Non-perturbative improvement of the axial current in $N_f = 3$ lattice QCD

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Motivation

Inherent $O(a)$ discretization errors of Wilson fermions are systematically removable via *Symanzik improvement*, by adding ...

- ... a dimension–5 term to the action (Sheikoleslami-Wohlert term $\propto c_{sw}$)
- ... dimension–4 terms to quark bilinear composite operators

Improvement & Renormalization pattern of the axial vector current

$$\left[(A_I)^a_\mu \right]_R(x) \;=\; Z_A \left[A^a_\mu(x) \;+\; a\, c_A\, \frac{1}{2} \left(\partial_\mu + \partial^*_\mu \right) P^a(x) \right]$$

$$A^a_\mu(x) \;=\; \bar{\psi}(x)\, T^a\, \gamma_\mu \gamma_5\, \psi(x) \qquad\qquad P^a(x) \;=\; \bar{\psi}(x)\, T^a\, \gamma_5\, \psi(x)$$

Prominent applications of the improved (& renormalized) axial current:

- PCAC quark masses, e.g., for tuning $N_f = 2 + 1(+1)$ simulations
- Pseudoscalar decay constants f_{PS}, e.g., for scale setting with f_K

$\Rightarrow$ Non-perturbative determination of improvement coefficient c_A desired

[for Z_A, see next talk by Christian Wittemeier]

Strategy

Preferable criteria for a sensible improvement condition:

1.) Large sensitivity for $L \gtrsim 0.8\,\mathrm{fm}$ and low-energy states with $E \ll a^{-1}$
$\rightarrow$ variation of boundary wave functions in PCAC with external states

2.) Imposing improvement conditions at all physical scales kept fixed
$\rightarrow$ define c_A on a *line of constant physics (LCP)*
$\Rightarrow$ $O(a)$ ambiguities disappear smoothly towards the continuum limit
$\Rightarrow$ avoid potentially large $O(a)$ ambiguities in c_A itself

By this approach, c_A is known in QCD with dynamical Wilson quarks for ...

- ... $N_f = 2$ with plaquette gauge action
  [ALPHA Collaboration, JHEP0503(2005)029, hep-lat/0503003]
- ... $N_f = 3$ with Iwasaki gauge action
  [ALPHA Collaboration & CP-PACS/JLQCD, JHEP0704(2007)092, hep-lat/0703006]

Here:

- $N_f = 3$ with tree-level Symanzik improved (aka "Lüscher-Weisz") gauge action
  [ALPHA Collaboration, Bulava, Della Morte, H. & Wittemeier, PoS LATTICE2013(2013)311, arXiv:1312.3591]

Strategy

1.) PCAC relation with different external states

Basic idea:

The PCAC quark mass, derived from an operator identity, is independent of external states and the insertion point up to cutoff effects

$$
\begin{aligned}
m(x;\alpha,\beta) &= r(x;\alpha,\beta) + a\, c_A \cdot s(x;\alpha,\beta) + O(a^2) \\
r(x;\alpha,\beta) &= \frac{\langle\, \alpha \,|\, \frac{1}{2}\,(\partial_\mu + \partial^*_\mu)\, A^a_\mu(x) \,|\, \beta \,\rangle}{2\,\langle\, \alpha \,|\, P^a(x) \,|\, \beta \,\rangle} \\
s(x;\alpha,\beta) &= \frac{\langle\, \alpha \,|\, \partial_\mu \partial^*_\mu P^a(x) \,|\, \beta \,\rangle}{2\,\langle\, \alpha \,|\, P^a(x) \,|\, \beta \,\rangle}
\end{aligned}
$$

- Continuum: m_{PCAC} independent of external states $|\,\alpha\,\rangle$, $|\,\beta\,\rangle$, and x
- Lattice: $O(a)$ ambiguities without improvement

$\Rightarrow$ Improvement condition:

From two sets of external states and insertion points:

$$
m(x;\alpha,\beta) \stackrel{!}{=} m(y;\gamma,\delta) \quad \Longleftrightarrow \quad -c_A \equiv \frac{\Delta r}{a\,\Delta s} = \frac{1}{a} \cdot \frac{r(x;\alpha,\beta) - r(y;\gamma,\delta)}{s(x;\alpha,\beta) - s(y;\gamma,\delta)}
$$

Strategy

1.) PCAC relation with different external states

Implementation in finite-volume QCD with Schrödinger functional BCs

(periodic BCs in space, Dirichlet in time; finite-volume renormalization scheme)

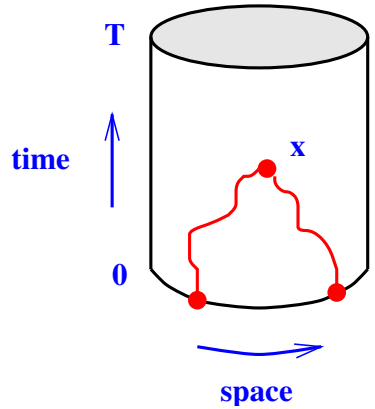
- Use correlators with *spatial trial wave functions* ω at the boundaries:

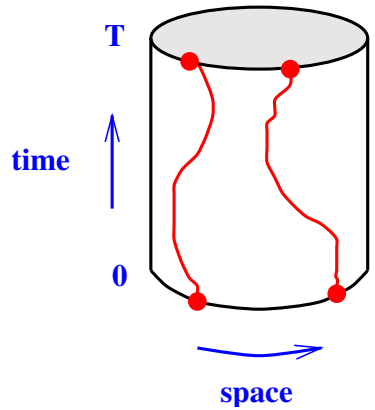
$$f_A(x_0;\omega) = -\frac{a^3}{3L^6}\sum_{\mathbf{x}}\langle A_0^a(x)\,\mathcal{O}^a(\omega)\rangle$$

$$f_P(x_0;\omega) = -\frac{a^3}{3L^6}\sum_{\mathbf{x}}\langle P^a(x)\,\mathcal{O}^a(\omega)\rangle$$

$$F_1(\omega',\omega) = -\frac{1}{3L^6}\langle \mathcal{O}'^a(\omega')\,\mathcal{O}^a(\omega)\rangle$$

$$\mathcal{O}^a(\omega) = a^6\sum_{\mathbf{x},\mathbf{y}}\bar{\zeta}(\mathbf{x})\,T^a\gamma_5\,\omega(\mathbf{x}-\mathbf{y})\zeta(\mathbf{y})$$





- Then (where also a value for x_0 must be specified):

$$r(x_0;\omega) = \frac{\frac{1}{2}\left(\partial_0+\partial_0^*\right)f_A(x_0;\omega)}{2\,f_P(x_0;\omega)} \qquad s(x_0;\omega) = \frac{\partial_0\partial_0^*\,f_P(x_0;\omega)}{2\,f_P(x_0;\omega)}$$

Strategy

1.) PCAC relation with different external states

Choose wave functions $\omega_{\pi^{(0)}}$ and $\omega_{\pi^{(1)}}$ s. th. operator $\mathcal{O}^a(\omega)$ couples only to the ground and first excited state in the pseudoscalar channel

Approximation of $\omega_{\pi^{(0)}}$ and $\omega_{\pi^{(1)}}$

- Employ a basis of three (spatially periodic) wave functions

$$\omega_i(\mathbf{x}) \;=\; N_i \sum_{\mathbf{n}\in\mathbb{Z}^3} \overline{\omega}_i\big(|\mathbf{x}-\mathbf{n}L|\big) \qquad i=1,\ldots,3$$

$$\overline{\omega}_1(r) \;=\; e^{-r/a_0} \qquad \overline{\omega}_2(r) \;=\; r\,e^{-r/a_0} \qquad \overline{\omega}_3(r) \;=\; e^{-r/(2a_0)}$$

  with normalization N_i and a_0 some physical length scale (set to $L/6$)

- $F_1(\omega_i', \omega_j)|_{i,j=1,2,3}$ becomes a positive & symmetric 3×3 matrix, whose eigenvalues $\lambda^{(0)} > \lambda^{(1)} > \lambda^{(2)}$ and (normalized) eigenvectors $\eta^{(0)}, \eta^{(1)}, \eta^{(2)}$ can be calculated by diagonalization

- Now approximate $\omega_{\pi^{(0)}}$ and $\omega_{\pi^{(1)}}$ by the 1st and 2nd eigenvectors:

$$\omega_{\pi^{(0)}} \;\approx\; \textstyle\sum_{i=1}^{3} \eta_i^{(0)}\omega_i \qquad\qquad \omega_{\pi^{(1)}} \;\approx\; \textstyle\sum_{i=1}^{3} \eta_i^{(1)}\omega_i$$

Strategy

2.) Line of constant physics

Simulations for c_A performed along a *line of constant physics (LCP)*

Constant physics condition:

Starting from an initial pair $(L/a, \beta)$ that fixes $L \equiv L_{phys}$, scale β to keep L constant towards smaller lattice spacings via PT formula ($g_0 < g_0'$)

$$\frac{a(g_0^2)}{a\big((g_0')^2\big)} = e^{-[\,g_0^{-2}-(g_0')^{-2}\,]/(2b_0)}\,\big[\,g_0^2/(g_0')^2\,\big]^{-b_1/(2b_0^2)} \times \big\{\,1 + q\cdot\big[\,g_0^2-(g_0')^2\,\big] + O\big((g_0')^4\big)\big\}$$

3–loop contribution to q (from the β–function) not known for LW action $\rightarrow$ only universal parts used

L/a	12	16	20	24
β	3.3	3.512	3.676	3.810

- $\beta \in [3.3, 3.4] \sim a \approx 0.09\,\text{fm} \rightarrow$ spatial volume of extent $L \approx 1.2\,\text{fm}$
- Mass-independent improvement / renormalization scheme:
  3 mass-degenerate quarks, where in practice κ is tuned s.th. the bare PCAC mass (with 1–loop c_A) is reasonably constant resp. just small

Simulations

Action

- Tree-level Symanzik improved (LW) gauge action
- NP'ly $O(a)$ improved three-flavour Wilson fermion action: $c_{sw}(g_0^2)$

[Bulava & Schaefer, NPB874(2013)188, arXiv:1304.7093]

Dynamical $N_f = 2 + 1$ simulations / Algorithm / Measurements

- Generation of gauge configurations by the openQCD code with Schrödinger functional BCs

  [Lüscher & Schaefer, CPC184(2013)519, arXiv:1206.2809]

  - quark doublet: HMC with frequency splitting of the quark determinant
  - stabilizing twisted-mass regulator not necessary in most cases
  - two- and three-level integration schemes
  - 3rd quark: Zolotarev rational approximation in RHMC algorithm, which is corrected for with stochastically estimated reweighting factors
- Computation of SF correlation functions and derived quantities

Schrödinger functional setup

- $\theta = 0$, vanishing background field
- $T = (3/2) \cdot L \rightarrow$ re-use configurations to also determine Z_A

[see next talk by Christian Wittemeier]

Results
Data ensembles

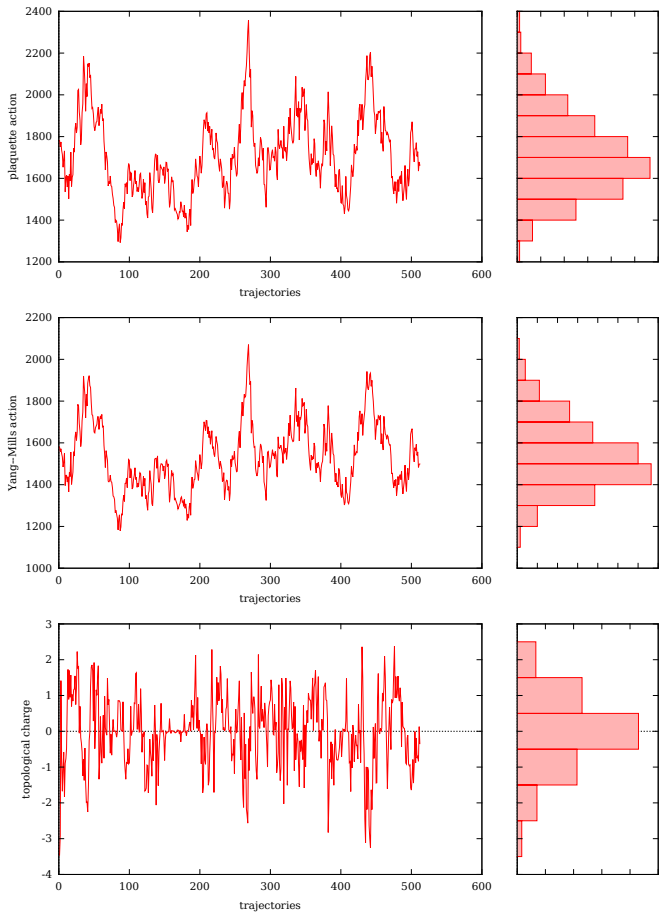
L/a	T/a	β	κ	N_{tr}	am_{PCAC}	$\overline{g}^2_{GF}(L)$
12	17	3.3	0.13652	5120	$-0.00096(71)$	$18.12(21)$
12	17	3.3	0.13660	6524	$-0.0086(6)$	$16.92(13)$
16	23	3.512	0.13700	10240	$0.0064(2)$	$16.49(13)$
16	23	3.512	0.13703	4096	$0.0056(3)$	$16.85(20)$
16	23	3.512	0.13710	12288	$0.0024(2)$	$16.11(14)$
20	29	3.676	0.13680	3548	$0.0139(2)$	$16.52(30)$
20	29	3.676	0.13700	7616	$0.0066(1)$	$15.54(14)$
24	35	3.810	0.13712	7724	$-0.00269(8)$	$13.90(11)$

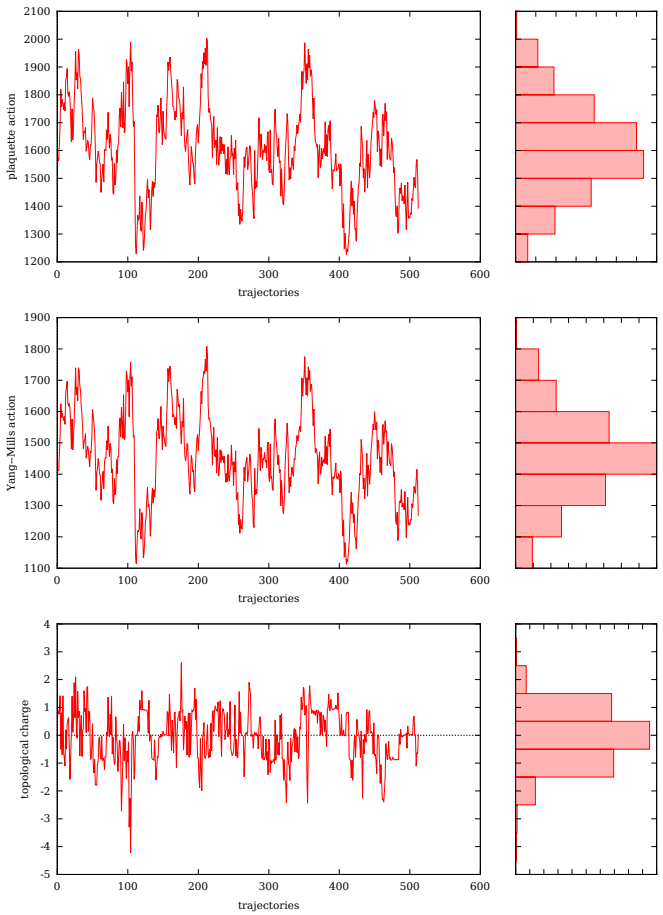
- Acceptance rates $\gtrsim 0.90$; trajectory length $= 2 \;\Rightarrow\; N_{MDU} = 2N_{tr}$
- Measurements: usually $N_{meas} = N_{tr}/4$, seperated by 8 MDU's
- am_{PCAC}, via projected correlators (see below), with c_A from 1–loop PT

  [Aoki, Frezzotti & Weisz, NPB540(1999)501, hep-lat/9808007]
- Check LCP by gradient flow coupling $\overline{g}^2_{GF} \propto t^2 \langle E(t, x_0) \rangle |^{x_0=T/2}_{t=(0.35L)^2/8}$

Results
Monte Carlo histories

Wilson plaquette, Yang-Mills action and topological charge densities, smoothed, i.e., evaluated at Wilson flow time $t = (c \cdot L)^2/8$ with $c = 0.35$



