

Cutoff effects of the gradient flow for fermions

Andrea Shindler^{a,*}

^a*Facility for Rare Isotope Beams & Physics Department, Michigan State University,
East Lansing, Michigan 48824, USA*

E-mail: shindler@frib.msu.edu

I analyze cutoff effects of the gradient flow for Wilson-type fermions. I show that with a proper choice of the higher dimensional fields in the Symanzik effective theory, $O(a)$ improvement of the action is achieved changing the initial conditions of the gradient flow equation.

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*Speaker

1. Introduction

In this contribution I perform an analysis of $O(a)$ cutoff effects of the gradient flow for Wilson-type fermions [1]. For a recent review on the applications to renormalization of the gradient flow see Ref. [2]. Discretization effects of the gradient flow for gauge fields [3–5] have been studied for example in Refs. [6, 7]. $O(a)$ cutoff effects affecting correlation functions containing flowed fermion fields have been analyzed in Ref. [1], where special improvement terms, needed to improve correlation functions of flowed fermion fields, have been derived. In the case of flowed correlation functions the Symanzik effective theory, beside the usual clover improvement term proportional to c_{sw} , contains an additional term proportional to c_{fl} . In this proceedings I discuss the reason for the presence of such additional term. I also show that with a proper choice of the higher dimensional fields the theory can be alternatively improved modifying the initial conditions of the gradient flow equations.

2. Cutoff effects of the gradient flow for fermions

The evolution with the flow time t for fermions is given by [1]

$$\begin{aligned} \partial_t \chi(x, t) &= \Delta \chi(x, t), & \partial_t \bar{\chi}(x, t) &= \bar{\chi}(x, t) \overleftarrow{\Delta}, \\ \chi(x, t = 0) &= \psi(x), & \bar{\chi}(x, t = 0) &= \bar{\psi}(x), \end{aligned} \quad (1)$$

where $\Delta = D_\mu D_\mu$ and the covariant derivative $D_\mu = \partial_\mu + B_\mu$ contain the flowed gauge field $B_\mu(t)$. The dynamics of correlation functions containing flowed fermion fields, χ and $\bar{\chi}$, can be described introducing an extra-dimension to the theory, for the flow time t , and introducing suitable Lagrange multipliers, that, once integrated out, constrain the flowed fields to satisfy the appropriate flow equations. The action of the 4 + 1 dimensional theory reads

$$S = S_G + S_{G,fl} + S_F + S_{F,fl}, \quad (2)$$

where $S_G + S_F$ is the standard QCD action and $S_{G,fl}$ contains the Lagrange multipliers for the gauge fields discussed for example in Refs. [4, 7]. For the fermion fields one has

$$S_{F,fl} = \int_0^\infty dt \int d^4x \left[\bar{\lambda}(x, t) (\partial_t - \Delta) \chi(x, t) + \bar{\chi}(x, t) \left(\overleftarrow{\partial}_t - \overleftarrow{\Delta} \right) \lambda(x, t) \right], \quad (3)$$

where λ and $\bar{\lambda}$ are the Lagrange multipliers that, once integrated out, impose to the flowed fermion fields to satisfy Eqs. (1). The energy-dimension of λ and $\bar{\lambda}$ is 5/2. With the local formulation it is possible to demonstrate the renormalizability of the modified theory [1, 4, 5] and discuss chiral symmetry and related Ward identities [1, 8, 9].

The discretization of the gauge action, provided it preserves the standard symmetries, is not relevant for this discussion. I choose a Wilson-type¹ discretization for the fermion part of the action and the flow time part of the fermion action is discretized with a step ϵ ($t = n\epsilon$)

$$S_{F,fl} = \epsilon \sum_{n \geq 0} a^4 \sum_x \left[\bar{\lambda}(x, t) \left(\partial_t - \nabla^2 \right) \chi(x, t) + \bar{\chi}(x, t) \left(\overleftarrow{\partial}_t - \overleftarrow{\nabla}^2 \right) \lambda(x, t) \right], \quad (4)$$

¹With Wilson-type discretization I denote all lattice actions based on the Wilson action, such as clover fermions.

where $\nabla^2 = \nabla_\mu^* \nabla_\mu$ with ∇_μ (and ∇_μ^*) the flowed forward (and backward) lattice covariant derivatives. The discrete derivative with respect with the flow time is given by

$$\partial_t \chi(x, t) = \frac{1}{\epsilon} (\chi(x, t + \epsilon) - \chi(x, t)) . \quad (5)$$

To analyze cutoff effects it is convenient to describe the theory close to the continuum limit with an effective continuum theory, the so-called Symanzik effective theory, with higher dimensional fields multiplying powers of the lattice spacing [10, 11]. The classification of the higher dimensional fields is obtained using standard discrete and chiral symmetry transformation properties of the fermion fields and the Lagrange multipliers [8].

