# Gauge field smearing and controlled continuum extrapolations

**Andreas Risch**[1]
andreas.risch@desy.de

Stefan Schaefer[1]
stefan.schaefer@desy.de

Rainer Sommer[1,2]
rainer.sommer@desy.de

[1]John von Neumann-Institut für Computing NIC
Deutsches Elektronen-Synchrotron DESY
Platanenallee 6, 15738 Zeuthen, Germany

[2]Institut für Physik
Humboldt-Universität zu Berlin
Newtonstr. 15, 12489 Berlin, Germany

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# Discretisation effects in lattice QCD with Wilson fermions

Two strategies to modify current CLS action ($O(a)$-improved Wilson fermions):

- Further **improvement** of action:
  W2/D234 fermion action[1]: additional irrelevant dim-6 operator[2]

$$\delta\mathscr{L} = -\frac{a^2}{6}\sum_\mu \overline{\Psi}\gamma_\mu\nabla_\mu\Delta_\mu\Psi$$

  provides full tree-level $O(a^2)$-improvement, shifts $\Gamma_i$ in SymEFT expansion[3]

$$\mathcal{O}(a) - \mathcal{O}(0) \sim \sum_i \hat{c}_i M_i a^2 (\alpha_s(a^{-1}))^{\Gamma_i} \qquad \alpha_s(a^{-1}) \sim (-\log(a\Lambda))^{-1}$$

  $\Gamma_i \to \Gamma_i + 1 \Rightarrow a^2 \log(a)$ lattice artefacts a bit further suppressed

- Smearing of gauge fields $U$ in Dirac operator (**UV filtering**): $D[\mathcal{S}[U]]$
  $\Rightarrow$ Reduces likelihood of finding small eigenvalues (related to explicit $\chi$SB breaking) and amount of renormalization[4]

  **Caveat**: Too much smearing destroys UV structure of lattice theory and makes continuum extrapolation unreliable

**What smearing strengths allow for controlled continuum extrapolations?**

- First focus on observable smearing $\langle O[\mathcal{S}[U]]\rangle$ in SU(3) Yang-Mills theory

[1] Alford et al. 1997.
[2] Sheikholeslami and Wohlert 1985.
[3] Husung et al. 2022; Husung et al. 2020.
[4] Hasenfratz et al. 2007.

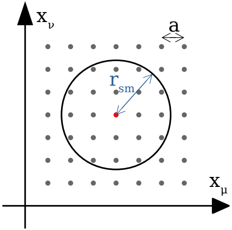
Yang-Mills continuum gradient flow[5]:

- Introduce gauge field $B_\mu(x, t_{\text{fl}})$ defined on $\mathbb{R}^4 \times [0, \infty)$:

$$\frac{\partial}{\partial t_{\text{fl}}} B_\mu(x, t_{\text{fl}}) = -\frac{\delta S_{\text{YM}}[B]}{\delta B_\mu(x, t_{\text{fl}})} \qquad B_\mu(x, 0) = A_\mu(x)$$

- $B_\mu(x, t_{\text{fl}})$ is spherically smoothed with a mean-square radius $r_{\text{sm}} = \sqrt{8 t_{\text{fl}}}$
- No additional renormalisation required[6]:

$$O(x, 0) \text{ finite } \Rightarrow O(x, t_{\text{fl}}) \text{ finite } \forall t_{\text{fl}} > 0$$




Lattice discretisation:

- Wilson gradient flow:

$$\frac{\partial}{\partial t_{\text{fl}}} V_\mu(x, t_{\text{fl}}) = -g_0^2 (\partial_{x,\mu} S[V])\, V_\mu(x, t_{\text{fl}}) \qquad V_\mu(x, 0) = U_\mu(x)$$

$$\partial_{x,\mu} f(U) = T^a \frac{\mathrm{d}}{\mathrm{d}s} f\left(e^{s X^a_{x,\mu}} U\right)\Big|_{s=0} \qquad X^a_{x,\mu}(y, \nu) = T^a \delta_{y,x} \delta_{\nu,\mu}$$

- Numerical integration of flow equation: Forward 3rd-order Runge-Kutta integration scheme, step size $\varepsilon < 0.01$

[5] Lüscher 2010.