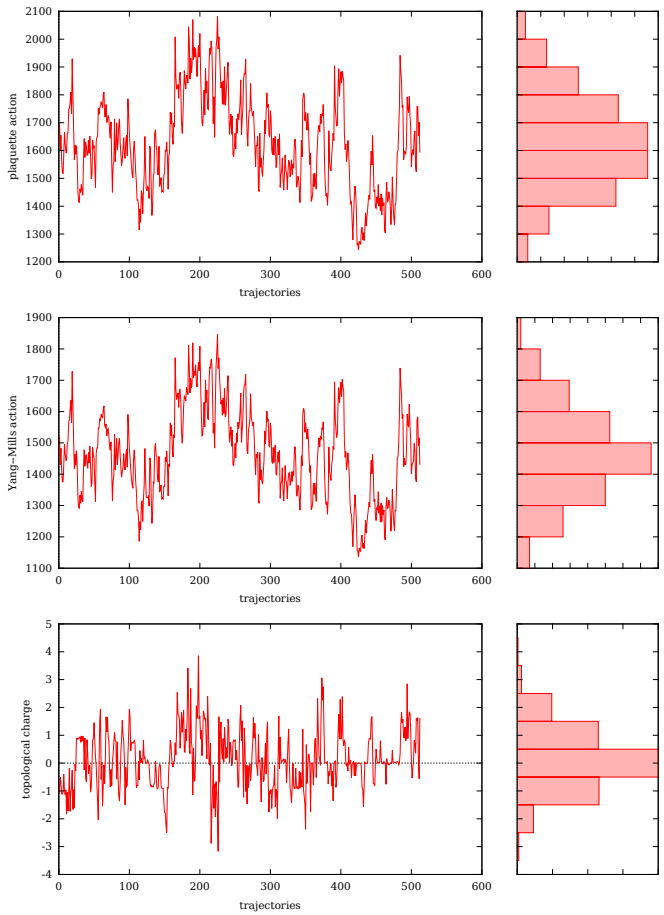


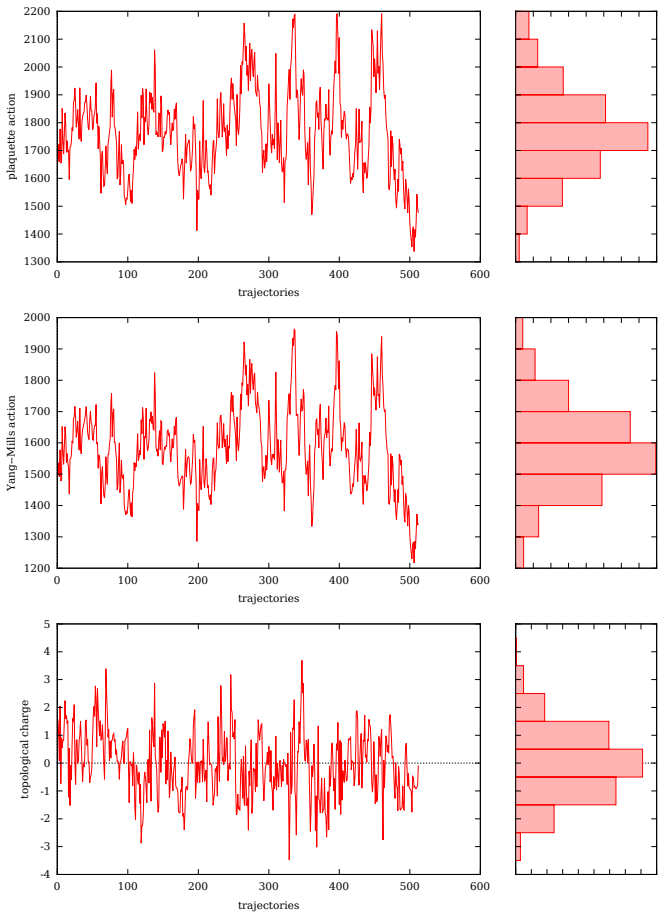
- $L/a = 12$, $T/a = 17$, $\kappa = 0.13652$
- 1024 MDU (replicum #1)

- $L/a = 12$, $T/a = 17$, $\kappa = 0.13652$
- 1024 MDU (replicum #2)

Results
Monte Carlo histories

Wilson plaquette, Yang-Mills action and topological charge densities, smoothed, i.e., evaluated at Wilson flow time $t = (c \cdot L)^2/8$ with $c = 0.35$



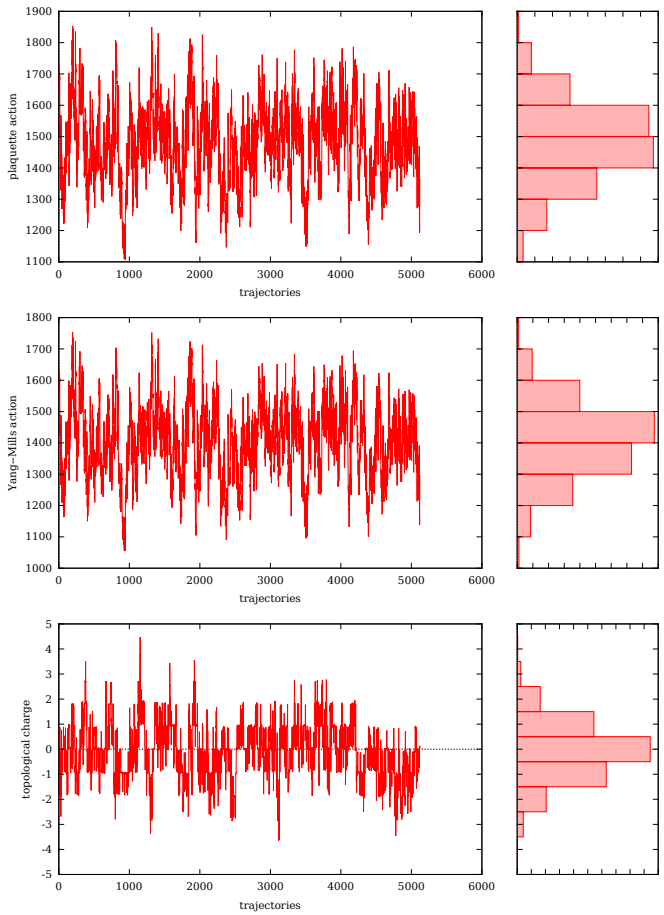


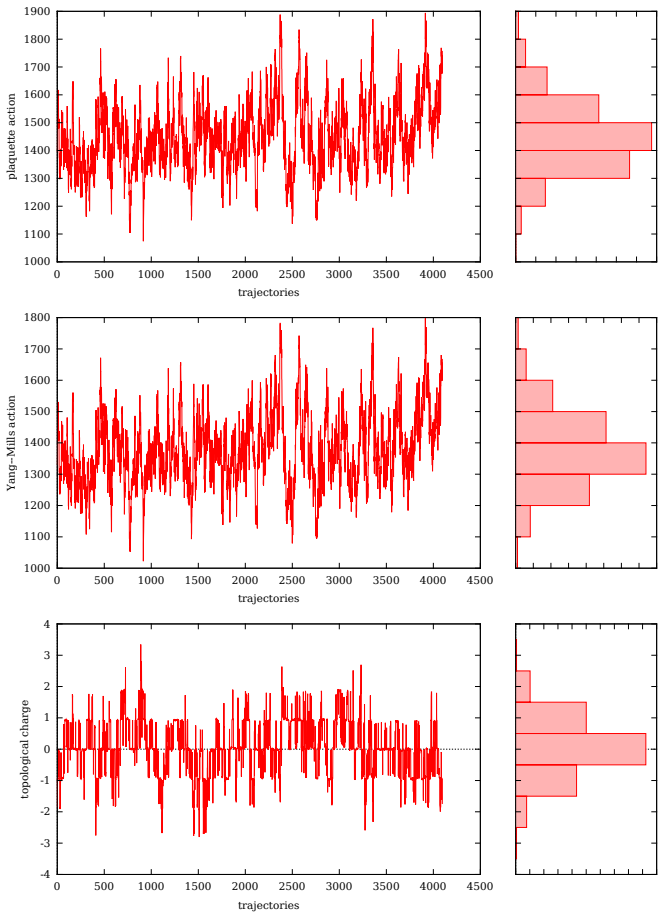
- $L/a = 12$, $T/a = 17$, $\kappa = 0.13652$
- 1024 MDU (replicum #3)

- $L/a = 12$, $T/a = 17$, $\kappa = 0.13652$
- 1024 MDU (replicum #4)

Results
Monte Carlo histories

Wilson plaquette, Yang-Mills action and topological charge densities, smoothed, i.e., evaluated at Wilson flow time $t = (c \cdot L)^2/8$ with $c = 0.35$



