On O(a^2) effects in gradient flow observables

Alberto Ramos

PH-TH CERN, CH-1211 Geneva 23, Switzerland
E-mail: alberto.ramos@cern.ch

Stefan Sint[*]

NIC, DESY-Zeuthen, Platanenallee 6 D-15738 Zeuthen, Germany
& School of Mathematics, Trinity College, Dublin 2, Ireland
E-mail: sint@maths.tcd.ie

In lattice gauge theories, the gradient flow has been used extensively both, for scale setting and for defining finite volume renormalization schemes for the gauge coupling. Unfortunately, rather large cutoff effects have been observed in some cases. We here investigate these effects to leading order in perturbation theory, considering various definitions of the lattice observable, the lattice flow equation and the Yang Mills lattice action. These considerations suggest an improved set-up for which we perform a scaling test in the pure SU(3) gauge theory, demonstrating strongly reduced cutoff effects. We then attempt to obtain a more complete understanding of the structure of O(a^2) effects by applying Symanzik's effective theory approach to the 4+1 dimensional local field theory with flow time as the fifth dimension. From these considerations we are led to a fully O(a^2) improved set-up the study of which is left to future work.

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[*]Speaker.

1. Yang-Mills gradient flow and running couplings

The gradient flow [1] allows for the definition of renormalized observables which are measurable with high statistical precision at relatively low computational costs. One may thus hope that this will allow for high precision in the calibration of the lattice scale and precision studies of the running coupling [2]. In both cases one starts from the observable $\langle E \rangle$,

$$\langle E(t,x) \rangle = -\frac{1}{2} \left\langle \text{tr} \left(G_{\mu\nu}(t,x) G_{\mu\nu}(t,x) \right) \right\rangle, \qquad G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \qquad (1.1)$$

and the gauge field B_μ at flow time t is obtained as the solution of the Yang-Mills gradient flow equation,

$$\partial_t B_\mu(t,x) = -\frac{\delta S[B]}{\delta B_\mu(x)} = D_\nu G_{\nu\mu}(t,x), \qquad B_\mu(0,x) = A_\mu(x), \qquad (1.2)$$

with the covariant derivative $D_\mu = \partial_\mu + [B_\mu, \cdot]$ and $A_\mu(x)$ the fundamental 4-dimensional gauge field. In [3] a perturbative all-order proof was given that gauge invariant observables like (1.1) are renormalized if expressed in terms of a renormalized gauge coupling, g^2. Given the perturbative expansion, $\langle E \rangle = \mathscr{E}_0 g^2 + \text{O}(g^4)$, one may thus introduce the renormalized gradient flow coupling,

$$\bar{g}_{\text{GF}}^2(q = 1/\sqrt{8t}) = \mathscr{N}^{-1} t^2 \langle E(t,x) \rangle, \qquad (1.3)$$

where the constant $\mathscr{N} = t^2 \mathscr{E}_0$ ensures the standard normalization of a coupling constant. The requirement that $g_{\text{GF}}^2(q)$ takes a particular value can also be seen as the implicit definition of the corresponding scale. In particular, the scale, t_0, defined by [1],

$$\left\{ t^2 \langle E(t) \rangle \right\}_{t=t_0} = 0.3, \qquad (1.4)$$

corresponds to a value $\bar{g}_{\text{GF}}^2(q = 1/\sqrt{8t_0}) = 8\pi^2/5 \approx 15.8$ (assuming $N = 3$ colours). Analogous considerations can be made in a finite space-time volume, leading to interesting finite volume schemes for renormalized couplings. In a symmetric (hyper-) box of physical size L^4 one then relates L to t by setting the ratio $c = \sqrt{8t}/L$ to a particular value, e.g. $c = 0.3$. Different schemes are obtained for different boundary conditions [4, 5, 6, 7] and values of c. Here we will focus on the pure gauge theory with either twisted periodic [6] or SF boundary conditions [5].

Relatively large cutoff effects have been found in t_0 [1] and step scaling functions of finite volume flow couplings related to $E(t,x)$ (e.g. [4]). We here present a systematic study of O(a^2) effects in $\mathscr{E}_0$, for various lattice gauge actions, lattice definitions of the observable $E(t,x)$ and of the lattice gradient flow equation. We start with the infinite volume case, then move to finite volume, which leads to further improvement conditions. We then sketch how full O(a^2) improvement à la Symanzik [8, 9, 10] can be achieved, based on the local $4+1$ dimensional field theory for gradient flow observables [3].

