The influence of gauge field smearing on discretisation effects

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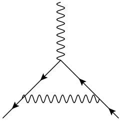
Motivation: The muon anomalous magnetic moment a_μ

- Magnetic moment of the muon $\vec{M}$:

$$\vec{M} = g_\mu \frac{e}{2m_\mu}\vec{S},$$

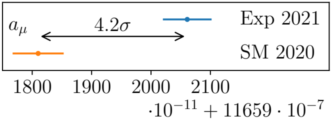
  g_μ gyromagnetic ratio



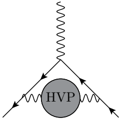
LO-QED

- Relativistic QM (Dirac equation): $g_\mu = 2$
- Anomalous magnetic moment (QFT effects): $a_\mu = \frac{g_\mu - 2}{2}$
- Experimental value: BNL + FNAL 2021[1] (0.35 ppm)
  vs. Standard Model prediction: Muon g-2 Theory Initiative 2020[2]

$$a_\mu^{\mathrm{Exp}} = 116592061(41) \cdot 10^{-11}$$
$$a_\mu^{\mathrm{SM}} = 116591810(43) \cdot 10^{-11}$$



  Precision observable
  $\Rightarrow$ indirect searches for new physics



LO-HVP

- Decomposition into $a_\mu^{\mathrm{SM}} = a_\mu^{\mathrm{QED}} + a_\mu^{\mathrm{QCD}} + a_\mu^{\mathrm{EW}}$
- Error of LO-HVP contribution $a_\mu^{\mathrm{HVP}} \subset a_\mu^{\mathrm{QCD}}$ is dominant

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[1] Abi et al. 2021.
[2] Aoyama et al. 2020.

Motivation: LO-HVP contribution to a_μ

LO-HVP contribution a_μ^{HVP}:

- From dispersion relation[3]:

$$a_\mu^{\mathrm{HVP}} = \frac{\alpha^2}{3\pi^2}\int_{4m_\pi^2}^{\infty} \mathrm{d}s\, \frac{K(s,m_\mu)}{s} R(s)$$

$$R(s) = \frac{\sigma(e^+e^- \to \mathrm{hadrons}(+\gamma))(s)}{(4\pi\alpha^2)/(3s)}$$

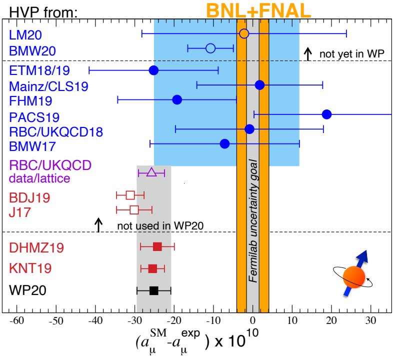
  Experimental input:
  Energy dependent cross section $\sigma(s)$

- From Lattice QCD in TMR ab-initio (time-momentum representation)[4]:

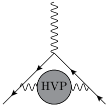
$$a_\mu^{\mathrm{HVP}} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^{\infty} \mathrm{d}t\, \widetilde{K}(t,m_\mu)\, C(t)$$

$$C(t)\,\delta^{kl} = -\int \mathrm{d}x^3\, \langle \mathcal{V}_\gamma^k(\vec{x},t)\, \mathcal{V}_\gamma^l(\vec{0},0)\rangle$$

  Experimental input:
  E.g. hadron masses, m_π, m_K, m_D, m_Ω



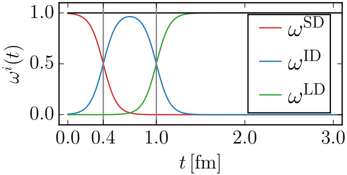
LO-HVP contribution to a_μ (Snowmass 2021[5]). Dispersion relation (red), Lattice QCD (blue).

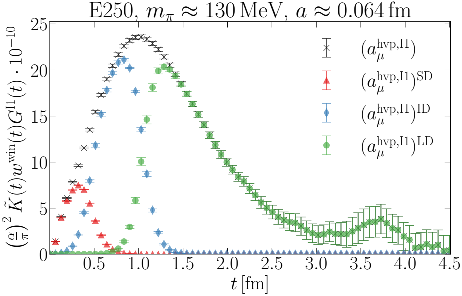


LO-HVP

[3] Aoyama et al. 2020.
[4] Bernecker and Meyer 2011; Francis et al. 2013; Della Morte et al. 2017.
[5] Colangelo 2022.