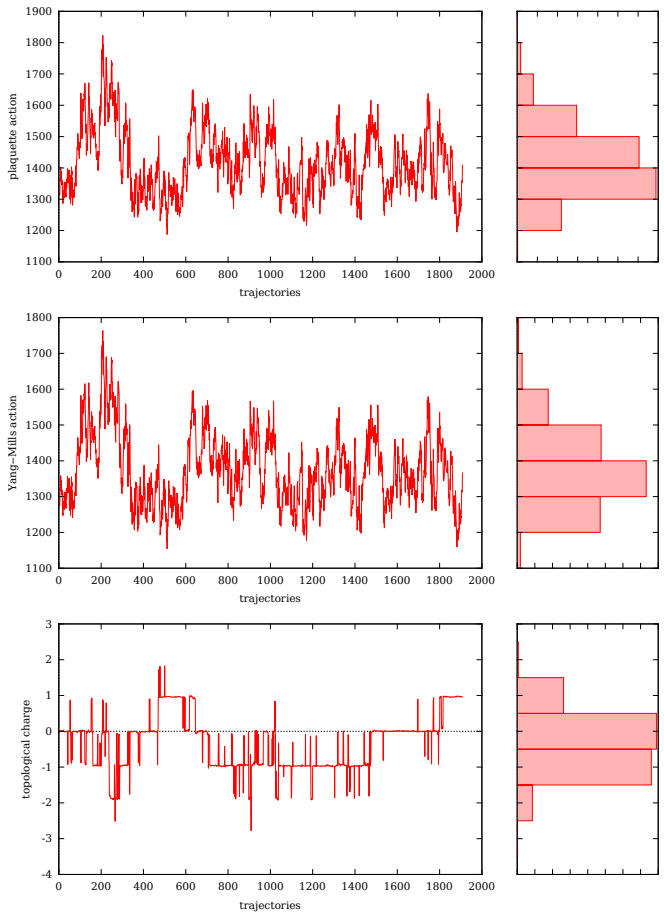


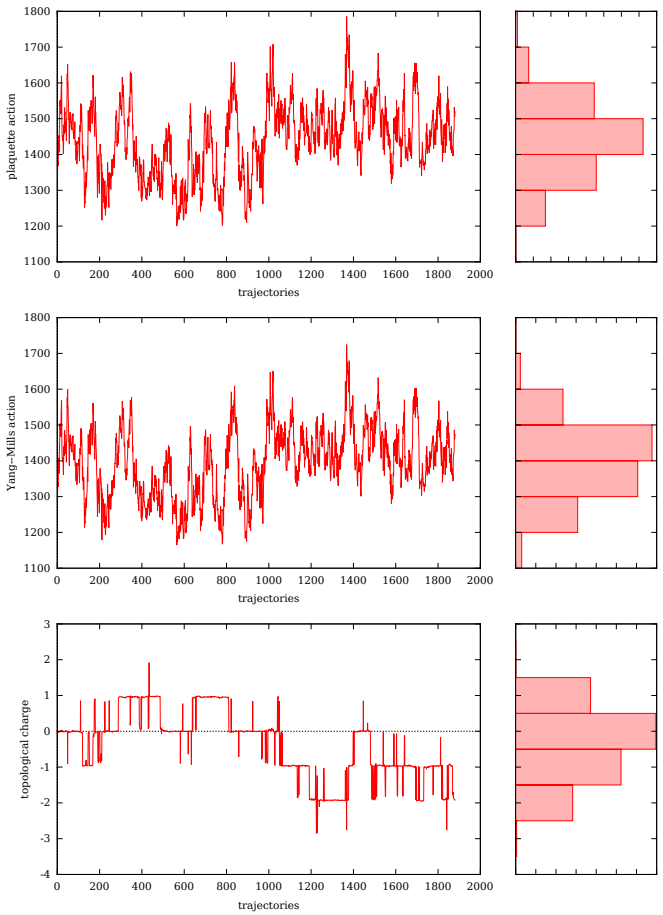
- $L/a = 16$, $T/a = 23$, $\kappa = 0.1370$
- 10240 MDU (replicum #1)

- $L/a = 16$, $T/a = 23$, $\kappa = 0.1371$
- 8192 MDU (replicum #1)

Results
Monte Carlo histories

Wilson plaquette, Yang-Mills action and topological charge densities, smoothed, i.e., evaluated at Wilson flow time $t = (c \cdot L)^2/8$ with $c = 0.35$



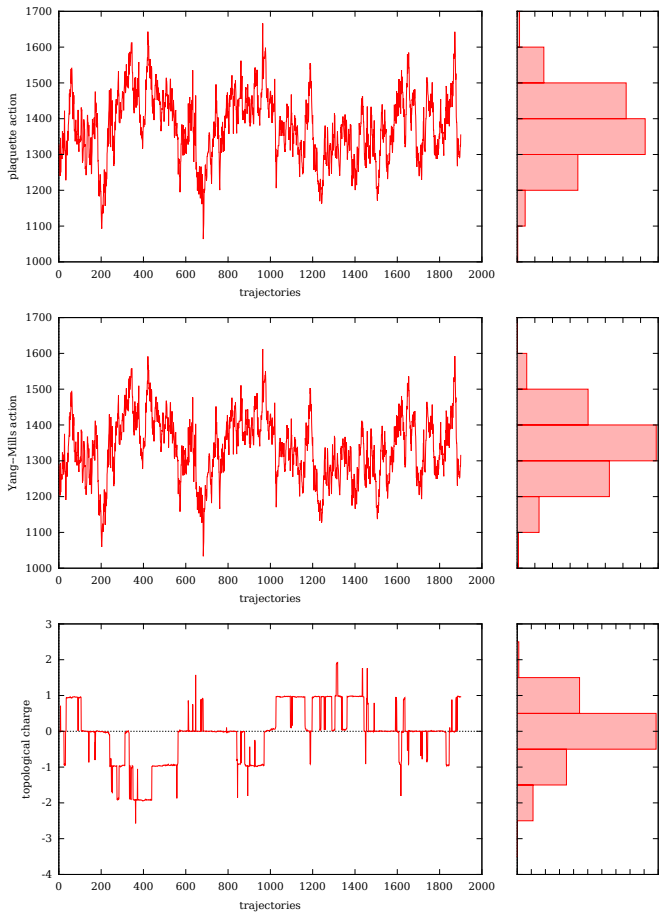


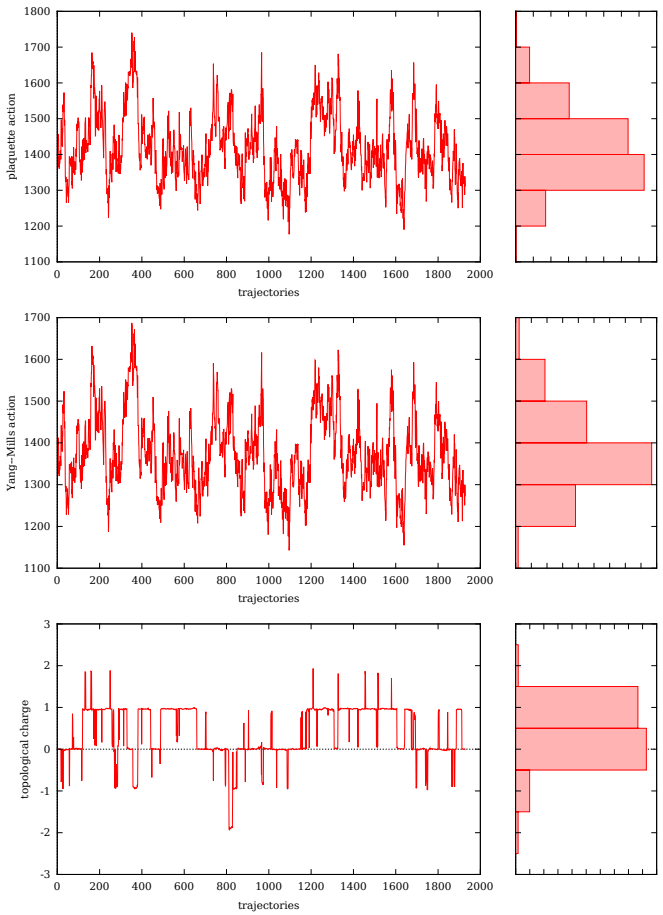
- $L/a = 20$, $T/a = 29$, $\kappa = 0.1370$
- $\approx$ 1900 MDU (replicum #1)

- $L/a = 20$, $T/a = 29$, $\kappa = 0.1370$
- $\approx$ 1900 MDU (replicum #2)

Results
Monte Carlo histories

Wilson plaquette, Yang-Mills action and topological charge densities, smoothed, i.e., evaluated at Wilson flow time $t = (c \cdot L)^2/8$ with $c = 0.35$