2. Infinite lattice

To study the expectation value $\langle E(t,x) \rangle$ in perturbation theory on the infinite lattice we must choose a discretization of the observable $E(t,x)$, a lattice action and a lattice version of the flow equation. At leading perturbative order one needs to expand $E(t,x)$ to second order in the B_μ fields,

relate these to the fundamental gauge field A_μ via the linearized lattice flow equation, and calculate the expectation value of the two A_μ fields, i.e. the gauge field propagator, for the chosen lattice action. The propagator is the inverse kernel for the action when expanded to second order in the gauge fields[1],

$$S = \frac{1}{2} \int_{-\pi/a}^{\pi/a} \mathrm{d}^4 p \, A_\mu^b(-p) K_{\mu\nu}(p,\lambda) A_\nu^b(p) + \mathrm{O}(A^3), \tag{2.1}$$

where λ is the gauge fixing parameter required for K to be invertible. Similarly, the gradient flow equation on the lattice,

$$\partial_t V_\mu(t,x) = -\partial_{x,\mu} \left(g_0^2 S_{\mathrm{lat}}[V] \right) V_\mu(t,x), \qquad V_\mu(0,x) = U_\mu(x), \tag{2.2}$$

with links parameterized by $V_\mu(t,x) = \exp\{aB_\mu(t,x)\}$, and expanded to first order in B_μ can be parameterized by the quadratic part of the corresponding lattice action, and thus by another kernel $K_{\mu\nu}(p,\alpha)$, with gauge parameter α. Finally, since the observable (1.1) has the form of an action density, another free action kernel can be used, however, this time without a gauge fixing term. Hence, we have 3 kernels $K_{\mu\nu}$ for action (a), observable (o) and flow (f). We have considered generic lattice actions with all 4- and 6-link Wilson loops, parameterized by coefficients c_i, $i = 0..3$ satisfying the normalization condition $c_0 + 8c_1 + 16c_2 + 8c_3 = 1^2$ [10]. This includes the Wilson plaquette action ($c_0 = 1$, $c_1 = c_2 = c_3 = 0$) and the tree-level O(a^2) improved Lüscher-Weisz action [10] ($c_0 = 5/3$, $c_1 = -1/12$, $c_2 = c_3 = 0$). For the observable we use either the corresponding lattice action densities or the action density obtained with the clover definition of $G_{\mu\nu}(t,x)$. For instance, the kernel corresponding to the Wilson plaquette action is given by,

$$K_{\mu\nu}(p,\lambda) = \hat{p}^2 \delta_{\mu\nu} + (\lambda - 1)\hat{p}_\mu \hat{p}_\nu, \qquad \hat{p}_\mu = \frac{2}{a} \sin\left(\frac{1}{2} a p_\mu \right), \tag{2.3}$$

with continuum limit

$$K_{\mu\nu}^{\mathrm{cont}}(p,\lambda) = p^2 \delta_{\mu\nu} + (\lambda - 1) p_\mu p_\nu, \tag{2.4}$$

and a small a-expansion of the form

$$K_{\mu\nu}(p,\lambda) = K_{\mu\nu}^{\mathrm{cont}}(p,\lambda) + a^2 R_{\mu\nu}(p,\lambda) + \mathrm{O}(a^4), \tag{2.5}$$

where

$$R_{\mu\nu}(p,\lambda) = -\frac{1}{12} p^4 \delta_{\mu\nu} + \frac{1}{24}(\lambda - 1) p_\mu p_\nu (p_\mu^2 + p_\nu^2). \tag{2.6}$$

Proceeding analogously for all kernels, we obtain the master equation

$$t^2 \mathscr{E}_0 = \frac{1}{2}(N^2 - 1) \int_{-\pi/a}^{\pi/a} \frac{\mathrm{d}^4 p}{(2\pi)^4} \, \mathrm{tr}\left[K^{(\mathrm{o})}(p,0) e^{-tK^{(\mathrm{f})}(p,\alpha)} K^{(\mathrm{a})}(p,\lambda)^{-1} e^{-tK^{(\mathrm{f})}(p,\alpha)} \right]. \tag{2.7}$$