An analysis of the Symanzik effective theory for fermions has already been performed in Ref. [1], and it is given by

$$S_{\text{eff}}[B, \chi, \bar{\chi}] = S_0[B, \chi, \bar{\chi}] + aS_1 + O(a^2), \quad (6)$$

where S_0 denotes the target continuum theory with renormalized parameters, and S_1 contains higher dimensional fields.

The $O(a)$ cutoff effects in the lattice action are distinguished in $S_{1,b}$ arising from the $t = 0$ boundary, and $S_{1,\text{fl}}$, arising from the bulk of the 4 + 1 dimensional theory

$$S_{1,b} = \int d^4x \sum_{i=1}^{n_b} O_i(x), \quad S_{1,\text{fl}} = \int_0^\infty dt \int d^4x \sum_{i=1}^{n_{\text{fl}}} Q_i(x, t). \quad (7)$$

The fields $Q_i(t, x)$ and $O_i(x)$ are made of space-time and/or flow-time derivatives and the fundamental degrees of freedom of the theory, including the Lagrange multipliers. To keep the action with zero dimension the fields $Q_i(t, x)$ must have dimension 7 while $O_i(x)$ dimension 5.

It is sufficient to improve classically the bulk action thanks to the observation that in perturbation theory flowed correlation functions generate only ‘‘tree diagrams’’ [5]. The standard Symanzik improvement program can be applied to the boundary term $S_{1,b}$.

A classical expansion in powers of a of the lattice fermion action (4) dictates the form of $S_{1,\text{fl}}$. Expanding the covariant laplacian $\nabla^* \nabla$

$$\nabla^* \nabla = D_\mu D_\mu \left(1 + \frac{a^2}{12} D_\mu D_\mu \right) + O(a^3), \quad (8)$$

one obtains the expected result that the leading corrections to the bulk action are of $O(a^2)$, i.e. $S_{1,\text{fl}} = 0$ and the first non-leading term of the effective theory is $S_{2,\text{fl}}$. Modifying the covariant derivatives following Eq. (8), $\nabla_\mu^* \nabla_\mu \rightarrow \nabla_\mu^* \nabla_\mu \left(1 - \frac{a^2}{12} \nabla_\mu^* \nabla_\mu \right)$, removes the $O(a^2)$ stemming from the gradient flow equation [12]. In this work I am only considering $O(a)$ cutoff effects, but it could become useful to monitor the continuum limit to include or exclude the $O(a^2)$ corrections to the flow equation. For this reason I define later a different gradient flow equation that includes the extra term in Eq. (8).

For a single flavor the $D = 5$ fields contributing to the boundary term $S_{1,b}$ are

$$O_1(x) = \bar{\psi}(x)\sigma_{\mu\nu}G_{\mu\nu}(x)\psi(x), \quad (9)$$

$$O_2(x) = \bar{\psi}(x)D_\mu D_\mu \psi(x) + \bar{\psi}(x)\overleftarrow{D}_\mu \overleftarrow{D}_\mu \psi(x), \quad (10)$$

$$O_3(x) = m\text{Tr} [G_{\mu\nu}G_{\mu\nu}], \quad (11)$$

$$O_4(x) = m\bar{\psi}(x) \left[\gamma_\mu D_\mu - \gamma_\mu \overleftarrow{D}_\mu \right] \psi(x), \quad (12)$$

$$O_5(x) = m^2 \bar{\psi}(x)\psi(x), \quad (13)$$

$$O_6(x) = \bar{\lambda}(x)\lambda(x), \quad (14)$$

$$O_7(x) = m \left(\bar{\lambda}(x)\psi(x) + \bar{\psi}(x)\lambda(x) \right), \quad (15)$$

$$O_8(x) = \bar{\lambda}(x)\gamma_\mu D_\mu \psi(x) - \bar{\psi}(x)\gamma_\mu \overleftarrow{D}_\mu \lambda(x), \quad (16)$$