[6] Lüscher and Weisz 2011.

# Gradient flow smearing and physical gradient flow

Gradient flow smearing:

- Preserve continuum physics $\Rightarrow r_{\mathrm{sm}} \to 0$ for $a \to 0$

$$r_{\mathrm{sm}} \propto a \quad \Leftrightarrow \quad \frac{r_{\mathrm{sm}}^2}{a^2} = \frac{8t_{\mathrm{fl}}}{a^2} = \mathrm{const}$$

- Smearing strengths up to $\frac{8t_{\mathrm{fl}}}{a^2} = 8$ have been used in practice

Physical gradient flow:

- Alteration of continuum limit

$$r_{\mathrm{sm}} = \mathrm{const} \quad \Leftrightarrow \quad \frac{t_{\mathrm{fl}}}{t_0} = \mathrm{const}$$

  $t_0$: reference flow time

- New observables become accessible

# Continuum extrapolation and small flow time expansion

- Lattice spacing parameter $\hat{a} \equiv \frac{a}{\sqrt{8t_0}}$, flow time parameter $\varepsilon = \frac{t_{\mathrm{fl}}}{t_0}$
- For **finite** dimensionless observable $\hat{O}(\hat{a}, \varepsilon)$:

$$\lim_{\hat{a}\to 0} \lim_{\varepsilon\to 0} \hat{O}(\hat{a}, \varepsilon) = \lim_{\varepsilon\to 0} \lim_{\hat{a}\to 0} \hat{O}(\hat{a}, \varepsilon)$$

$\Rightarrow$ combined Symanzik and small flow time expansion possible:

$$\hat{O} = \sum_{i,j\geq 0} c_{ij} \hat{a}^i \varepsilon^j$$

- Continuum limit can be altered by a physical gradient flow:

$$\hat{a} = 0 \quad \Rightarrow \quad \hat{O} = c_{00} + \sum_{j>0}^{n} c_{0j} \varepsilon^j$$

- Primarily interested in the effect of smearing: smearing strength $\frac{8t_{\mathrm{fl}}}{a^2} = \frac{\varepsilon}{\hat{a}^2}$

$$\hat{O} = \sum_{i,j\geq 0} c_{ij} \hat{a}^{i+2j} \left(\frac{\varepsilon}{\hat{a}^2}\right)^j = \sum_{i,j\geq 0} c_{ij} \hat{a}^{i+2j} \left(\frac{8t_{\mathrm{fl}}}{a^2}\right)^j$$

- Continuum limit independent of smearing:

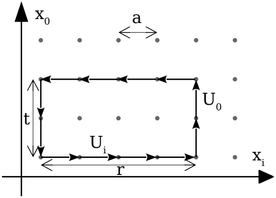
$$\hat{a} = 0 \quad \Rightarrow \quad \hat{O} = c_{00}$$

- Advantage: data at various small $(\hat{a}, \varepsilon)$ can be used to determine the coefficients $c_{ij}$

# Wilson loops and Creutz ratios

Planar rectangular Wilson loops of size $r \times t$:

$$W(r,t) = \left\langle \operatorname{tr} \left( \prod_{(x,\mu)\in\gamma(r,t)} U_\mu(x) \right) \right\rangle$$




- Related to e.g. mesonic correlation functions via hopping parameter expansion
- Caveat: diverge in the continuum limit

More suitable: **Creutz ratios**[7]:

$$\chi(r,t) = -\frac{\partial}{\partial t}\frac{\partial}{\partial r}\ln(W(r,t))$$