Evaluation of the trace over Lorentz indices and extension of the momentum integrals to infinity leads to

$$t^2 \mathscr{E}_0 = \frac{3(N^2-1)}{128\pi^2} \left\{ 1 + \frac{a^2}{t} \left[\left(d_1^{(\mathrm{o})} - d_1^{(\mathrm{a})} \right) J_{4,-2} + \left(d_2^{(\mathrm{o})} - d_2^{(\mathrm{a})} \right) J_{2,0} - 2d_1^{(\mathrm{f})} J_{4,0} - 2d_2^{(\mathrm{f})} J_{2,2} \right] \right\} \tag{2.8}$$

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[1] We decompose e.g. $A_\mu(x) = A_\mu^b T^b$ with summation over $b = 1, \ldots, N^2 - 1$ understood and anti-hermitian generators T^b, normalized by $\mathrm{tr}\,(T^a T^b) = -1/2$.

[2] In the literature c_2 and c_3 are sometimes interchanged. We here follow the convention where c_2 multiplies the "bent rectangles" or "chairs", and c_3 the "parallelograms".

where corrections are O(a^4) and

$$J_{n,m} = \frac{t^{(m+n)/2} \int_{-\infty}^{\infty} d^4p\, e^{-2tp^2} p^n p^m}{\int_{-\infty}^{\infty} d^4p\, e^{-2tp^2}}, \qquad p^n\Big|_{n=2,4,\dots} = \sum_{\mu} p_{\mu}^n, \qquad p^{-n} = 1/p^n. \qquad (2.9)$$

All momentum integrals can be evaluated analytically,

$$J_{2,0} = 1, \quad J_{2,2} = 3/2, \quad J_{4,0} = 3/4, \quad J_{4,-2} = 1/2, \qquad (2.10)$$

so that the coefficients of the leading O(a^2) effects can be combined,

$$t^2 \mathscr{E}_0 = \frac{3(N^2-1)}{128\pi^2} \left\{ 1 + \frac{a^2}{t}\left(d^{(\mathrm{o})} - d^{(\mathrm{a})} - 3d^{(\mathrm{f})}\right) + \mathrm{O}(a^4) \right\}. \qquad (2.11)$$

Each d-coeffcient takes a particular value e.g. for the Wilson-plaquette, Lüscher-Weisz or the clover kernel (or linear combinations thereof). Examples are

$$d^{(\mathrm{a,o,f})} = \begin{cases} -\frac{1}{24}, & \text{plaquette (pl),} \\ \frac{1}{72}, & \left(= -\frac{1}{24} - \frac{2}{3}c_1\right) \quad \text{Lüscher-Weisz (lw),} \\ -\frac{5}{24}, & \text{Clover (cl),} \end{cases} \qquad (2.12)$$

in agreement with [11]. Obviously, there are many ways to cancel a single O(a^2) term, e.g. by linear combination of plaquette and clover definitions of the observable, or by a τ-shift [12]. However, such recipes are of limited use as they only cancel the leading cutoff in a particular observable. Symanzik improvement is more ambitious in that it aims at improving the action and composite fields by local counterterms such that leading cutoff effects are eliminated in all observables. Not so long ago most people (including the authors) would have expected that tree-level O(a^2) improvement of flow observables could be achieved by combining an O(a^2) improved action, an O(a^2) improved observable and the gradient of an O(a^2) improved action for the flow (possibly up to a boundary counterterm, cf. [2]). Hence, using the Lüscher-Weisz action [10] for all three kernels should then achieve tree-level O(a^2) improvement. However, the above results show that this choice leads to a non-vanishing coefficient,

$$d^{\mathrm{total}} = d^{(\mathrm{o})} - d^{(\mathrm{a})} - 3d^{(\mathrm{f})} = -\frac{1}{24}, \qquad (2.13)$$

indicating that this expectation was too naive. It is also worth mentioning that the seemingly small cutoff effects observed in [1] with the clover observable are due to an accidental cancellation between cutoff effects of clover observable, Wilson flow and Wilson action.