$$O_9(x) = \partial_t (\bar{\chi}(x,t)\chi(x,t))|_{t=0}, \quad (17)$$

where the first 5, O_1, \dots, O_5 , are the standard terms from the unflowed theory [11], and the additional 4, O_6, \dots, O_9 , are the new contributions stemming from the gradient flow equation. For on-shell $O(a)$ improvement one can use the field equations for ψ , (and $\bar{\psi}$), χ , (and $\bar{\chi}$), while the field equations for λ , (and $\bar{\lambda}$) are equivalent to impose the gradient flow equation. The total number of conditions is 4, leaving 5 total independent fields. From the first 5 fields, $O_1 - O_5$, I make the standard choice [11] to select O_1, O_3 and O_5 . In Ref. [1], for the additional fields $O_6 - O_9$, the choice is to select O_6 and O_7 . The field $O_6 = \bar{\lambda}\lambda$ is multiplied by the improvement coefficient $c_{\bar{\lambda}}$, while O_7 is responsible for the mass dependent cutoff effects removed by the improvement coefficients b_χ .² In this study I select instead O_7 and O_8 . Our choice is dictated by the following observation. If I write explicitly the terms of the summation over ϵ of Eq. (4)

$$\begin{aligned} S_{F,\text{fl}} = & a^4 \sum_x \left[\bar{\lambda}(x)\chi(x,\epsilon) - \bar{\lambda}(x)\chi(x,t=0) - \epsilon \bar{\lambda}(x)\nabla^2 \chi(x,t=0) + \right. \\ & \left. + \bar{\chi}(x,\epsilon)\lambda(x) - \bar{\chi}(x,t=0)\lambda(x) - \epsilon \bar{\psi}(x)\nabla^2 \lambda(x) \right] + \dots \end{aligned} \quad (18)$$

the second and the fifth terms contain the fermion fields defined by the initial conditions of the gradient flow equations. The lattice version of the fields O_7 and O_8 can then be included in the lattice action modifying the initial conditions. If I now modify the initial conditions

$$\begin{aligned} \chi(x,t)|_{t=0} &= \left(1 + \frac{a}{2}c_1\gamma_\mu D_\mu + \frac{a}{2}c_2m \right) \psi(x), \\ \bar{\chi}(x,t)|_{t=0} &= \bar{\psi}(x) \left(1 - \frac{a}{2}c_1\gamma_\mu \overleftarrow{D}_\mu + \frac{a}{2}c_2m \right). \end{aligned} \quad (19)$$

the second and fifth terms in Eq. (18) change as follows

$$\bar{\lambda}(x)\chi(x,t=0) \rightarrow \bar{\lambda}(x) \left(1 + \frac{a}{2}c_1\gamma_\mu D_\mu + \frac{a}{2}c_2m \right) \psi(x), \quad (20)$$

$$\bar{\chi}(x,t=0)\lambda(x) \rightarrow \bar{\psi}(x) \left(1 - \frac{a}{2}c_1\gamma_\mu \overleftarrow{D}_\mu + \frac{a}{2}c_2m \right) \lambda(x). \quad (21)$$

The modified form of the action $S_{F,\text{fl}}$ now contains automatically the fields O_7 and O_8 .

²With more than one flavor there is an additional $D = 5$ field responsible to the term proportional to \bar{b}_χ .

The conclusion is that the $O(a)$ improvement of the theory can be obtained modifying the initial conditions at finite lattice spacing. With this formulation one does not need to determine the coefficient c_{fl} and one does not need to compute additional correlation functions with the space-time insertion of the term $c_{\text{fl}}\bar{\lambda}\lambda$.

3. Tree-level analysis

To study cutoff effects I first consider standard Wilson fermions at tree-level of perturbation theory. In the next Sec. 3.1 I extend this analysis to include flowed fermion fields.

In momentum space the standard Wilson fermion tree-level propagator is given by

$$\tilde{S}_{\text{W}}(p) = \frac{-i\not{p} + M(p)}{\not{p}^2 + M(p)^2}, \quad (22)$$

where $M(p) = m + \frac{1}{2}a\hat{p}^2$, $\hat{p}_\mu = \frac{1}{a}\sin(ap_\mu)$ and $\hat{p}_\mu = \frac{2}{a}\sin(\frac{ap_\mu}{2})$. The only step needed to renormalize the quark propagator is a redefinition of the quark mass. Using the pole mass definition, $m \rightarrow m(1 + \frac{1}{2}am)$, it is equivalent to include the field O_5 in the lattice theory. At leading order in the lattice spacing a the quark propagator now reads (see for example Ref. [13, 14])

$$S(x, y) \rightarrow \int \frac{d^4p}{(2\pi)^4} e^{ip(x-y)} \frac{-i\not{p} + m}{p^2 + m^2} (1 - am) + \frac{1}{2}a\delta^{(4)}(x - y) + O(a^2). \quad (23)$$