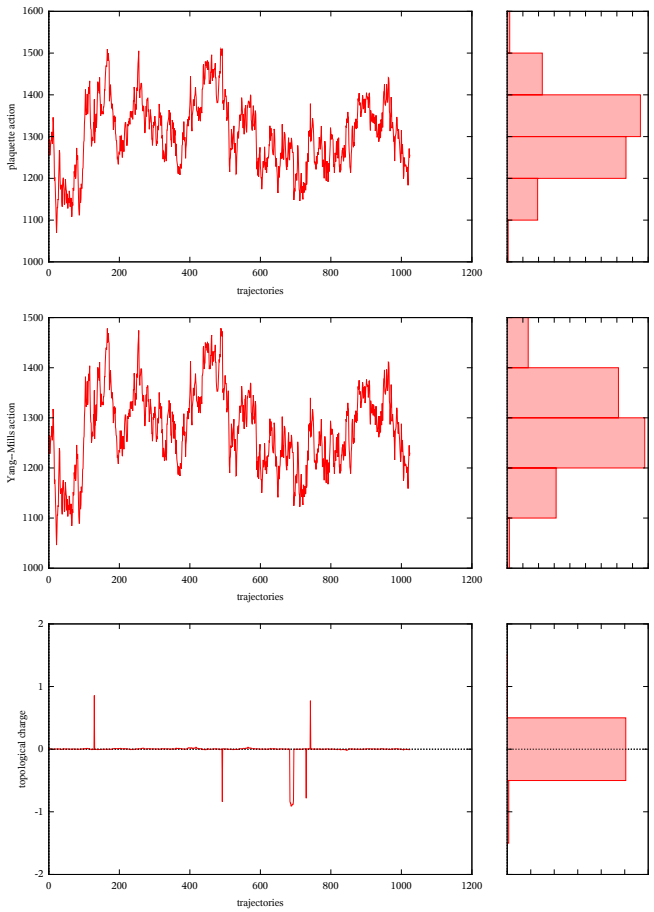


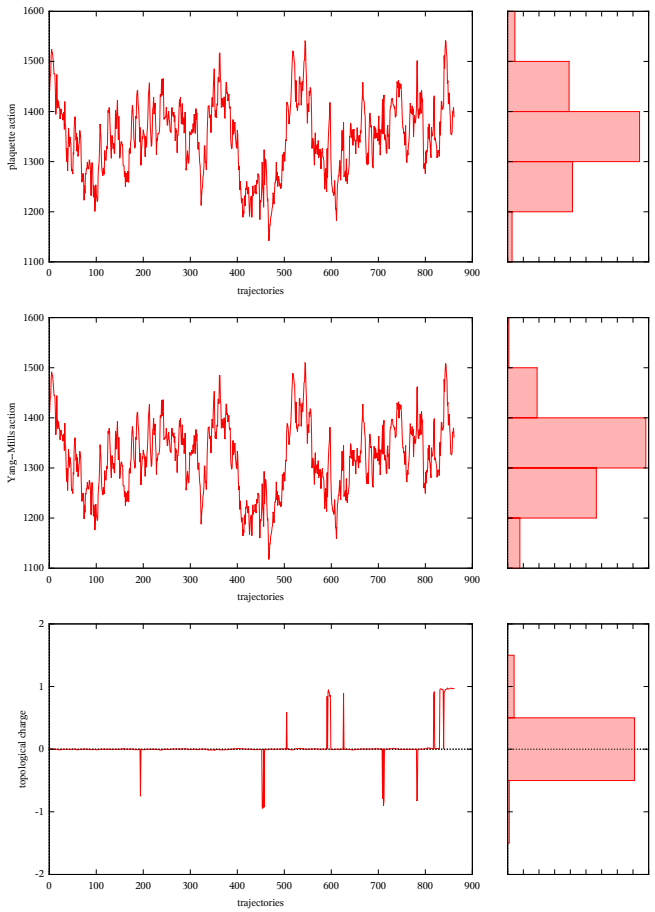
- $L/a = 20$, $T/a = 29$, $\kappa = 0.1370$
- $\approx$ 1900 MDU (replicum #3)

- $L/a = 20$, $T/a = 29$, $\kappa = 0.1370$
- $\approx$ 1900 MDU (replicum #4)

Results
Monte Carlo histories

Wilson plaquette, Yang-Mills action and topological charge densities, smoothed, i.e., evaluated at Wilson flow time $t = (c \cdot L)^2/8$ with $c = 0.35$



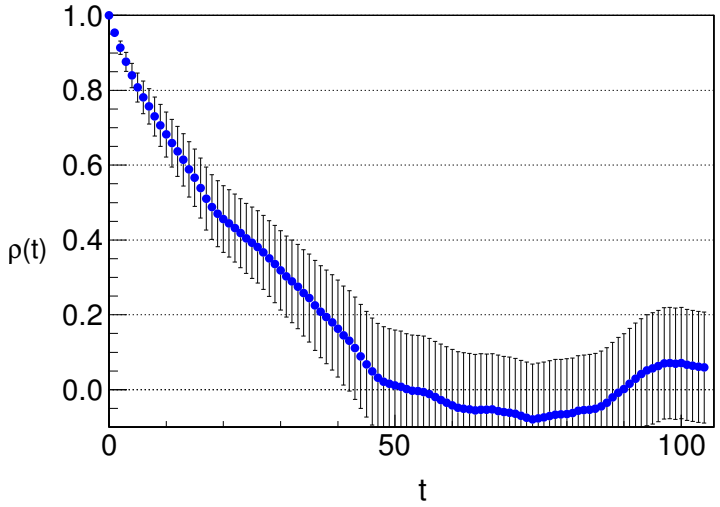


- $L/a = 24$, $T/a = 35$, $\kappa = 0.13712$
- 2048 MDU (replicum #1)

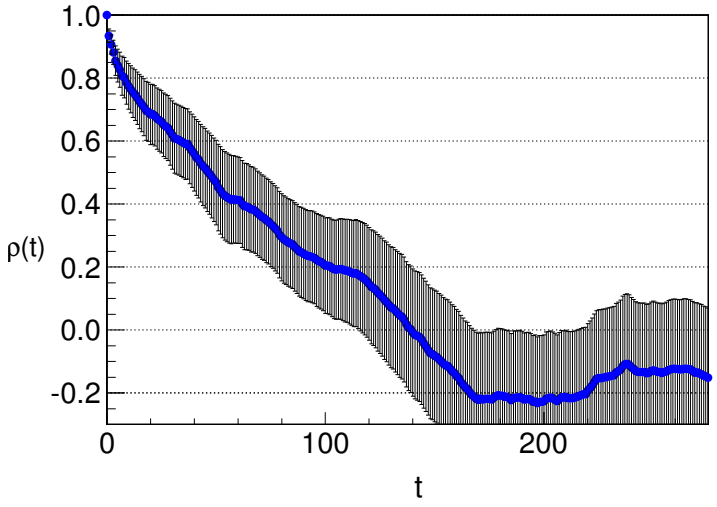
- $L/a = 24$, $T/a = 35$, $\kappa = 0.13712$
- 2048 MDU (replicum #2)

Results
Analysis of autocorrelations

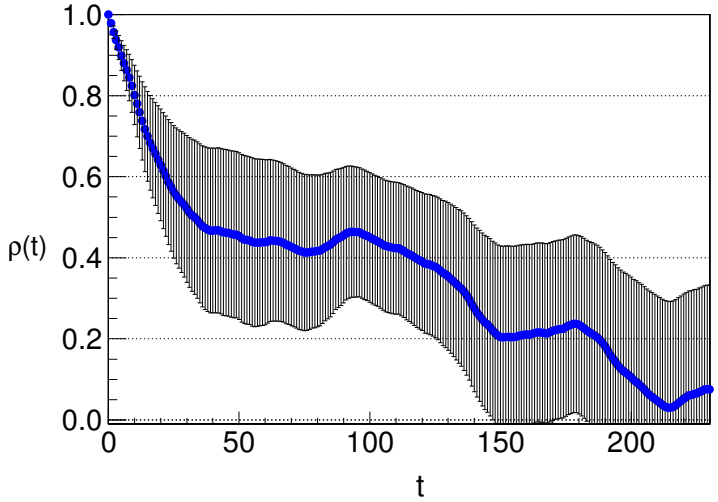
Normalized autocorrelations functions $\rightarrow$ Largest autocorrelation times at:



- $L/a = 20$, $T/a = 29$, $\kappa = 0.1370$
- Smoothed action: $\tau_{\text{int}} \approx 20 - 30$



- $L/a = 20$, $T/a = 29$, $\kappa = 0.1370$
- Topol. charge: $\tau_{\text{int}} \approx 60 - 70$



- $L/a = 24$, $T/a = 35$, $\kappa = 0.13712$
- Smoothed action: $\tau_{\text{int}} \approx 100$
- Q_{top} does not tunnel through sectors, i.e., it is frozen to 0

Results

Determination of the eigenvectors $\eta^{(0)}$ and $\eta^{(1)}$ of the matrix $F_1(\omega_i', \omega_j)$

- They have a well-defined continuum limit along a LCP, as long as the wave functions depend on physical scales only
  $\rightarrow$ no considerable dependence on the lattice spacing observed
- We thus fix the vectors for once from the analysis of a representative data ensemble and regard this as *part of the improvement condition*
  $\rightarrow$ our choice is from $L/a = 16$ and $\kappa = 0.13703$, giving

$$\eta^{(0)} = \big(0.5317(3)\,,\, 0.5977(1)\,,\, 0.6000(2)\big)$$
$$\eta^{(1)} = \big(0.843(5)\,,\, -0.31(6)\,,\, -0.44(6)\big)$$