- TMR allows to define window contributions $(a_\mu^{\mathrm{HVP}})^i$ with $i \in \{\mathrm{SD}, \mathrm{ID}, \mathrm{LD}\}$[6]:
  $$(a_\mu^{\mathrm{HVP}})^i = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty \mathrm{d}t\, \omega^i(t)\, \widetilde{K}(t, m_\mu)\, C(t)$$
  Smoothed window functions $\omega^i(t)$

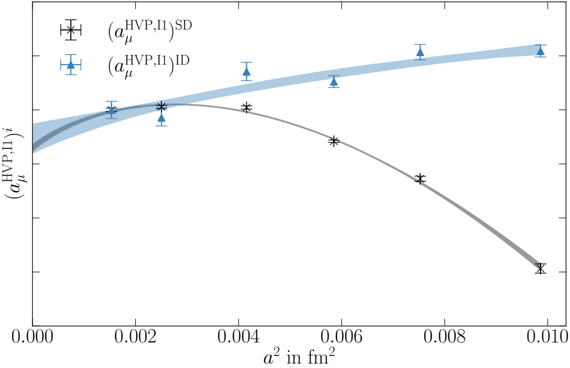


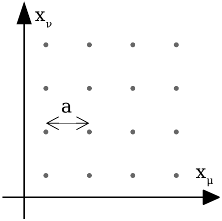


TMR integrand for the isovector contribution to a_μ^{HVP} together with the short (SD), intermediate (ID) and long-distance (LD) contributions[7]

- $(a_\mu^{\mathrm{HVP}})^{\mathrm{SD}}$: Sizable discretisation effects (UV cutoff)
- $(a_\mu^{\mathrm{HVP}})^{\mathrm{LD}}$: Sizable finite volume effects (IR cutoff) and noise problem

[6] Blum et al. 2018.
[7] Cè et al. 2023.





Continuum extrapolations of $(a_\mu^{\mathrm{HVP,I1}})^{\mathrm{SD}}$ and $(a_\mu^{\mathrm{HVP,I1}})^{\mathrm{ID}}$ at the SU(3)-symmetric point normalised to the finest ensemble.[8]

- Extrapolation of $(a_\mu^{\mathrm{HVP,I1}})^{\mathrm{SD}}$ highly problematic: Non-monotonous, strong curvature, uncontrolled higher order contributions in a
- **For reliable continuum extrapolations of short distance observables discretisation effects have to be reduced!**

[8]Image provided by Simon Kuberski

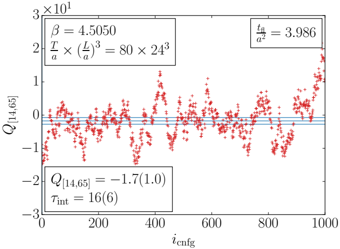
Reduction of discretisation effects

Add gauge ensembles at finer lattice spacings:

- Obtain data points closer to continuum value
- **Caveat**: Critical slowing down of MC algorithms towards continuum limit[9]
  $\Rightarrow$ Simulations at finer lattice spacings become disproportionally expensive:

  $$\text{costs} \propto a^{-p} \text{ at fixed } L \text{ where } p > 6$$

  (naive volume scaling: $p = 4$)



Topological charge as a function of MC time

Modify lattice discretisation to obtain a flatter continuum extrapolation:

- Evaluation of action becomes more expensive (by constant factor)
- Current CLS (Coordinated Lattice Simulations) action has not been modified for the last 20 years
- **Caveat:** Establishing a new action requires generation of a large set of new gauge ensembles
  $\Rightarrow$ Huge computational effort (several 100 MCoreH) and human effort (several man-years)

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[9] Schaefer et al. 2011.

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[10] (tree-level $O(a^2)$-improved) adding irrelevant dim-6 operator[11]

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

- Smearing of gauge fields U in Dirac operator (**UV filtering**): $D[\mathcal{S}[U]]$
  $\Rightarrow$ Reduces likelihood of finding small eigenvalues (related to explicit χSB breaking) and amount of renormalization[12]

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

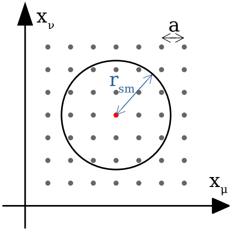
What smearing strengths allow for a controlled continuum extrapolation?

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

[10] Alford et al. 1997.
[11] Sheikholeslami and Wohlert 1985.
[12] Hasenfratz et al. 2007.

Gradient flow smearing

Gradient flow formalism[13]:



- In free theory: Define smeared gauge field $B_\mu(x, t_{\text{fl}})$ with $t_{\text{fl}} \geq 0$ using heat kernel $K(z, t_{\text{fl}})$ as:

$$B_\mu(x, t_{\text{fl}}) = \int \mathrm{d}^4 y\, K(x-y, t_{\text{fl}})\, A_\mu(y)$$

$$K(z, t_{\text{fl}}) = \int \frac{\mathrm{d}p^4}{(2\pi)^4}\, e^{ipz}\, e^{-t_{\text{fl}} p^2} = \frac{e^{-\frac{z^2}{4 t_{\text{fl}}}}}{(4\pi t_{\text{fl}})^2}$$

  $\Rightarrow$ High momentum modes are damped

  $\Rightarrow$ $B_\mu(x, t_{\text{fl}})$ is spherically smoothed with a mean-square radius $r_{\text{sm}} = \sqrt{8 t_{\text{fl}}}$

- Non-perturbative gauge-covariant formulation:

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

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu] \qquad D_\mu = \partial_\mu + [B_\mu, \cdot]$$

  $\Rightarrow$ Integration of flow equation required

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

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

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[13] Lüscher 2010; Lüscher and Weisz 2011.