3. Finite volume: the GF coupling with twisted periodic b.c.'s

We now pass to a finite volume and consider the gradient flow coupling (1.3) with twisted periodic boundary conditions for the gauge field [6] Since this finite volume scheme preserves translation invariance, the the trace algebra is the same as infinite volume, with the generalized momenta of the twisted periodic set-up. What changes are the momentum integrals which become momentum sums. The result can be cast in the same form as eq. (2.8) with the important difference
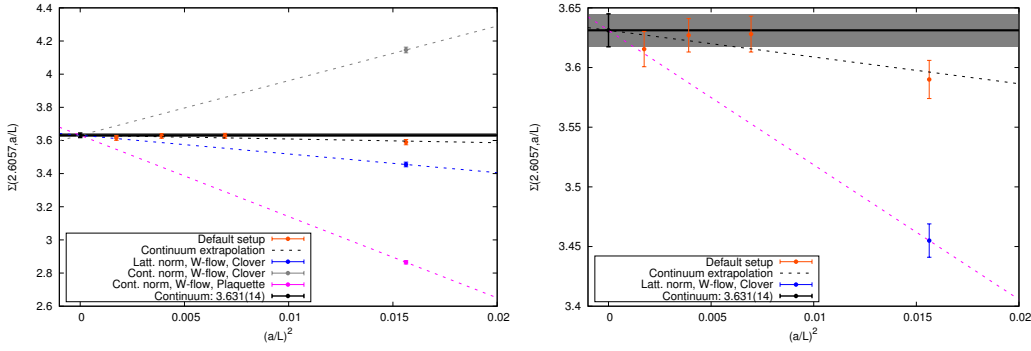
Figure 1: The step-scaling function computed with the "default" set-up using an improved observable, action and the chair flow. For comparison we have included several data points at the coarsest lattice spacing with alternative discretizations. The definition with the clover observable and the Wilson flow fares second best and is shown again in the right panel.

that the numbers $J_{n,m}$ become functions of $c = \sqrt{8t}/L$, with the infinite volume result recovered in the limit $c \to 0$. As functions of c the different lattice sums are linearly independent and give thus rise to more stringent improvement conditions, as each their coefficients must vanish separately. Our results indicate that tree-level O(a^2) improvement cannot be achieved with the Lüscher-Weisz flow. However, with a generic lattice action for the flow we found a 1-parameter family of flows such that tree level O(a^2) improvement is achieved for this finite volume coupling. Our choice was to set $c_3 = 0$ and to include only the bent rectangles/chairs with coefficient c_2. With the choice for the coefficients,

$$c_0 = 1, \qquad c_1 = -1/12, \qquad c_2 = 1/24, \tag{3.1}$$

this defines what we will call the "chair flow".

4. Scaling test in pure SU(3) gauge theory

We have implemented the chair flow in the open-QCD code [14] and performed a scaling test, using the LW action and, for the observable, the step-scaling function for the finite volume coupling with SF boundary conditions and $c = 0.3$ [5]. In this case the expectation value $\langle E(t,x) \rangle$ retains an x_0-dependence. In order to minimize the (small) influence from the time boundaries we set $x_0 = T/2$ and $T = L$. Moreover, the (colour-) magnetic and electric components of $G_{\mu\nu}$ contribute differently. After some experimentation with perturbative data we chose to only use the magnetic components, i.e.

$$-\frac{1}{2} \langle \operatorname{tr} G_{kl}(x,t) G_{kl}(x,t) \rangle |_{x_0=T/2} = \mathcal{N}(c,a/L) \bar{g}_{\mathrm{GF}}^2(L). \tag{4.1}$$

We then computed the step-scaling function $\Sigma(u,a/L) = \bar{g}_{\mathrm{GF}}^2(2L)$ at $u = \bar{g}_{\mathrm{GF}}^2(L) = 2.6057$ for lattice sizes $L/a = 8, 12, 16, 24$ and with scale factor $s = 2$. The results shown in figure 1 show indeed a strong reduction of cutoff effects for the improved data with the chair flow. On the coarsest lattice the cutoff effects are reduced by a factor 4 or so with respect to the second best definition with the Wilson flow and the clover observable.