The last constant term is a contact term term proportional to $\delta^{(4)}(x - y)$, while the residual $O(am)$ contribution can be removed improving the observable, i.e. the fermion fields in this case. Improving the fermion fields

$$\begin{cases} \psi_{\text{I}}(x) = \psi(x) \left(1 + \frac{a}{2}b_\psi m\right) \\ \bar{\psi}_{\text{I}}(x) = \bar{\psi}(x) \left(1 + \frac{a}{2}b_\psi m\right), \end{cases} \quad (24)$$

with the tree-level value $b_\psi^{(0)} = 1$, the improved propagator reads

$$\langle \psi_{\text{I}}(x)\bar{\psi}_{\text{I}}(y) \rangle = S_{\text{I}}(x - y) = \int \frac{d^4p}{(2\pi)^4} \frac{-i\not{p} + m}{p^2 + m^2} + \frac{1}{2}a\delta^{(4)}(x - y) + O(a^2). \quad (25)$$

This result confirms the expectation of the Symanzik program. I have improved the theory and the observable and I obtain an $O(a)$ improved result, excluding contact terms.³

3.1 Tree-level analysis of the flowed fermion propagator

At finite lattice spacing the flowed fermion propagator is computed solving the discretized version of the gradient flow equation (18)

$$\tilde{S}_{\text{W}}(p, t, s) = e^{-\hat{p}^2(t+s)} \frac{-i\not{p} + M(p)}{\not{p}^2 + M(p)^2}. \quad (26)$$

³To remove also the contact term one can modify the fermion field, $\psi(x) \rightarrow \left(1 + \frac{a}{4}c_q (\not{D} + m)\right) \psi(x)$, with tree-level value $c_q^{(0)} = -1$, as discussed in Ref. [13, 15].

Expanding in powers of a and rescaling the quark mass, $m \rightarrow m(1 + 1/2am)$, one obtains

$$\tilde{S}_W(p, t, s) = e^{-p^2(t+s)} \left(1 + \frac{a^2 p^2}{12}(t+s) \right) \frac{-i\not{p} + m}{p^2 + m^2} (1 - am) + \frac{1}{2} a e^{-p^2(t+s)} \left(1 + \frac{a^2 p^2}{12}(t+s) \right) + \dots, \quad (27)$$

where, beside the $O(a)$, the equation shows also the $O(a^2)$ resulting from the expansion of the ∇^2 term. Modifying the gradient flow differential operator as discussed earlier, $\nabla_\mu^* \nabla_\mu \rightarrow \nabla_\mu^* \nabla_\mu \left(1 - \frac{a^2}{12} \nabla_\mu^* \nabla_\mu \right)$ subtracts those particular $O(a^2)$ effects. Only numerical experiments can test the effectiveness to use the improved laplacian operator and first numerical tests have been shown in Ref. [12].

I now drop all the $O(a^2)$ terms and continue the analysis retaining from Eq. (27) only the $O(a)$ terms. Following Ref. [1] to improve the observable I first need to improve the fermion fields as follows

$$\begin{cases} \chi_1(x, t) = \left(1 + \frac{a}{2} b_\chi m \right) \chi(x, t) \\ \bar{\chi}_1(x, t) = \bar{\chi}(x, t) \left(1 + \frac{a}{2} b_\chi m \right), \end{cases} \quad (28)$$

with a tree-level value $b_\chi^{(0)} = 1$. The propagator now is

$$\tilde{S}_1(p, t, s) = e^{-p^2(t+s)} \frac{-i\not{p} + m}{p^2 + m^2} + \frac{1}{2} a e^{-p^2(t+s)} + O(a^2). \quad (29)$$

The propagator is still affected by $O(a)$ cutoff effects which are the remnant of the contact term in Eq. (23). The gradient flow regulates the contact term generating a new $O(a)$ term parametrized, in the Symanzik effective theory, by a new $D = 5$ field. Following Ref. [1] the additional $O(a)$ cutoff effects are removed tuning the coefficient of $O_6 = \bar{\lambda}\lambda$, denoted as c_fl . In practice the term $c_\text{fl} O_6$ is inserted in the correlation functions with tree-level value $c_\text{fl}^{(0)} = 1/2$.