Creutz ratios

Creutz ratios in the continuum:

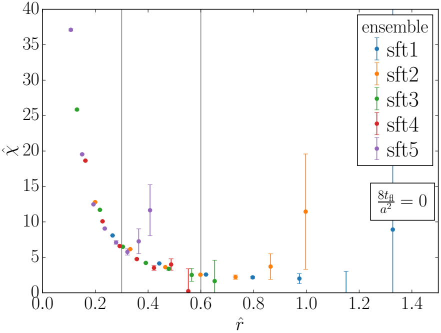
- Planar rectangular Wilson loop of size $r \times t$:

$$W(r,t) = \left\langle \operatorname{tr}\left(P \exp\left(\mathrm{i} \oint_{\gamma(r,t)} \mathrm{d}x_\mu A_\mu(x)\right)\right)\right\rangle$$

- Creutz ratios:

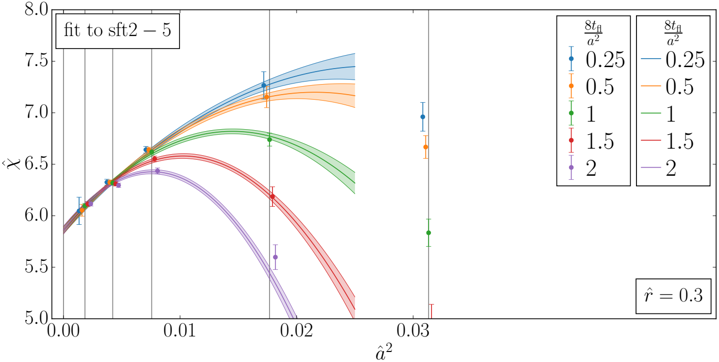
$$\chi(r,t) = -\frac{\partial}{\partial t}\frac{\partial}{\partial r} \ln\left(W(r,t)\right)$$

- Determine force between two static quarks: $\chi(r,t) \to F_{\overline{\mathrm{q}}\mathrm{q}}(r)$ for $t \to \infty$
- Creutz ratios probe physics at different distances
  $\Rightarrow$ Allows to study influence of smearing at different physical distances
- Focus on diagonal Creutz ratios $\chi(r) := \chi(r,r)$ with $r = t$



Creutz ratios $\hat{\chi} \equiv \chi \cdot t_0$ as functions of the distance $\hat{r} \equiv \frac{r}{\sqrt{8t_0}}$ on different ensembles

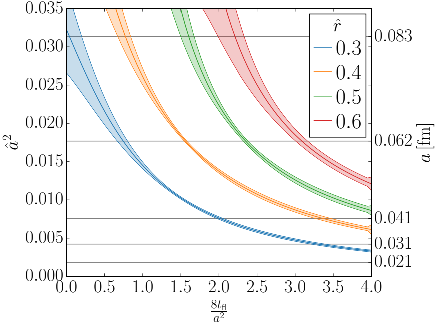
Continuum extrapolations of Creutz ratios



Continuum extrapolations of Creutz ratio $\hat{\chi} \equiv \chi \cdot t_0$ at a distance $\hat{r} \equiv \frac{r}{\sqrt{8t_0}}$ ($r = 0.14\,\mathrm{fm}$) as a function of the lattice spacing $\hat{a}^2 \equiv \frac{a^2}{8t_0}$

- 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
- Loose criterion for a controlled continuum extrapolation: Monotony
  $\Rightarrow$ Track position of maximum as a function of $\frac{8t_{\mathrm{fl}}}{a^2}$

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 $\frac{8t_{\rm fl}}{a^2}$ for several distances $\hat{r} \equiv \frac{r}{\sqrt{8t_0}}$

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

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 $r \geq 0.14\,\mathrm{fm}$ $\frac{8t_{\mathrm{fl}}}{a^2} \leq 1$ seems acceptable
- 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[14] $\frac{8t_{\mathrm{fl}}}{a^2} = 4$

[14] Borsanyi 2021.