- **Finite** continuum limit (no renormalisation required)
  $\Rightarrow$ Combined continuum extrapolation and small flow time expansion possible
- Determine force between two static quarks: $\chi(r,t) \to F_{\bar{q}q}(r)$ for $t \to \infty$
- Use central differences to obtain $O(a^2)$ lattice artefacts:

$$\chi\left(t+\frac{a}{2}, r+\frac{a}{2}\right) = \frac{1}{a^2}\ln\left(\frac{W(t+a,r)\cdot W(t,r+a)}{W(t,r)\cdot W(t+a,r+a)}\right)$$

- Focus on diagonal Creutz ratios $\chi(r) := \chi(r,r)$

[7] Creutz 1980.

# SU(3) gauge ensembles and scale setting

SU(3) Yang Mills theory gauge ensembles:

- Wilson plaquette action
- Temporal open boundary conditions[8] (alleviate topology freezing)
- Scale setting via reference flow time[9] $t_0$:

$$E(x,t_{\text{fl}}) = -\frac{1}{2}\sum_{\mu,\nu}\text{tr}\left(G^{\text{clv}}_{\mu\nu}(x,t_{\text{fl}})\,G^{\text{clv}}_{\mu\nu}(x,t_{\text{fl}})\right) \qquad t_{\text{fl}}^2\left\langle E(x,t_{\text{fl}})\right\rangle\Big|_{t_{\text{fl}}=t_0} = 0.3$$

- $t_0^{\text{phys}}$ via Sommer parameter[10]: $r_0^{\text{phys}} = 0.5\,\text{fm} \Leftrightarrow t_0^{\text{phys}} = 0.0268(3)\,\text{fm}^2$
- Lattice spacings between 0.08 and 0.02 fm, spatial extent $L = 1.9 - 2\,\text{fm}$

| ensemble | $\beta$ | $T/a$ | $L/a$ | $a$ [fm] | $L$ [fm] | $t_0/a^2$ |
|---|---|---|---|---|---|---|
| sft1 | 6.0662 | 80 | 24 | 0.0820(5) | 1.968(12) | 3.990(9) |
| sft2 | 6.2556 | 96 | 32 | 0.0616(4) | 1.971(12) | 7.070(17) |
| sft3 | 6.5619 | 96 | 48 | 0.04031(26) | 1.935(12) | 16.52(6) |
| sft4 | 6.7859 | 192 | 64 | 0.03010(19) | 1.927(12) | 29.60(10) |
| sft5 | 7.1146 | 320 | 96 | 0.01987(13) | 1.908(12) | 67.94(23) |

SU(3) gauge ensembles[11].

[8] Lüscher and Schaefer 2011.
[9] Lüscher 2010.
[10] Sommer 1994.
[11] Husung et al. 2018.

# Computation of Creutz ratios

From Monte Carlo simulation:

- Compute quantities in lattice units:

$$(\chi \cdot a^2)\left(\frac{r}{a}\right) \quad \text{for } \frac{r}{a} = 1.5, 2.5, \ldots \qquad\qquad \frac{8t_0}{a^2}$$

- Combine to dimensionless quantities:

$$\hat{r} = \frac{r}{\sqrt{8t_0}} = \frac{r}{a} \cdot \left(\frac{8t_0}{a^2}\right)^{-\frac{1}{2}} \qquad\qquad \hat{\chi}(\hat{r}) = \chi(r) \cdot 8t_0 = (\chi \cdot a^2)\left(\frac{r}{a}\right) \cdot \frac{8t_0}{a^2}$$