Then:

$$c_A \equiv -\frac{1}{a}\cdot\frac{r(x_0;\omega_{\pi^{(1)}}) - r(x_0;\omega_{\pi^{(0)}})}{s(x_0;\omega_{\pi^{(1)}}) - s(x_0;\omega_{\pi^{(0)}})}$$

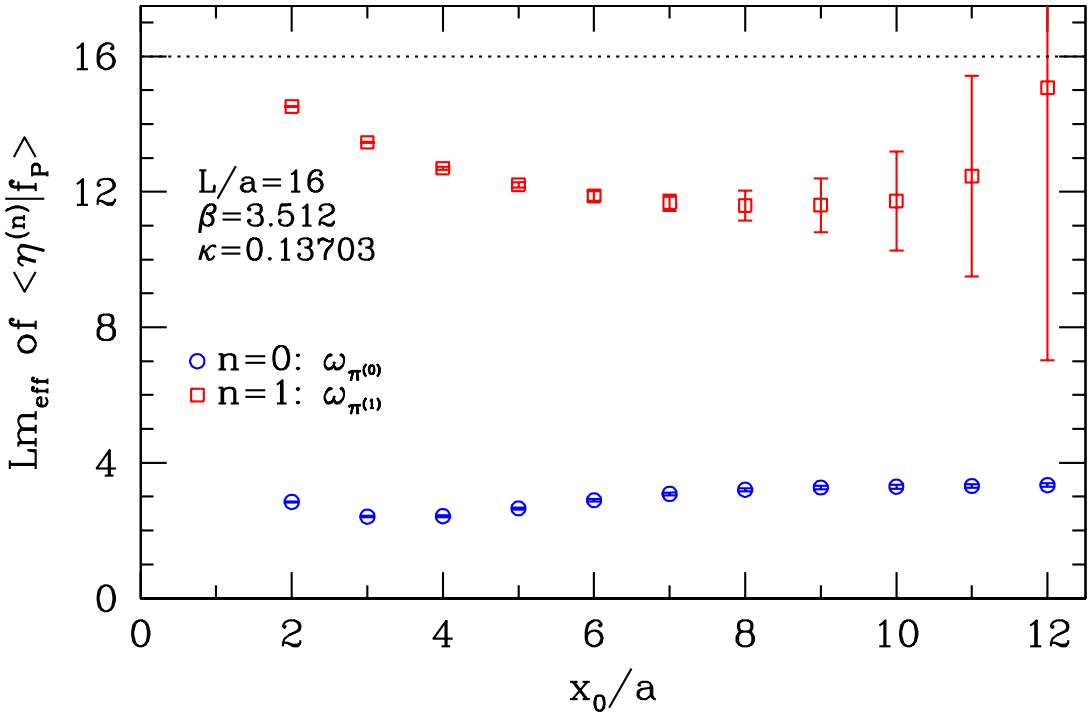
$$r(x;\omega) = \frac{\frac{1}{2}\left(\partial_0 + \partial_0^*\right) f_A(x_0;\omega)}{2\, f_P(x_0;\omega)} \qquad s(x;\omega) = \frac{\partial_0\partial_0^*\, f_P(x_0;\omega)}{2\, f_P(x_0)}$$

($\omega_{\pi^{(0)}}, \omega_{\pi^{(1)}}$ define the states β, δ above, while $|\alpha\rangle, |\gamma\rangle$ have vacuum quantum numbers)

Results

Representative data ensemble with $L/a = 16$, $\beta = 3.512$ and $\kappa = 0.13703$

With the eigenvectors, project the CFs to the (approximate) ground & 1st excited state: $f_{A/P}(x_0; \omega_{\pi^{(0)}})$, $f_{A/P}(x_0; \omega_{\pi^{(1)}})$ $\rightarrow$ effective mass of f_P

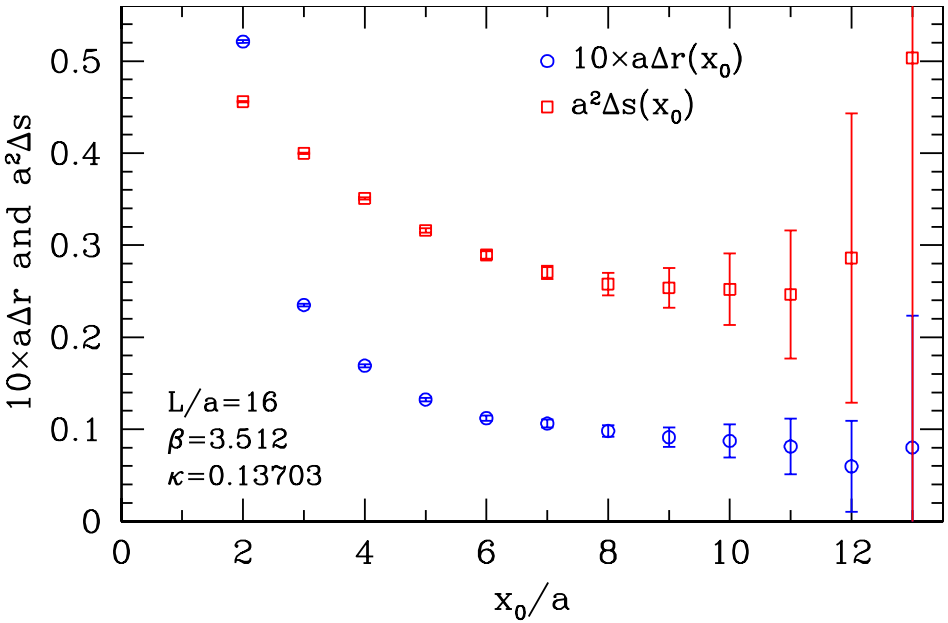


- The two states are clearly separated up to $x_0 \approx 12a$
- Energy of 1st excited state still acceptably below the cutoff a^{-1}
  $\rightarrow$ smaller volumes may introduce significant residual $O(a^2)$ effects
- Sensitivity to c_A: $a\Delta s = a[s(x_0; \omega_{\pi^{(1)}}) - s(x_0; \omega_{\pi^{(0)}})] = a(m^2_{\pi^{(1)}} - m^2_{\pi^{(0)}})$

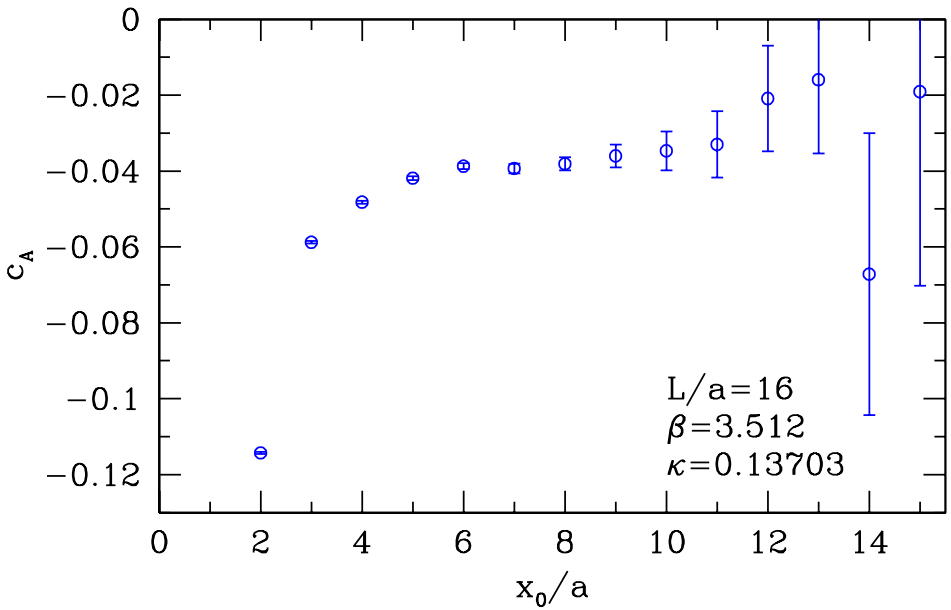
Results

Representative data ensemble with $L/a = 16$, $\beta = 3.512$ and $\kappa = 0.13703$