Appendix

SU(3) gauge ensembles

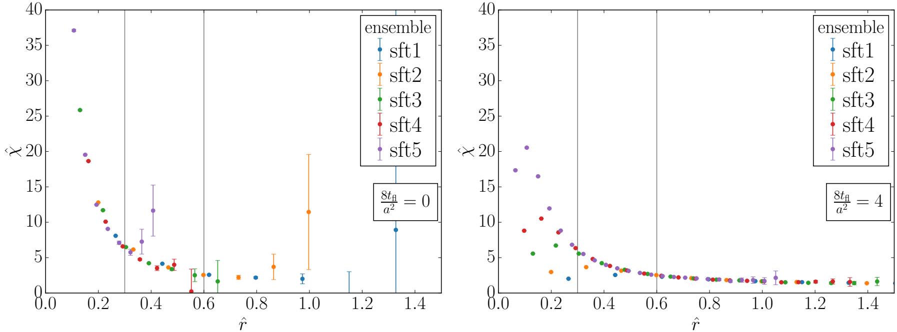
SU(3) Yang-Mills theory gauge ensembles:

- Wilson plaquette action
- Open temporal boundary conditions[15] (alleviate topology freezing)
- Scale setting via reference flow time t_0[16]
- Lattice spacings between 0.08 and 0.02 fm
- Constant spatial extent $L = 2\,\mathrm{fm}$

ensemble	β	T/a	L/a	a [fm]	L [fm]
sft1	6.0662	80	24	0.0834(4)	2.00(1)
sft2	6.2556	96	32	0.0624(4)	2.00(1)
sft3	6.5619	96	48	0.0411(2)	1.97(1)
sft4	6.7859	192	64	0.0312(2)	2.00(1)
sft5	7.1146	320	96	0.0206(2)	1.98(2)

SU(3) gauge ensembles[17]

[15] Lüscher and Schaefer 2011.
[16] Lüscher 2010.
[17] Husung et al. 2018.



Creutz ratios $\hat{\chi} \equiv \chi \cdot t_0$ as functions of the distance $\hat{r} \equiv \frac{r}{\sqrt{8t_0}}$ on different ensembles and gradient flow times $\frac{8t_{fl}}{a^2}$

Influence of gradient flow smearing $\frac{8t_{fl}}{a^2} = \text{const}$:

- Reduces statistical error
- Alters path to continuum and hence discretisation effects

Focus on region $0.3 \le \frac{r}{\sqrt{8t_0}} \le 0.6 \Leftrightarrow 0.14\,\text{fm} \le r \le 0.24\,\text{fm}$, where discretisation effects are not uncontrollably large and the statistical error is sufficiently small

Combined continuum extrapolation and small flow time expansion

Continuum extrapolation of $\hat{\chi}(\hat{r})$ with $\hat{\chi} \equiv \chi \cdot t_0$ at fixed distance $\hat{r} \equiv \frac{r}{\sqrt{8t_0}}$

- Double expansion in lattice spacing $\hat{a} \equiv \frac{a}{\sqrt{8t_0}}$ (Symanzic effective theory) and in flow time parameter $\varepsilon \equiv \frac{t_{\mathrm{fl}}}{t_0}$ (small flow time expansion):

$$\hat{\chi} = \sum_{i=0}^{n} c_i \hat{a}^i + O(\hat{a}^{n+1}) \qquad c_i = \sum_{i=0}^{m} c_{ij} \varepsilon^j + O(\varepsilon^{m+1})$$

- Truncated fit ansatz:

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

  Physical gradient flow $\varepsilon > 0$ alters continuum limit:

$$\hat{\chi}_{\mathrm{tr}}(\hat{a} = 0, \varepsilon) = c_{00} + c_{01}\varepsilon + c_{02}\varepsilon^2$$

- Rearrange terms to obtain smearing expansion with $\frac{\varepsilon}{\hat{a}^2} = \frac{8t_{\mathrm{fl}}}{a^2} = \mathrm{const}$:

$$\hat{\chi}_{\mathrm{tr}}\left(\hat{a}, \frac{8t_{\mathrm{fl}}}{a^2}\right) = d_0 + d_2\hat{a}^2 + d_4\hat{a}^4$$

  Coefficients d_i depend on smearing strength $\frac{8t_{\mathrm{fl}}}{a^2}$:

$$d_0 = c_{00} \quad d_2 = c_{20}\left(1 + \frac{c_{01}}{c_{20}}\frac{8t_{\mathrm{fl}}}{a^2}\right) \quad d_4 = c_{40}\left(1 + \frac{c_{21}}{c_{40}}\frac{8t_{\mathrm{fl}}}{a^2} + \frac{c_{02}}{c_{40}}\frac{64t_{\mathrm{fl}}^2}{a^4}\right)$$

  Gradient flow smearing $\frac{8t_{\mathrm{fl}}}{a^2} > 0$ does not alter continuum limit:

$$\hat{\chi}_{\mathrm{tr}}\left(\hat{a} = 0, \frac{8t_{\mathrm{fl}}}{a^2}\right) = d_0 = c_{00}$$

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