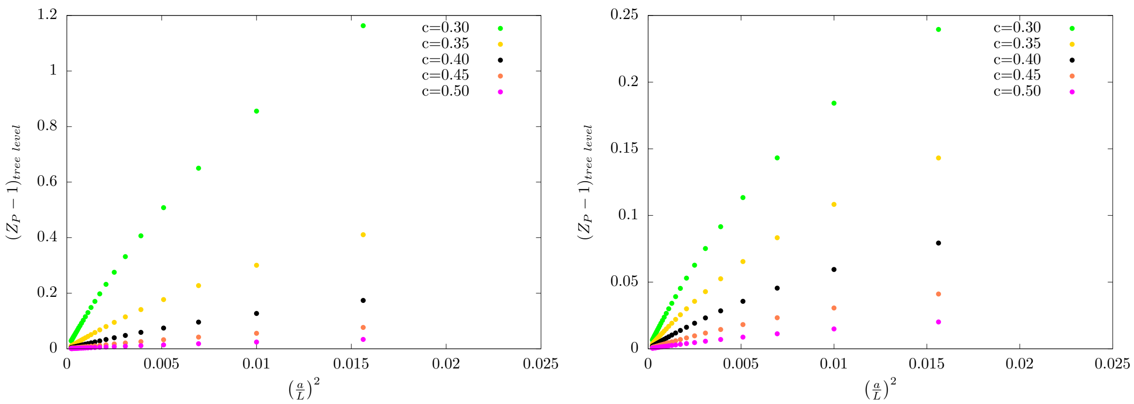
2. The pseudoscalar density as a test case

For definiteness we now specialize to $\Gamma = \gamma_5$, i.e. the pseudoscalar density with renormalization factor Z_P which is related to the quark mass renormalization. We have evaluated the lowest order (tree-level) expressions, using the χSF Wilson Dirac operator both for fundamental and flowed fermion fields. In this way, the orbifold technique very much simplifies the computation of the flowed fermion propagator in time-momentum representation and the correlation function is then easily evaluated. At this point we note that the right hand sides in Eqs (18) are, by definition, taken equal to the tree-level expression. This means that we would obtain $Z_P = 1$ by definition in all cases. In order to study the cutoff effects at the lowest order we therefore agree to take the continuum limit $a/L \to 0$ of the right hand sides in Eqs.(18). For the axial current, we set $Z_A = 1$ at tree-level, while for the conserved (point-split) vector current $Z_{\tilde{V}} = 1$ holds exactly.

2.1 Numerical set-up

We used lattice sizes $\frac{T}{a} \times \left(\frac{L}{a}\right)^3$, with aspect ratio $\rho = \frac{T}{L} = 1$, and even L/a ranging from 8 to 64. We set $x_0 = y_0 = T/2$ and the remaining free parameter, the flow time parameter was chosen from $c \in \{0.3, 0.35, 0.4, 0.45, 0.5\}$.

In Figures 1a and 1b we show the continuum limit of the second (i.e. "ii")) definition from (18) using the axial, the local and point-split vector currents, and in the Figure 2 the definition "i" which makes use of the pseudo-scalar density. By comparing all these three plots we can see the same quadratic behaviour of the cut-off effects but for fixed values of a/L there is an evident difference in the order of magnitude, which makes the last picture with the pseudo scalar current the best candidate for a suitable finite volume renormalization scheme so far.



(a) Renormalization condition (ii) with axial current

(b) Renormalization condition (ii) with vector current

Figure 1

Keeping the value of $c = 0.3$ fixed in the renormalization condition of type "i" (Figure 2), we now investigate how large are the changes in the cut off effects of Z_P if we change the definition of the flow. We keep χSF boundary conditions for the flowed fermion fields and consider the differences between the Laplacian definition of the flow (3), the one with the Wilson-Dirac operator

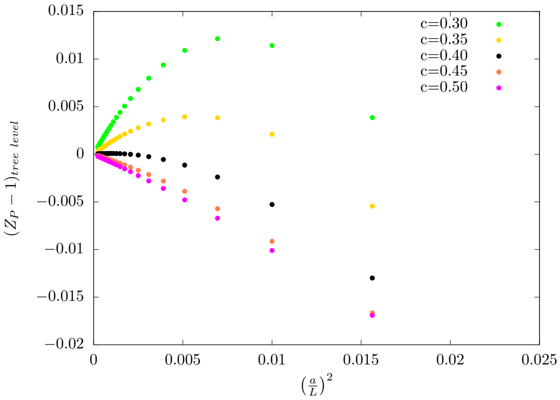
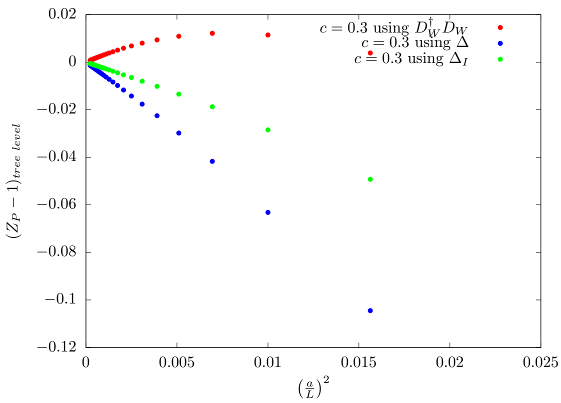