I now show that the same cancellation takes place modifying the initial boundary conditions as discussed in Sec. 2 (see Eq. (20)). With the new boundary conditions (20) the lattice flowed fermion propagator is

$$\tilde{S}(p, t, s) = e^{-\hat{p}^2(t+s)} \left(1 + \frac{a}{2} c_1^{(0)} i\not{\hat{p}} + \frac{a}{2} c_2^{(0)} m \right) (i\not{\hat{p}} + M(p))^{-1} \left(1 + \frac{a}{2} c_1^{(0)} i\not{\hat{p}} + \frac{a}{2} c_2^{(0)} m \right). \quad (30)$$

After rescaling the quark mass, the remaining $O(a)$ effects in the propagator are removed tuning the tree-level values of the improvement coefficients to $c_1^{(0)} = -1/2$ and $c_2^{(0)} = 1/2$. It is maybe convenient to rewrite the initial conditions as

$$\begin{aligned} \chi(x, t)|_{t=0} &= \left(1 + \frac{a}{2} c_\chi (\gamma_\mu D_\mu + m) + \frac{a}{2} c_m m \right) \psi(x), \\ \bar{\chi}(x, t)|_{t=0} &= \bar{\psi}(x) \left(1 - \frac{a}{2} c_\chi (\gamma_\mu \overleftarrow{D}_\mu + m) + \frac{a}{2} c_m m \right), \end{aligned} \quad (31)$$

where $c_\chi = c_1$ and $c_m = c_2 - c_1$, with tree-level values $c_\chi^{(0)} = -1/2$ and $c_m^{(0)} = 1$. It is possible to show that the improvement coefficients c_χ and c_m are related to c_fl and b_χ . The term proportional to c_χ can be implemented numerically using any lattice form of the Dirac operator, while the term proportional to c_m can be either included in the initial conditions as in Eq. (31) or as a multiplicative factor in flowed correlators as done in Ref. [1] with b_χ . A form of the initial conditions that avoids

including the quark mass is

$$\begin{aligned}\chi(x,t)|_{t=0} &= \left(1 + \frac{a}{2}c_\chi\gamma_\mu D_\mu\right)\psi(x), \\ \bar{\chi}(x,t)|_{t=0} &= \bar{\psi}(x)\left(1 - \frac{a}{2}c_\chi\gamma_\mu \overleftarrow{D}_\mu\right),\end{aligned}\tag{32}$$

where also in this case the term proportional to the mass is added to the correlation functions but with a different improvement coefficient than b_χ . Different choices of the lattice Dirac operator in the initial conditions generate different higher order cutoff effects and only numerical studies can provide an indication on which choice is better in terms of $O(a^2)$ effects.

4. Final remarks

The gradient flow for Wilson-type fermions simplifies the process of renormalization and improvement of flowed correlators [1]. Matrix elements of flowed operators renormalize multiplicatively and can be improved at the classical level, provided the lattice QCD action at the boundary $t = 0$ is $O(a)$ improved. The price to pay is some additional $O(a)$ boundary, $t = 0$, terms which are related to the use of flowed fermion fields. I have shown that these $O(a)$ effects are a remnant of the $O(a)$ proportional to contact terms in the unflowed theory. I have also shown that using the modified gradient flow equation

$$\begin{aligned}\partial_t\chi(x,t) &= \nabla_\mu^*\nabla_\mu\left(1 - \frac{a^2}{12}\nabla_\mu^*\nabla_\mu\right)\chi(x,t), \\ \chi(x,t)|_{t=0} &= \left(1 + \frac{a}{2}c_\chi\gamma_\mu D_\mu\right)\psi(x),\end{aligned}\tag{33}$$

and the corresponding for $\bar{\chi}$, flowed observables are $O(a)$ improved, provided the lattice QCD action is also non-perturbatively $O(a)$ improved. The modified lattice version of the Laplacian in Eq. (33) is $O(a^2)$ improved [12]. Only numerical tests can indicate whether the use of the improved Laplacian and the specific choice of the lattice covariant derivatives is useful to decrease discretization errors. The remaining $O(am)$ terms are removed multiplying flowed correlators with the proper rescaling factor for fermion fields as discussed in Ref. [1]. With the GF equations (33) it is not necessary to determine additional correlation functions to have an $O(a)$ improved lattice theory [1]. It would be interesting to test if chiral Ward identities can be used to estimate c_χ as done for c_{fl} .

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