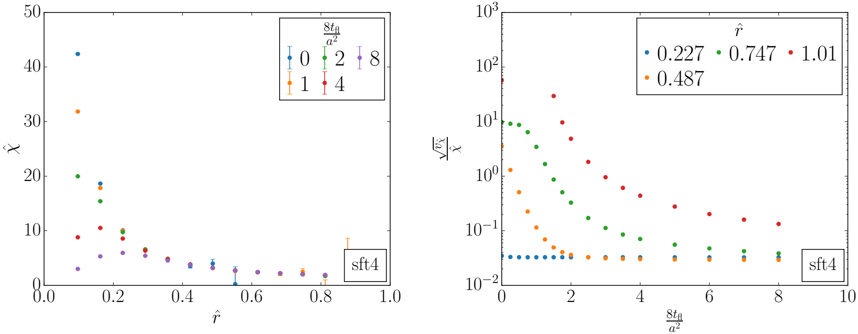
- Gradient flow smearing of $(\chi \cdot a^2)(\frac{r}{a})$:

$$\frac{8t_{\text{fl}}}{a^2} = 0,\ 0.25,\ 0.5,\ \ldots,\ 2,\ 2.5, \ldots,\ 3.5,\ 4,\ 5,\ 6,\ 7,\ 8$$

- Physical gradient flow of $(\chi \cdot a^2)(\frac{r}{a})$:

$$\frac{8t_{\text{fl}}}{a^2} = \frac{8t_0}{a^2} \times 0.0146 \times j\,, \quad j \in \{0,\ 1,\ \ldots,\ 4\}$$

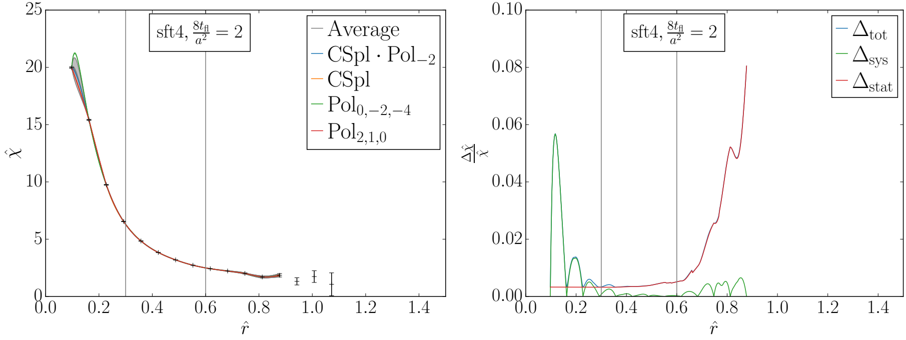
# Creutz ratios and gradient flow smearing




Dimensionless Creutz ratio $\hat{\chi}$ and relative variance $\frac{\sqrt{v_{\hat{\chi}}}}{\hat{\chi}}$ as functions of the flow time $\frac{8t_{fl}}{a^2}$ and the distance $\hat{r}$ on sft4.

- Short distance behaviour $\propto \frac{1}{\hat{r}^2}$ smoothed at distances $r \lessapprox \sqrt{8t_{fl}}$
- $\frac{\sqrt{v_{\hat{\chi}}}}{\hat{\chi}}$ smaller at smaller distances $\hat{r}$, shrinks with growing $\frac{8t_{fl}}{a^2}$
- Smearing does not lead to an arbitrary large reduction of the $\frac{\sqrt{v_{\hat{\chi}}}}{\hat{\chi}}$

# Interpolation model averaging for $(\chi \cdot a^2)\left(\frac{r}{a}\right)$

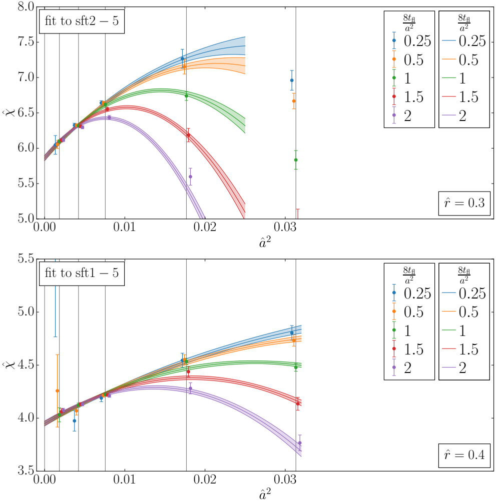



Dimensionless Creutz ratio $\hat{\chi}$ as a function of the distance $\hat{r}$ on the ensemble sft4 with a gradient flow time $\frac{8t_{\mathrm{fl}}}{a^2} = 2$ for various interpolation models.