Figure 2: Renormalization condition (i) with pseudo-scalar density

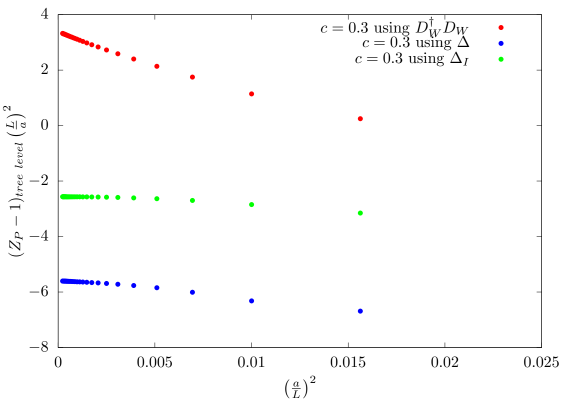
(7) and an O(a^2) improved Laplacian:

$$\Delta_I = \sum_{\mu=0}^{3} \nabla_\mu^* \nabla_\mu \left(1 - \frac{a^2}{12} \nabla_\mu^* \nabla_\mu\right) , \quad \Delta_I \xrightarrow{a\to 0} \Delta^{\text{cont}} + O(a^4) . \tag{19}$$

The results are shown in Figure 3.



(a) Renormalization condition (i) with pseudo-scalar density



(b) Coefficients of leading a^2-effects.

Figure 3

3. Conclusions and further prospects

We have considered a few options for finite volume renormalization schemes for fermion bilinear operators, including the pseudoscalar density as required for the renormalization of quark masses. As a first quality criterion, we have evaluated the cutoff effects at tree level. These vary considerable but there are clearly options where they are reasonably small, say, a few percent at most on the smaller lattices. We are currently implementing different versions of the fermion flow in a simulation program and hope to soon perform tests in the quenched approximation. It remains to be seen whether the fermionic gradient flow can provide an interesting improvement over the current status based on the standard SF schemes.

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References

[1] K. Jansen et al., Phys. Lett. B **372** (1996), 275-282 doi:10.1016/0370-2693(96)00075-5 [arXiv:hep-lat/9512009 [hep-lat]].

[2] M. Lüscher, JHEP **08** (2010), 071 [erratum: JHEP **03** (2014), 092] doi:10.1007/JHEP08(2010)071 [arXiv:1006.4518 [hep-lat]].

[3] M. Dalla Brida and A. Ramos, Eur. Phys. J. C **79** (2019) no.8, 720 doi:10.1140/epjc/s10052-019-7228-z [arXiv:1905.05147 [hep-lat]].

[4] M. Lüscher, JHEP **04** (2013), 123 doi:10.1007/JHEP04(2013)123 [arXiv:1302.5246 [hep-lat]].

[5] S. Sint, Nucl. Phys. B **421** (1994), 135-158 doi:10.1016/0550-3213(94)90228-3 [arXiv:hep-lat/9312079 [hep-lat]].

[6] I. Campos et al. [ALPHA], Eur. Phys. J. C **78** (2018) no.5, 387 doi:10.1140/epjc/s10052-018-5870-5 [arXiv:1802.05243 [hep-lat]].

[7] C. Monahan and K. Orginos, PoS **Lattice2013** (2014), 443 doi:10.22323/1.187.0443 [arXiv:1311.2310 [hep-lat]].

[8] S. Sint, Nucl. Phys. B **847** (2011), 491-531 doi:10.1016/j.nuclphysb.2011.02.002 [arXiv:1008.4857 [hep-lat]].

[9] M. Lüscher and P. Weisz, JHEP **02** (2011), 051 doi:10.1007/JHEP02(2011)051 [arXiv:1101.0963 [hep-th]].

[10] M. Boers, JHEP **01** (2021), 204 doi:10.1007/JHEP01(2021)204 [arXiv:2011.05316 [hep-th]].

[11] M. Dalla Brida, T. Korzec, S. Sint and P. Vilaseca, Eur. Phys. J. C **79** (2019) no.1, 23 doi:10.1140/epjc/s10052-018-6514-5 [arXiv:1808.09236 [hep-lat]].