Left: $a\,\Delta r(x_0)$ & $a^2\Delta s(x_0)$



Right: local / "effective" $c_A(x_0)$

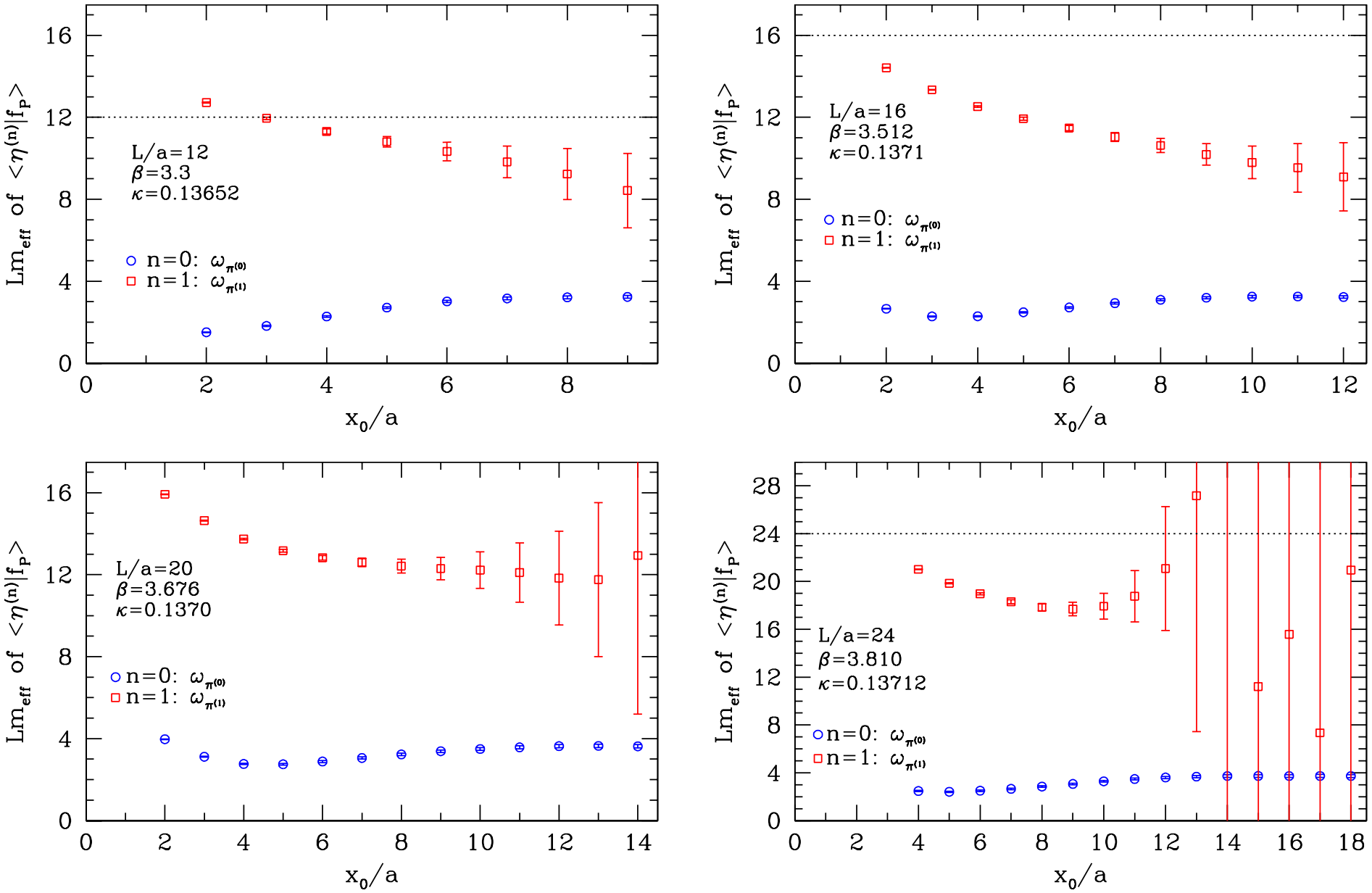


- Final definition of c_A from the improvement condition:
  Fix $x_0 = L/3$, as it is already in the asymptotic regime, still has good signal-to-noise ratio, and states with energy gap dominate the CFs

- Little variation for $x_0 \gtrsim 5a$ indicates that high-energy states, which could contribute large $O(a)$ ambiguities, are reasonably suppressed

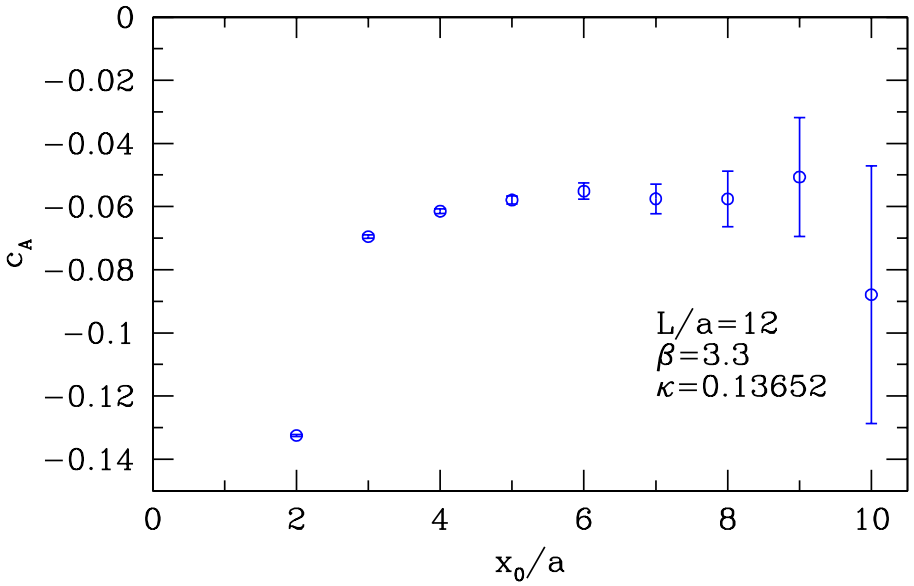
Results

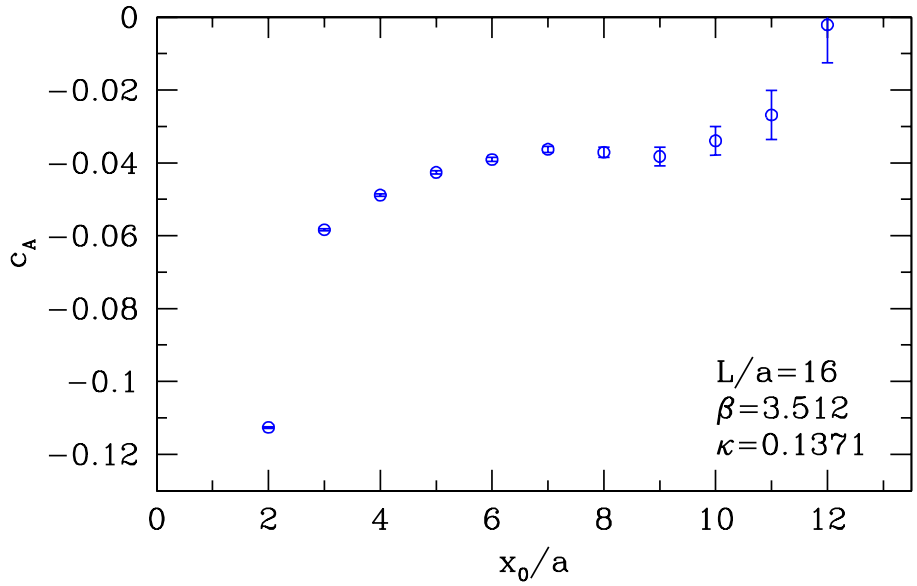
Effective mass of projected CFs from the scaled / matched lattices