- Continuum extrapolation of $\hat{\chi}(\hat{r})$ at fixed $\hat{r}$ requires interpolation
- Average over interpolation models, add systematic error
- Interpolation difficult at boundaries
- Focus in region $0.3 \leq \hat{r} \leq 0.6$

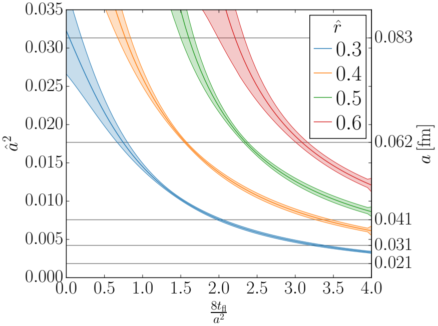
# Continuum extrapolations of smeared Creutz ratios $\hat{\chi}(\hat{r})$

- Fit ansatz: Truncation of Symanzik and small flow time expansion
  $$\hat{\chi}_{\mathrm{tr}} = c_{00} + c_{20}\hat{a}^2 + c_{40}\hat{a}^4 + c_{01}\varepsilon + c_{21}\hat{a}^2\varepsilon + c_{02}\varepsilon^2$$
- Combine data from smearing and physical flow
- Continuum limit independent of $\frac{8t_{\mathrm{fl}}}{a^2}$ by construction
- For larger $\frac{8t_{\mathrm{fl}}}{a^2}$ smearing extrapolations show non-monotonic behaviour
- **Monotony** as a loose criterion for a **controlled continuum extrapolation**:
  $\Rightarrow$ Track location of maximum as a function of $\frac{8t_{\mathrm{fl}}}{a^2}$




Continuum extrapolations of smeared Creutz ratio $\hat{\chi}$ at distances $\hat{r} = 0.3/0.4$ ($r = 0.14/0.18\,\mathrm{fm}$) as a function of the lattice spacing $\hat{a}^2$

# Monotony criterion for a controlled continuum extrapolation




| $\hat{r}$ | $r$ [fm] |
|---|---|
| 0.3 | 0.14 |
| 0.4 | 0.18 |
| 0.5 | 0.23 |
| 0.6 | 0.28 |

Location of the maximum of $\hat{\chi}(\hat{a})$ as a function of the smearing strength $\frac{8t_{\mathrm{fl}}}{a^2}$ for several distances $\hat{r}$

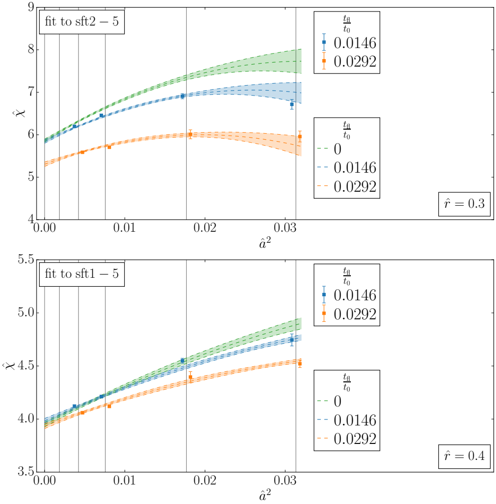
- Monotonic extrapolation at distance $\hat{r}$ when point $\left(\frac{8t_{\mathrm{fl}}}{a^2}, \hat{a}^2\right)$ below corresponding curve
- Larger distances $\hat{r}$ allow for more smearing $\frac{8t_{\mathrm{fl}}}{a^2}$
- Considering lattice spacings $a \leq 0.06\,\mathrm{fm}$:
  For correct physics above e.g. $r = 0.14\,\mathrm{fm}$ choose $\frac{8t_{\mathrm{fl}}}{a^2} \leq 1$