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5. Symanzik O(a^2) improvement of flow observables

Despite the impressive reduction of lattice artefacts seen with the chair flow it remains unclear whether this set-up is improved in the sense of Symanzik [8, 9, 10]. To apply the Symanzik programme to gradient flow observables it is essential to use a local formulation of the theory. This is achieved by the $4+1$ dimensional set-up discussed by Lüscher and Weisz [3], with the flow time t as additional coordinate. The $4+1$ dimensional lattice action is

$$S = S_{\text{lat}}[U] + \int_0^\infty dt\, a^4 \sum_x \text{tr}\left(L_\mu(t,x)\left\{ \left(\partial_t V_\mu(t,x)\right)V_\mu(t,x)^\dagger + \partial_{x,\mu}\left(g_0^2 S_{\text{lat}}[V]\right)\right\}\right). \tag{5.1}$$

The continuum limit of this action is the starting point for the Symanzik expansion. O(a^2) counterterms could arise from 3 sources, namely the observable, the 4-dimensional boundary at $t=0$, and O(a^2) counterterms in the $4+1$-dimensional bulk. Following the reasoning by Lüscher in the fermionic case [13], we expect classical O(a^2) improvement for both the observable and the flow to *completely* remove O(a^2) effects from these sources, i.e. to all orders in the coupling! This leaves us with possible boundary effects, generated by dimension 6 terms at $t=0$. If these do not involve the field $L_\mu(t,x)$ they must be of the same form as the standard improvement counterterms in the 4-dimensional theory. Requiring improvement for non-flow observables fixes this freedom. After use of the flow equation we are thus left with the following candidate counterterms[3],

$$\text{tr}\left\{L_\mu(t,x)L_\mu(t,x)\right\}|_{t=0}, \qquad \text{tr}\left\{L_\mu(t,x)D_\nu G_{\nu\mu}(x,t)\right\}|_{t=0}, \tag{5.2}$$

which may or may not be required for O(a^2) improvement. How to best implement these counterterms and whether both are really required is left to future work. Our explicit calculations suggest that they do not contribute at tree-level of perturbation theory.

6. Classical expansion of flow equation

It remains to perform out the classical a^2-expansion of the lattice flow equation, where $V_\mu(t,x)$ is related by a path ordered exponential to the continuum gauge field B_μ. We performed this calculation with the gradient of a lattice action with free parameters c_0, c_1 and c_2. Unfortunately it turns out that the chair flow does not seem to be O(a^2) improved. During the calculation we however noticed that the O(a^2) effects for the Lüscher-Weisz gradient flow ($c_0 = 5/3$, $c_1 = -1/12$, $c_2 = c_3 = 0$) have a simple structure:

$$\partial_t B_\mu = D_\nu G_{\nu\mu} - \frac{1}{12}a^2 D_\mu^2 D_\nu G_{\nu\mu} + O(a^3). \tag{6.1}$$

This suggests a simple modification of the lattice flow equation,

$$a^2\left(\partial_t V_\mu(x,t)\right)V_\mu(x,t)^\dagger = -\left(1 + \frac{1}{12}a^2 \nabla_\mu^* \nabla_\mu\right)\partial_{x,\mu}\left(g_0^2 S_{\text{lat}}[V]\right), \tag{6.2}$$

where ∇_μ and ∇_μ^* denote the covariant adjoint lattice derivative operators. While this "Zeuthen flow" removes all O(a^2) effects from the flow equation, it still remains to be put to a numerical test.

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[3]We thank A. Patella for pointing out to us the possibility of a term quadratic in L_μ.

7. Conclusions

We have carried out a detailed investigation of tree-level O(a^2) effects in gradient flow observables derived from $E(x,t)$. This led to the definition of the chair flow, which eliminates O(a^2) tree-level effects from the flow equation, in all cases considered. Furthermore, a quenched scaling test showed remaining cutoff effects to be very small. In order to see whether this provides a complete solution for *any* flow observable we took to Symanzik O(a^2) improvement in the $4+1$ dimensional set-up: a couple of candidate counterterm remain to be investigated, but do not seem to contribute in the explicit tree-level calculations. Symanzik improvement requires the classical a^2-expansion of both observables and flow equation. It turns out that the chair flow is not fully O(a^2) improved, i.e. the cancellation seen in the explicit calculation might be specific to the observables considered. Finally we proposed the fully O(a^2) improved "Zeuthen flow" as a simple modification of the Lüscher-Weisz gradient flow, which still needs to be tested numerically.

Acknowledgments

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