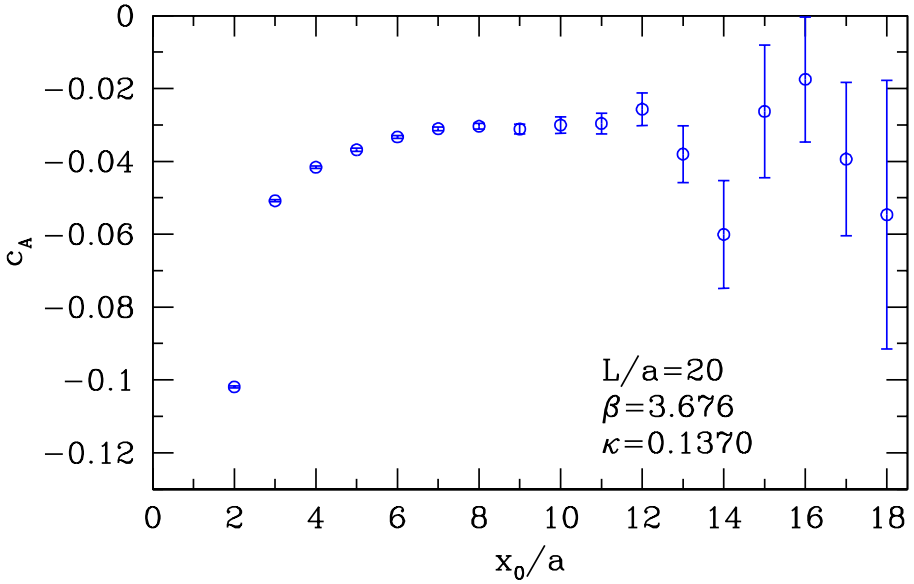


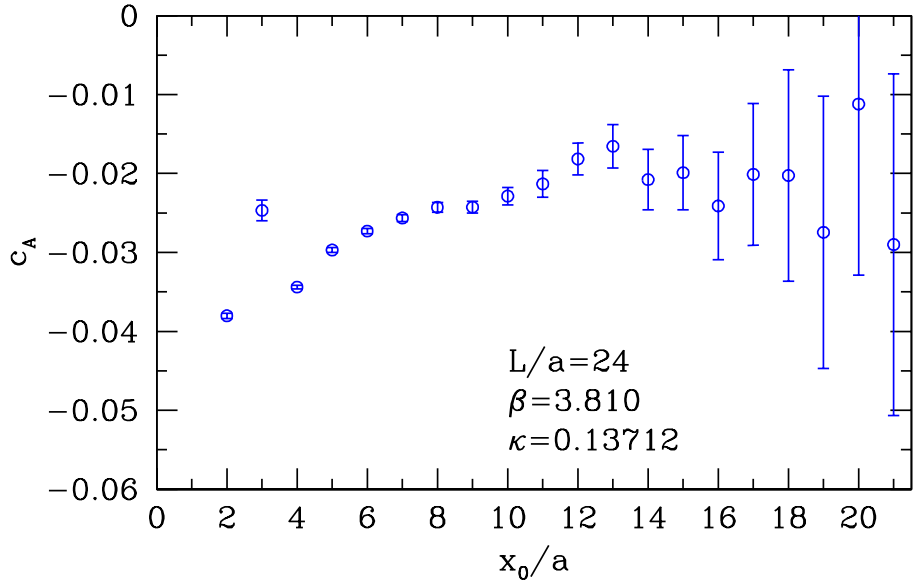
Results

Effective $c_A(x_0)$ from the scaled / matched lattices









Results

Observation from our MC histories on the smoothed Q_{top}:

The simulations with $L/a = 24$ (i.e., at smallest a) *sample the non-trivial topological sectors insufficiently*

$\Rightarrow$ Apply two kinds of analyses to compute c_A:

1.) Analysis including all topological charge sectors, but excluding the $L/a = 24$, $\beta = 3.81$ data ensemble

2.) Analysis restriced to sector with fixed topological charge, $Q_{top} = 0$

$$\langle O \rangle \big|_{Q_{top}=0} = \frac{\langle O \cdot \delta_{Q_{top},0} \rangle}{\langle \delta_{Q_{top},0} \rangle} \qquad \delta_{Q_{top},0} \equiv \Theta(Q_{top} + 0.5)\,\Theta(0.5 - Q_{top})$$

(Note: Ward identities should hold in any topological sector)

Error estimation:

- binned Jackknife of concatenated data from different replica (bin size larger than resp. comparable to τ_{int} and $> 50 - 100$ bins)
- checked with Γ–method studying autocorrelation functions

[Wolff, CPC156(2004)143, hep-lat/0306017]

Results

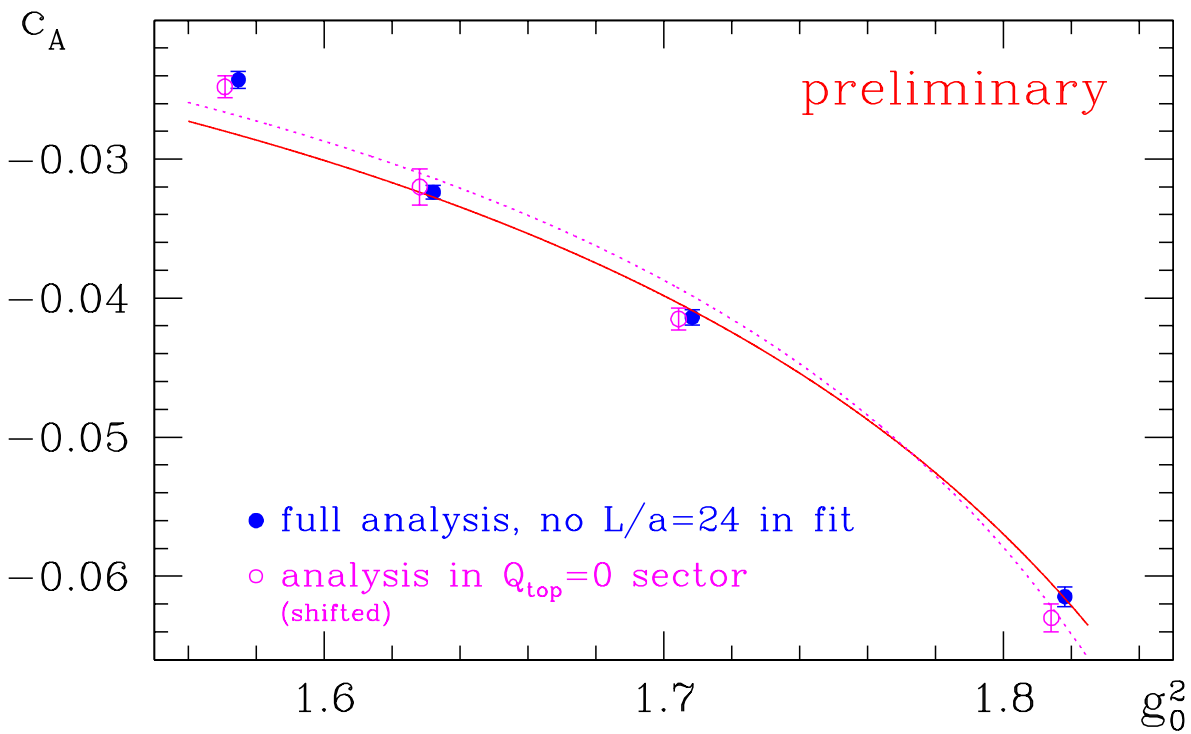
c_A as function of g_0^2

lattice	β	κ	$c_A(L/3)$	$c_A(L/3)\|_{Q_{top}=0}$
$12^3 \times 17$	3.3	0.13652	$-0.0615(7)$	$-0.0630(10)$
$12^3 \times 17$	3.3	0.13660	$-0.0604(5)$	—
$16^3 \times 23$	3.512	0.13700	$-0.0425(7)$	$-0.0410(11)$
$16^3 \times 23$	3.512	0.13703	$-0.0408(7)$	—
$16^3 \times 23$	3.512	0.13710	$-0.0414(6)$	$-0.0415(8)$
$20^3 \times 29$	3.676	0.13680	$-0.0353(6)$	$-0.0345(19)$
$20^3 \times 29$	3.676	0.13700	$-0.0324(5)$	$-0.0320(13)$
$24^3 \times 35$	3.810	0.13712	$-0.0243(6)$	$-0.0248(8)$

- ✓ Analysis restriced to the sector with zero topological charge yields consistent results (with larger statistical errors though)
- ✓ Small violations (approximately within $|am_{PCAC}| < 0.015$) of the "constant quark mass condition" negligible

Results

c_A as function of g_0^2



Smooth interpolation based on functional form constrained to 1–loop PT:

$$c_A(g_0^2) \;=\; -0.006033\, g_0^2 \times \frac{1 - 0.19(2)\, g_0^2}{1 - 0.486(3)\, g_0^2}$$

- Fit function is from analysis over all topological sectors, but excluding the $L/a = 24$ data point owing to the missing topology sampling
- Compatible to fit in the trivial sector with all ensembles

Conclusions & Outlook

- ✓ Non-perturbative improvement condition for c_A via PCAC and approximate projection method by wave functions, resembling ground & 1st excited external pseudoscalar states, works well

- ✓ By variation of boundary wave functions in Schrödinger functional correlation functions, a (enhanced) sensitivity $\propto m^2_{\pi^{(1)}} - m^2_{\pi^{(0)}}$ on c_A can be obtained

2do: Re-analysis of a few data ensembles with the fully available statistics

2do: Investigation of uncertainties due to deviating from the LCP

($\rightarrow$ e.g., adding a further ensemble with $L/a = 16$, $\beta = 3.47$)

2do: Determination of Z_A from the same ensembles

($\rightarrow$ talk by C. Wittemeier)