# Continuum extrapolations of physically flowed Creutz ratios $\hat{\chi}(\hat{r})$

- Fit ansatz: Truncation of Symanzic and small flow time expansion

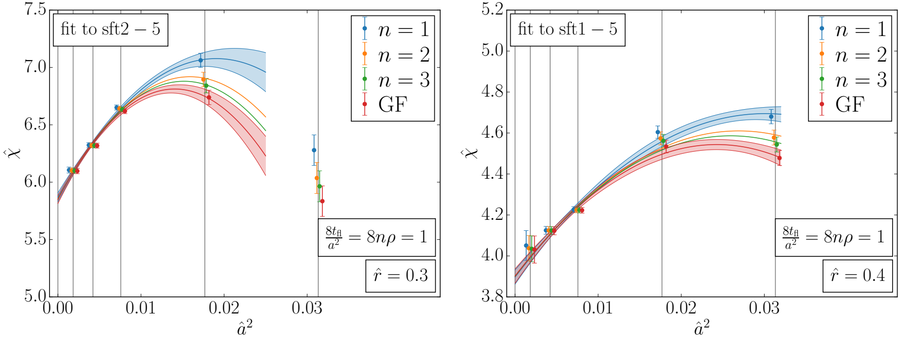
$$\hat{\chi}_{\mathrm{tr}} = c_{00} + c_{20}\hat{a}^2 + c_{40}\hat{a}^4 + c_{01}\varepsilon + c_{21}\hat{a}^2\varepsilon + c_{02}\varepsilon^2$$

- Combine data from smearing and physical flow
- Continuum limit depends on $\varepsilon = \frac{t_{\mathrm{fl}}}{t_0}$
- Monotonous continuum extrapolation for considered range of $\varepsilon$ and $\hat{r}$




Continuum extrapolations of physically flowed Creutz ratio $\hat{\chi}$ at distances $\hat{r} = 0.3/0.4$ ($r = 0.14/0.18\,\mathrm{fm}$) as a function of the lattice spacing $\hat{a}^2$

# Comparison of gradient flow and stout smearing




Continuum extrapolations of stout smeared Creutz ratio $\hat{\chi}$ at distances $\hat{r} = 0.3/0.4$ ($r = 0.14/0.18\,\mathrm{fm}$) as a function of the lattice spacing $\hat{a}^2$

- Gradient flow smearing too expensive in combination with dynamical fermions $\Rightarrow$ Replace by stout smearing with small step number $n$ and $\frac{8t_{\mathrm{fl}}}{a^2} = 8n\rho$
- Stout smearing: Location of maximum shifted to somewhat larger $\hat{a}^2$
- $n = 3$ stout (almost) reproduces gradient flow
- Even $n = 1$ might be sufficient

# Conclusions and Outlook

- Short distance observables may suffer from sizeable discretisation effects
- Large discretisation effects impede controlled continuum extrapolations
- Smearing may reduce discretisation effects, but too much smearing alters short distance behaviour significantly
- **We have performed the first systematic study of the influence of smearing on the continuum extrapolation**
- For $r \geq 0.14\,\text{fm}$ $\frac{8t_{\text{fl}}}{a^2} \leq 1$ seems acceptable
- Single stout smearing step with $\rho = \frac{1}{8}$ also possible for $\frac{8t_{\text{fl}}}{a^2} = 1$
- We will corroborate this considering various observables with fermions and fixing the smearing to the found range
- Bigger smearing radii have been used in the past, e.g. BMW $g-2$ computation[12] $\frac{8t_{\text{fl}}}{a^2} = 4$

[12] Borsanyi 2021.

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